# 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.

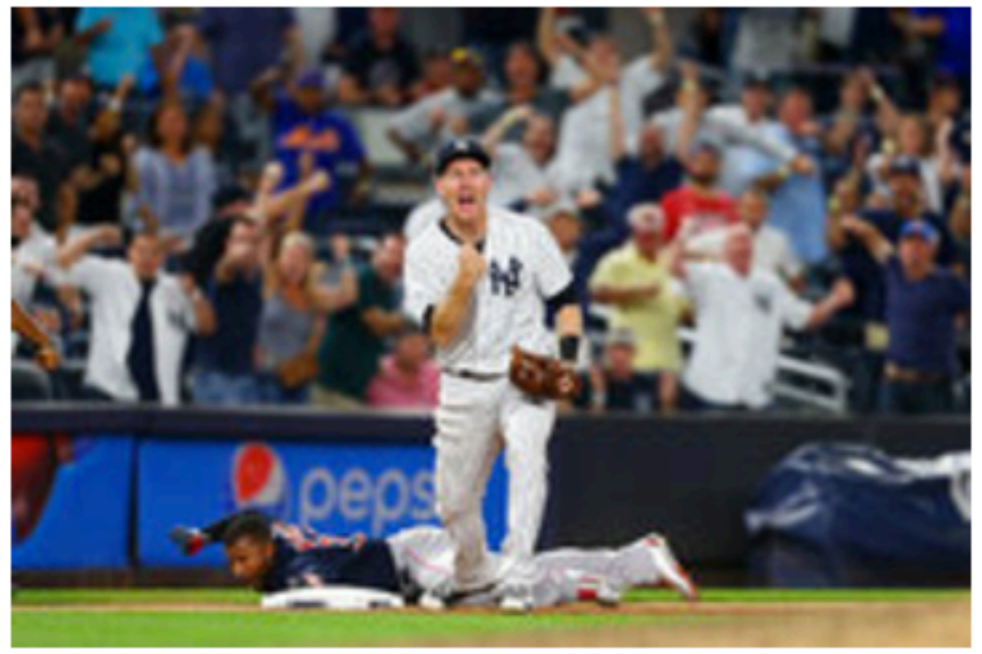
By GINA KOLATA

→ 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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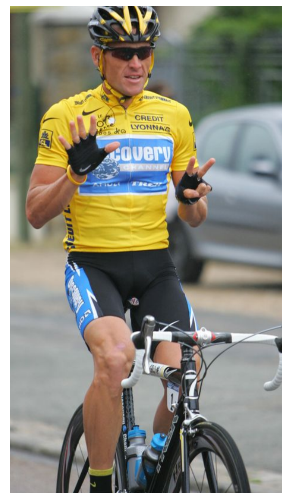

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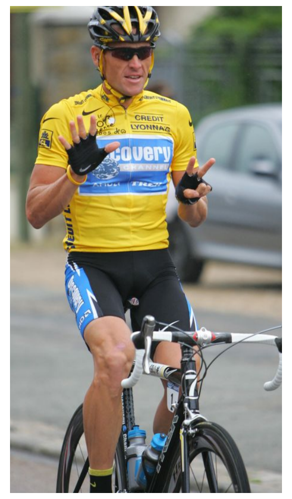

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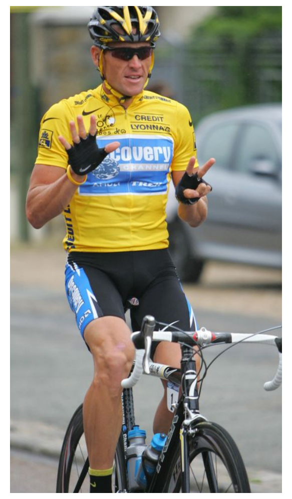

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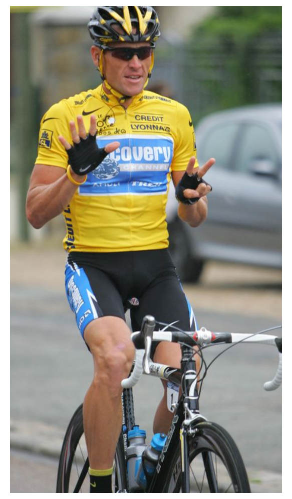

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? ?

- 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.

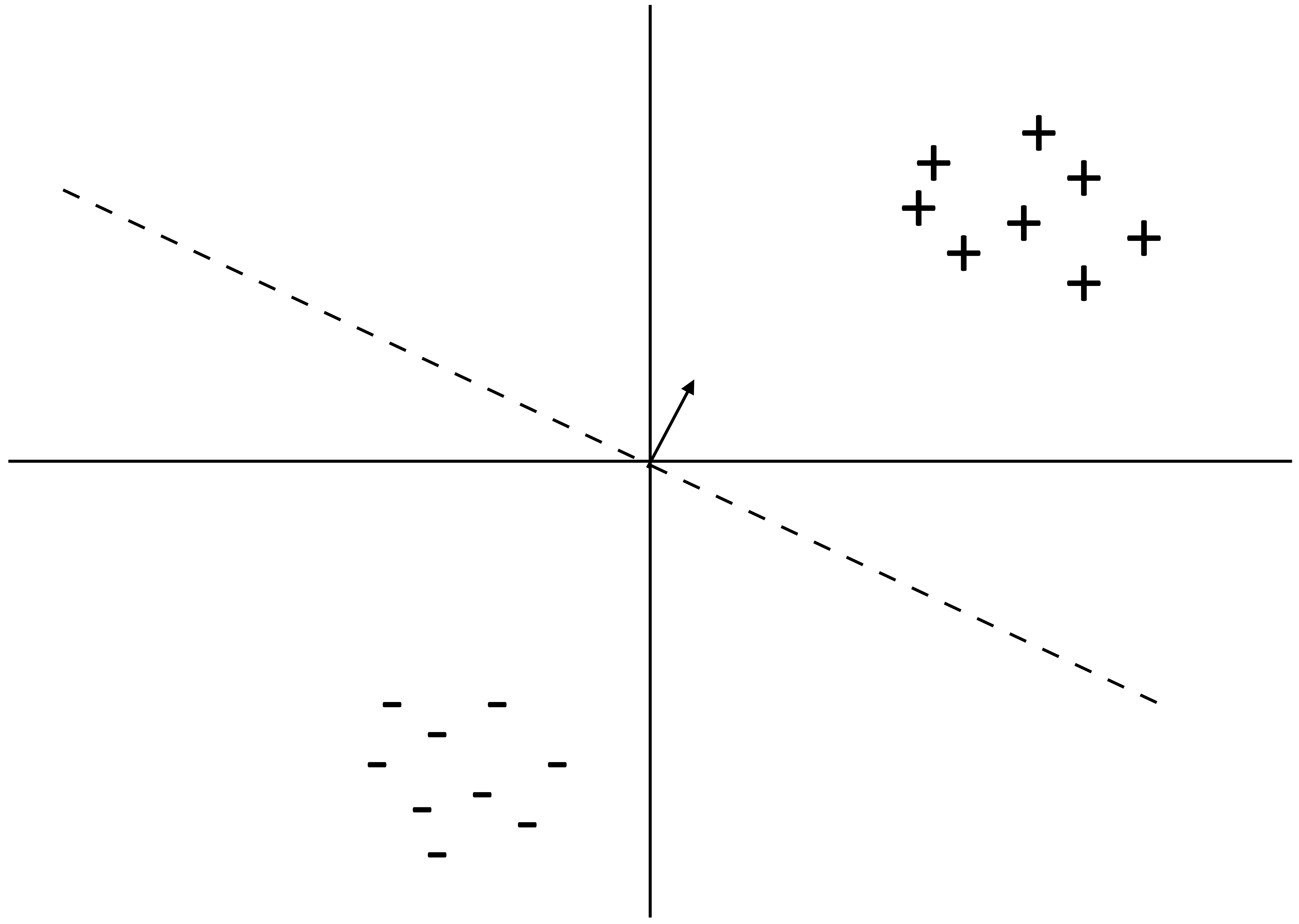
3) Where did James go after he went to the grocery store?
A) his deck
B) his freezer
C) a fast food restaurant
D) his room

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

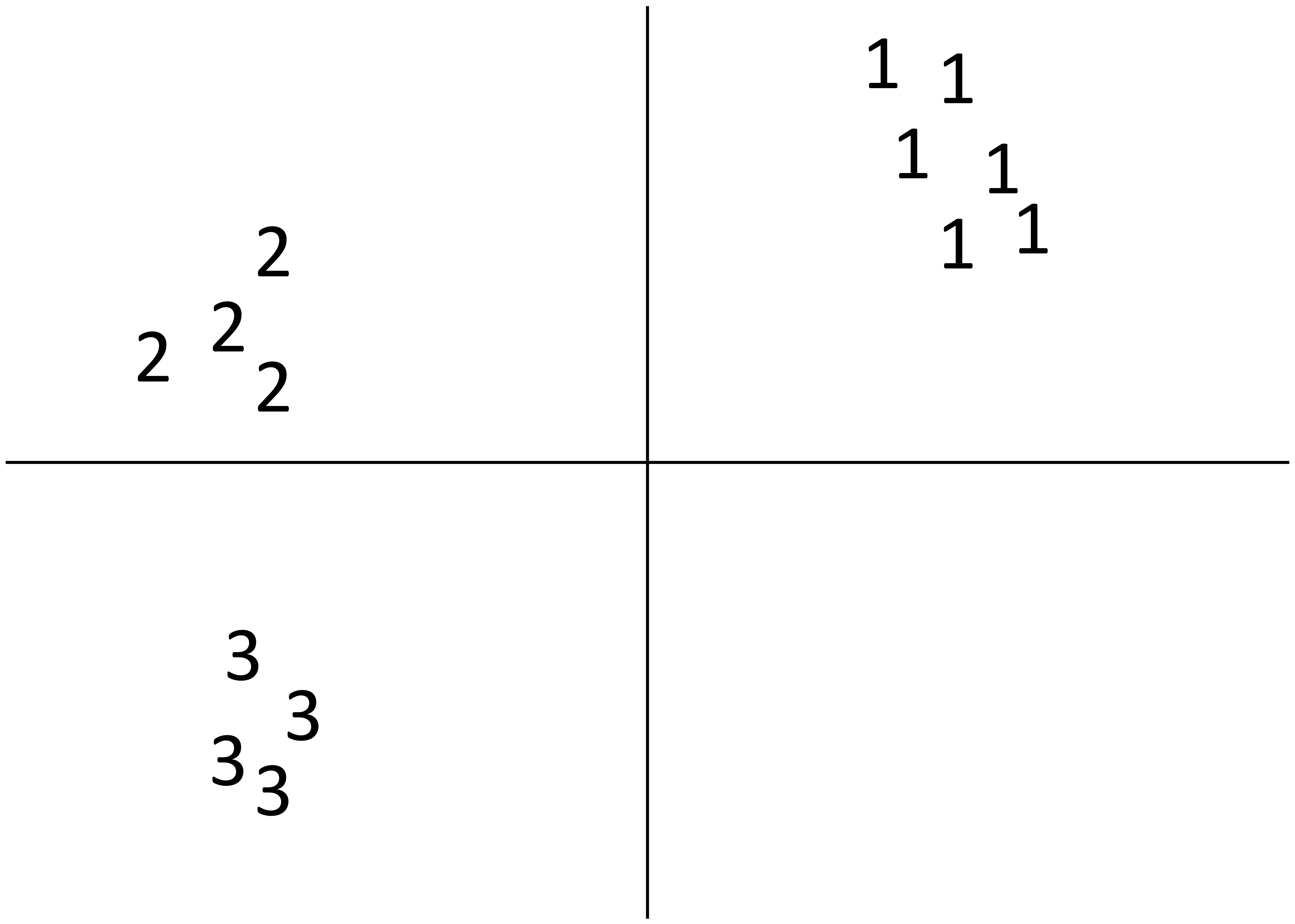
Richardson (2013)

# Binary Classification

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

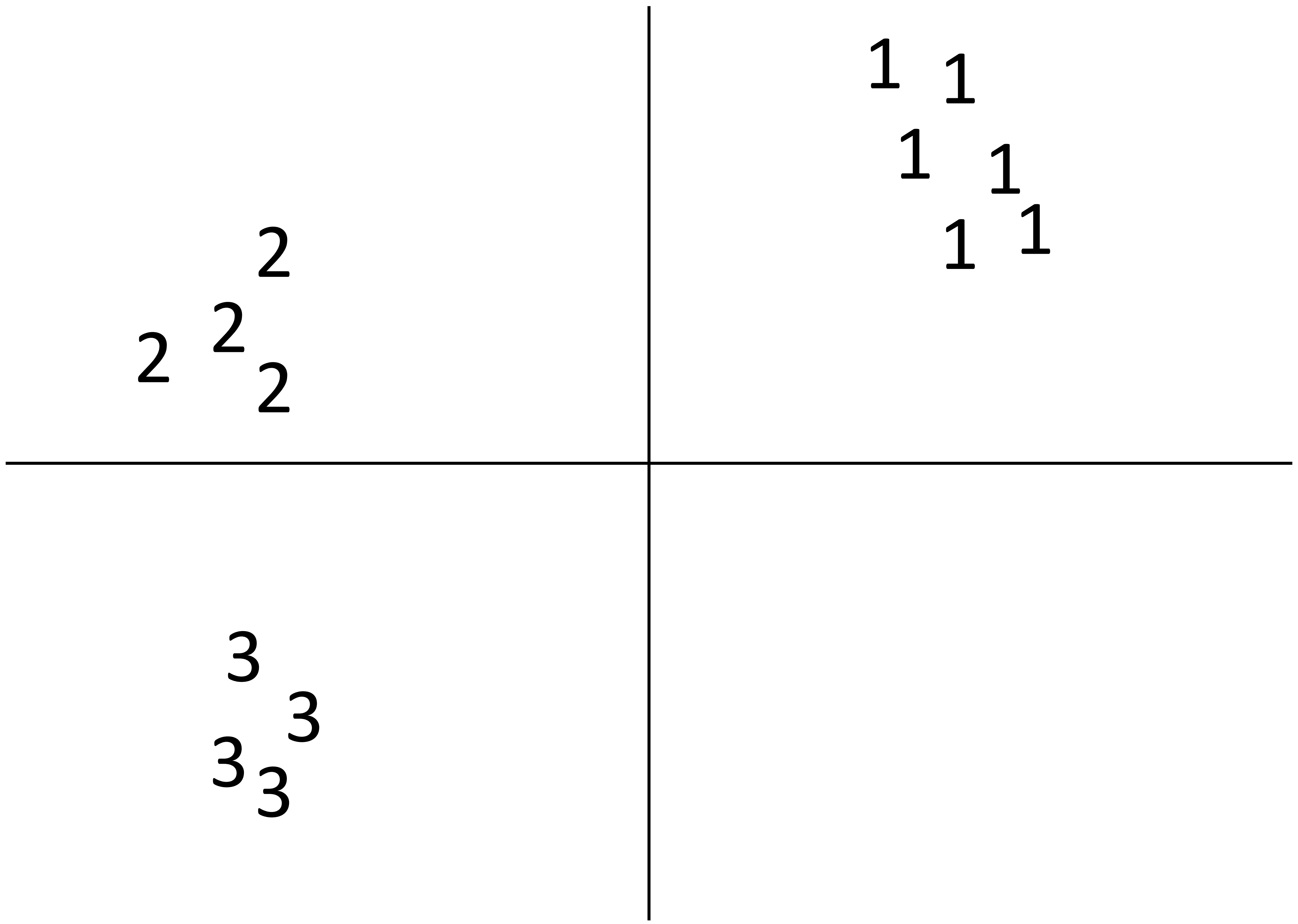


# Multiclass Classification



# Multiclass Classification

- Can we just use binary classifiers here?



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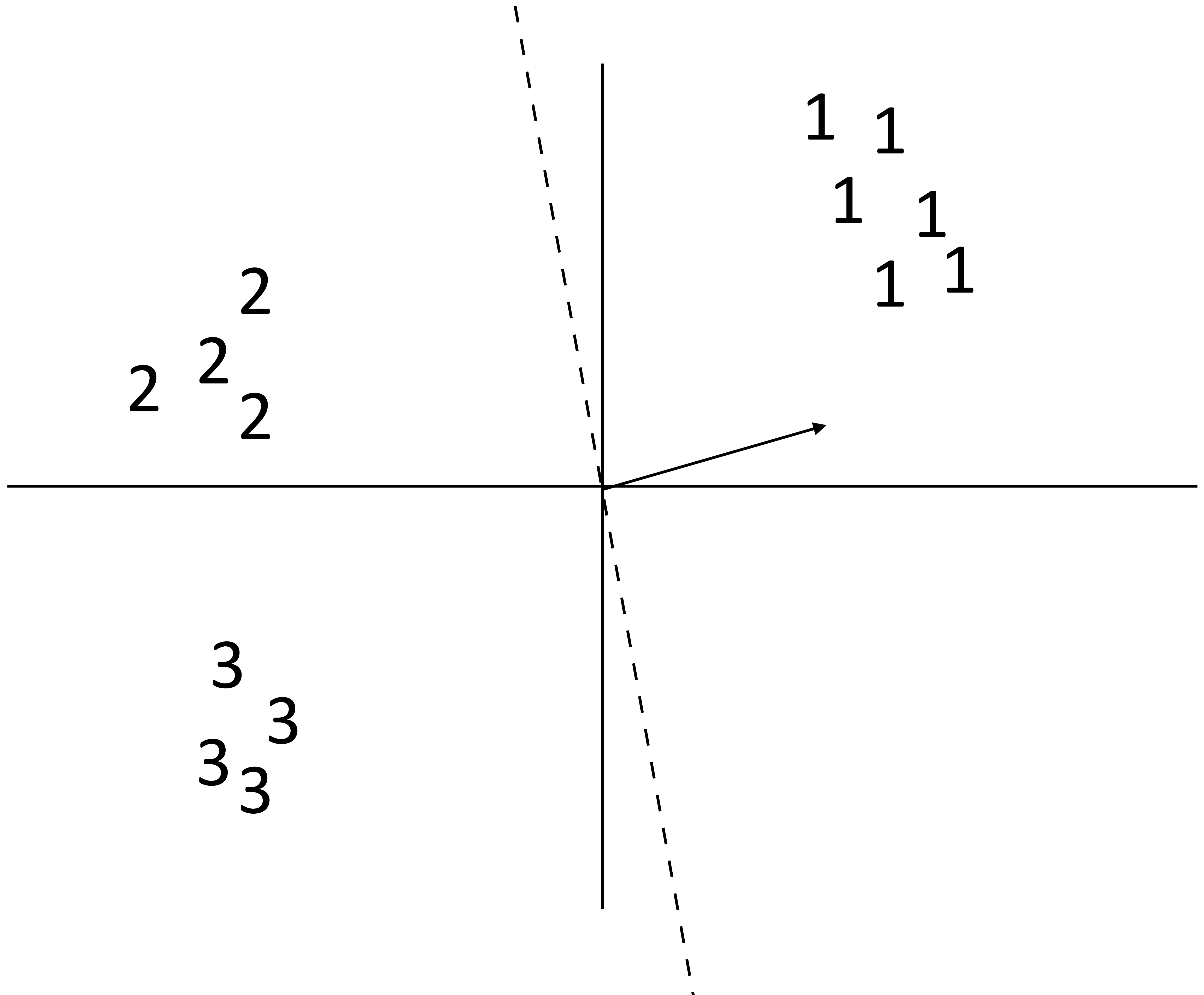

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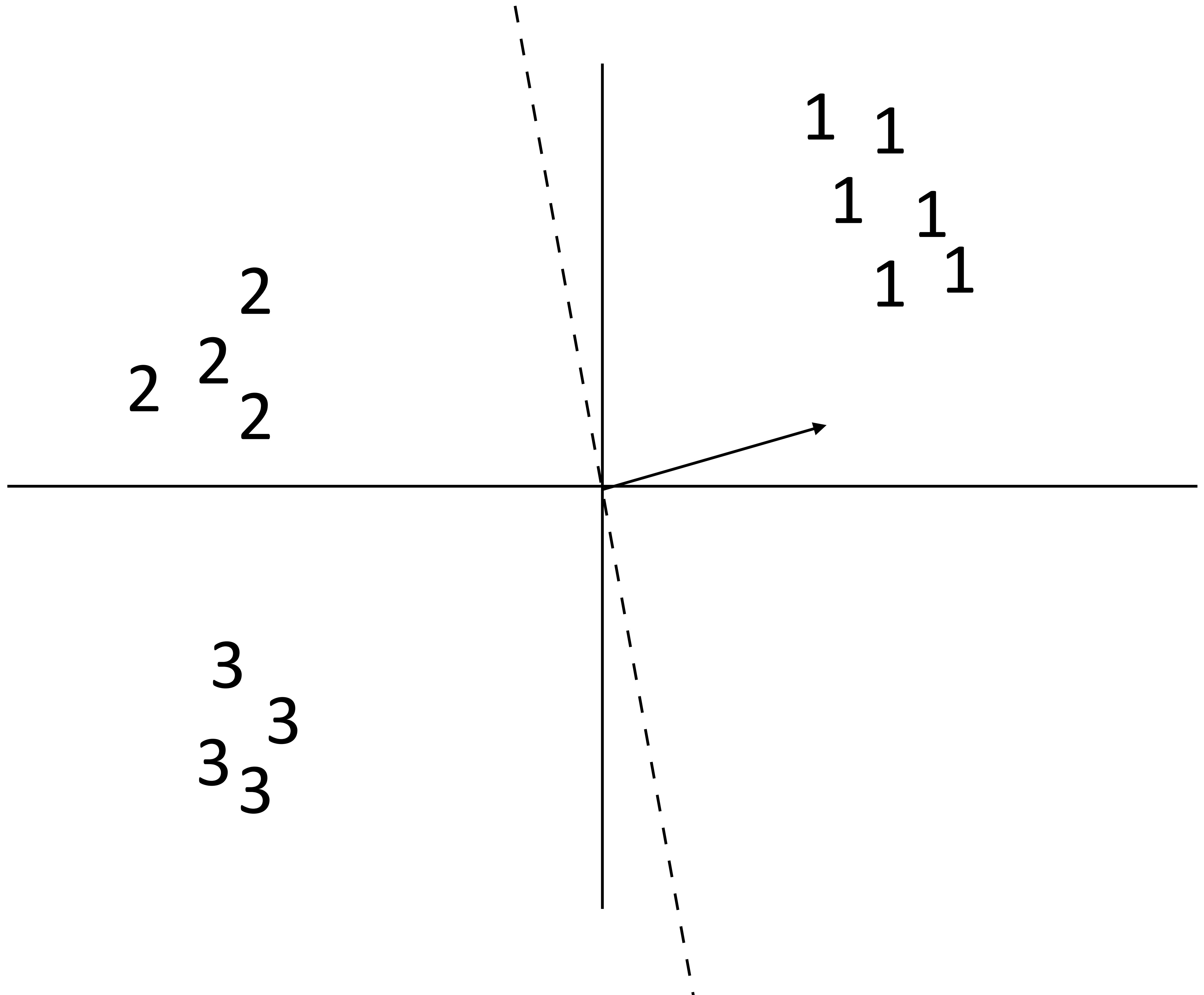
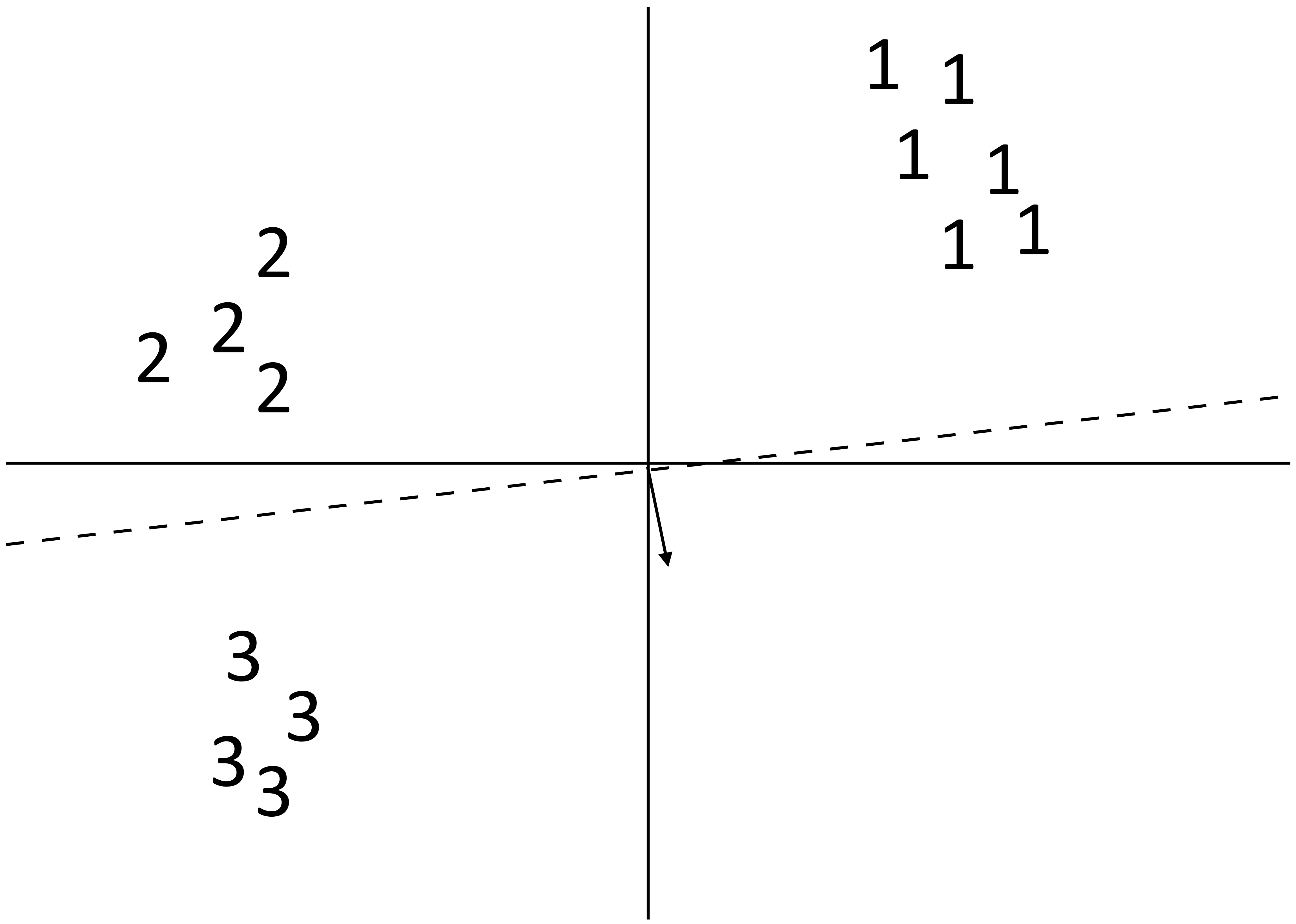
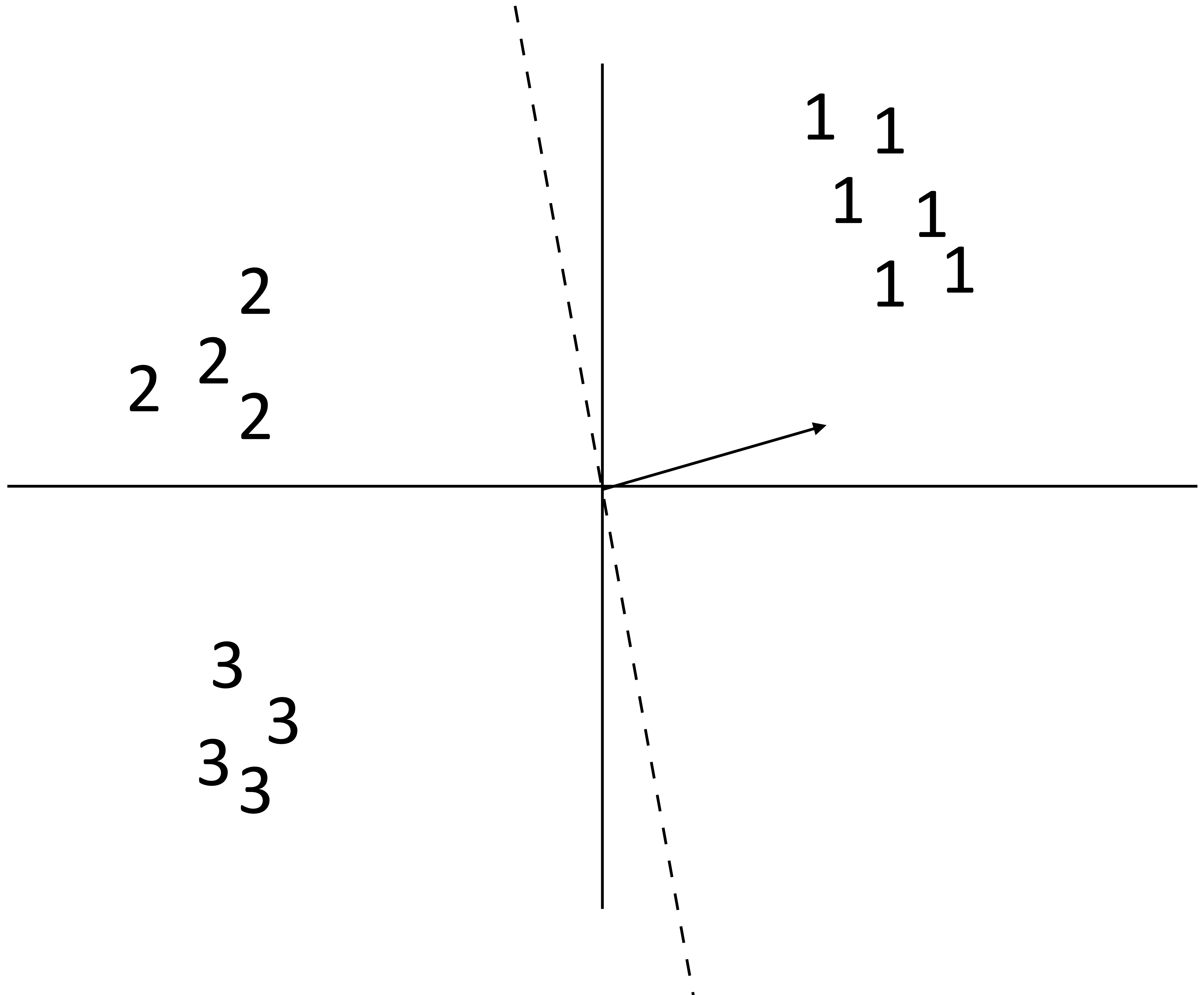
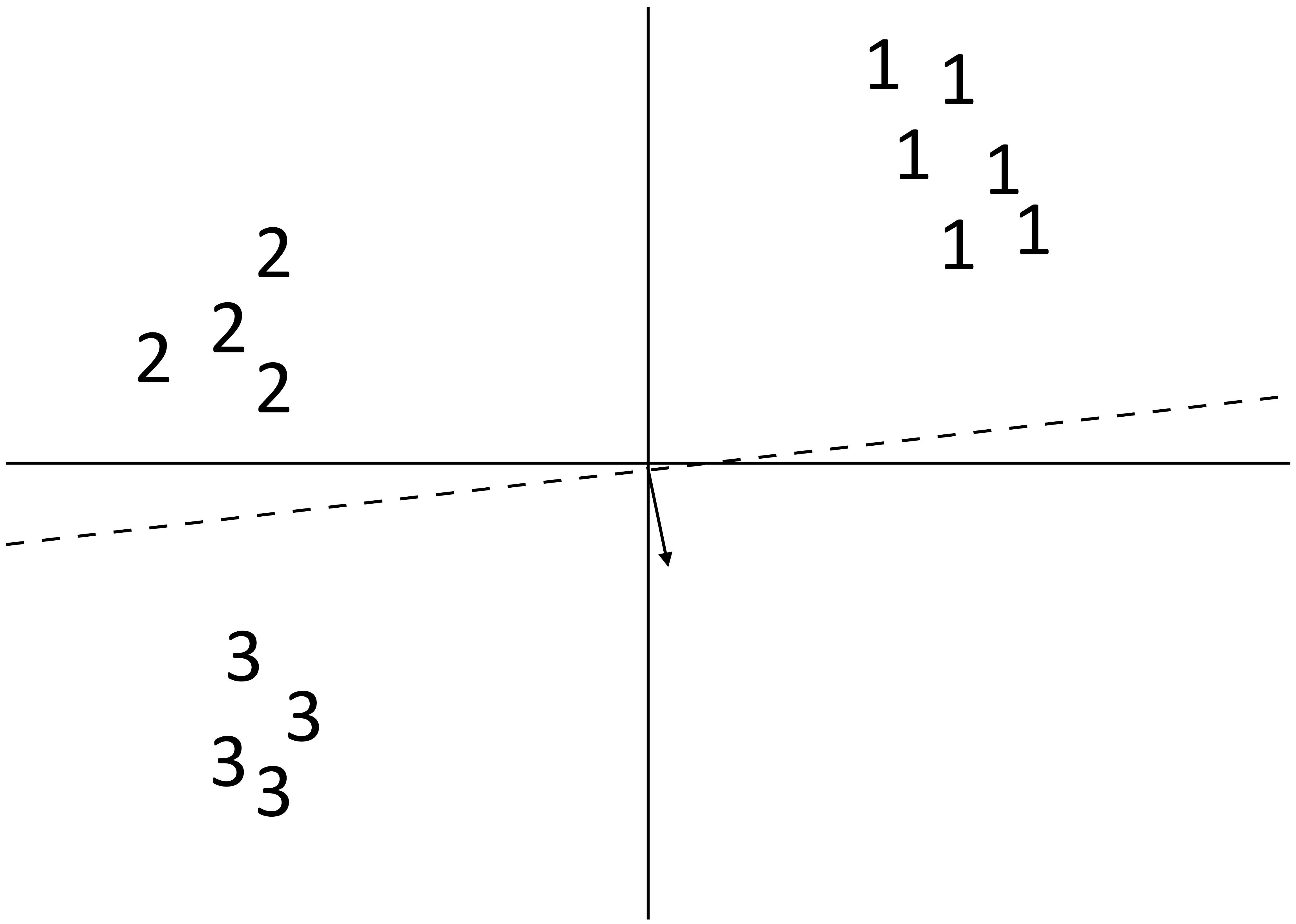


# Multiclass Classification

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



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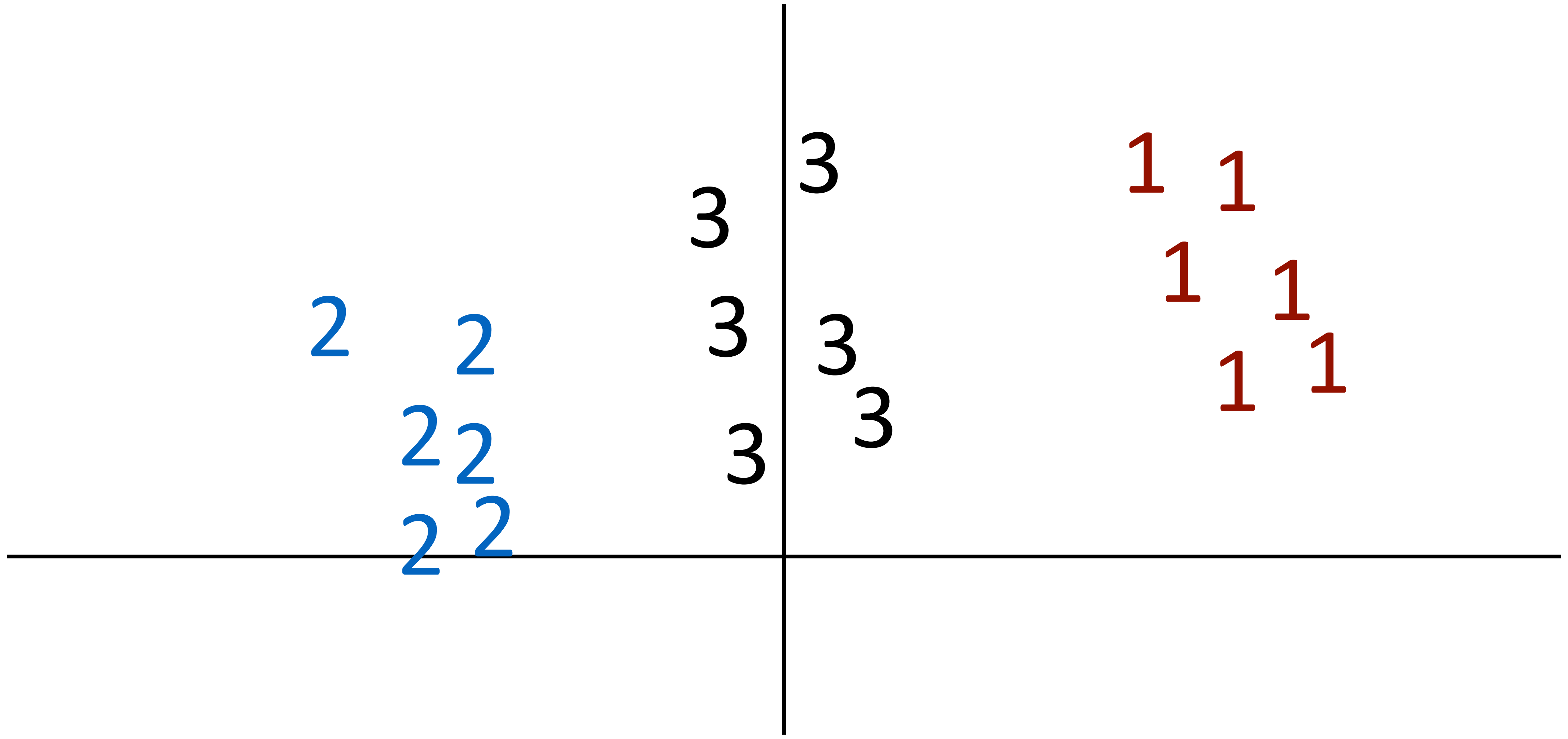

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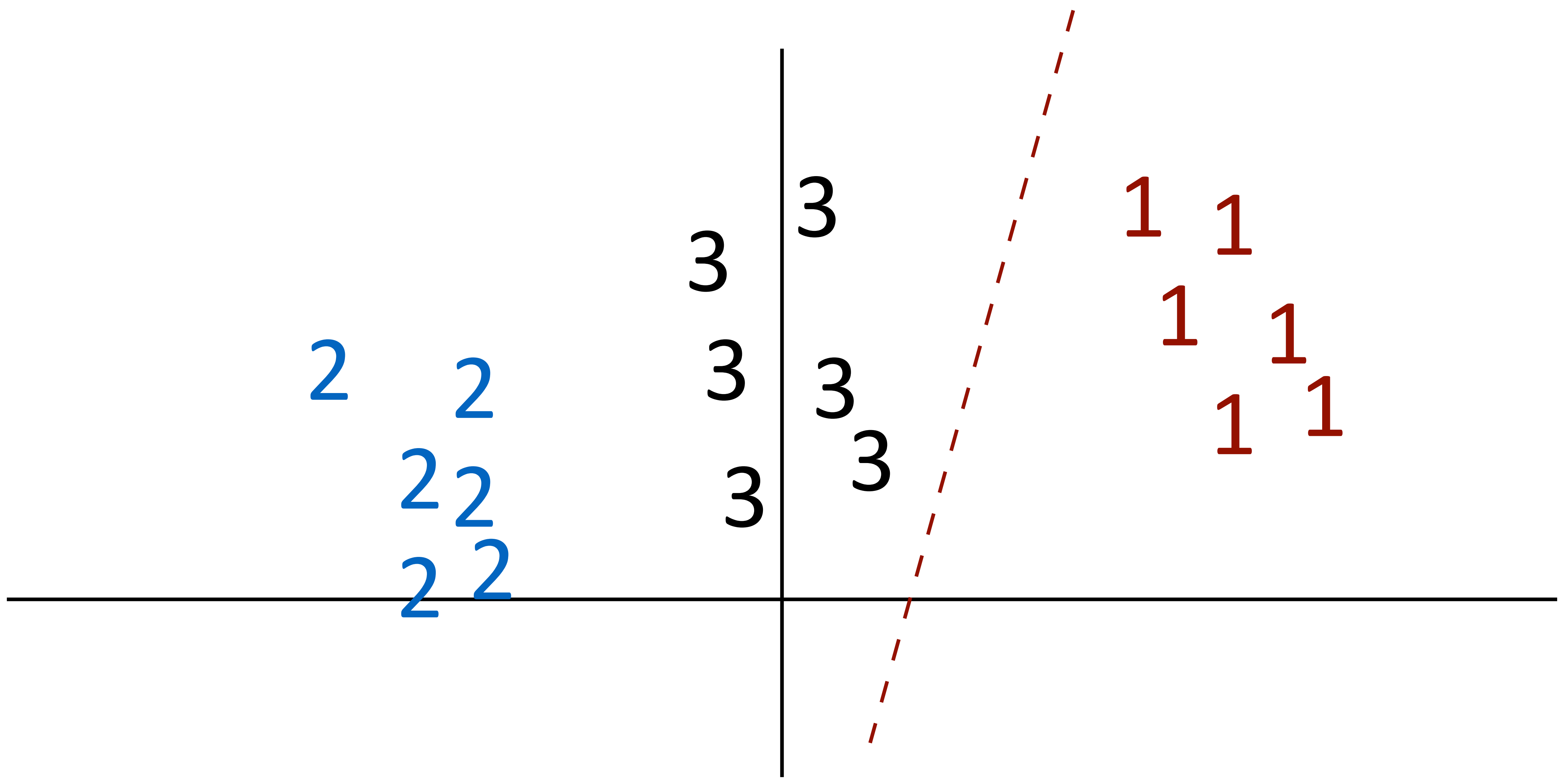

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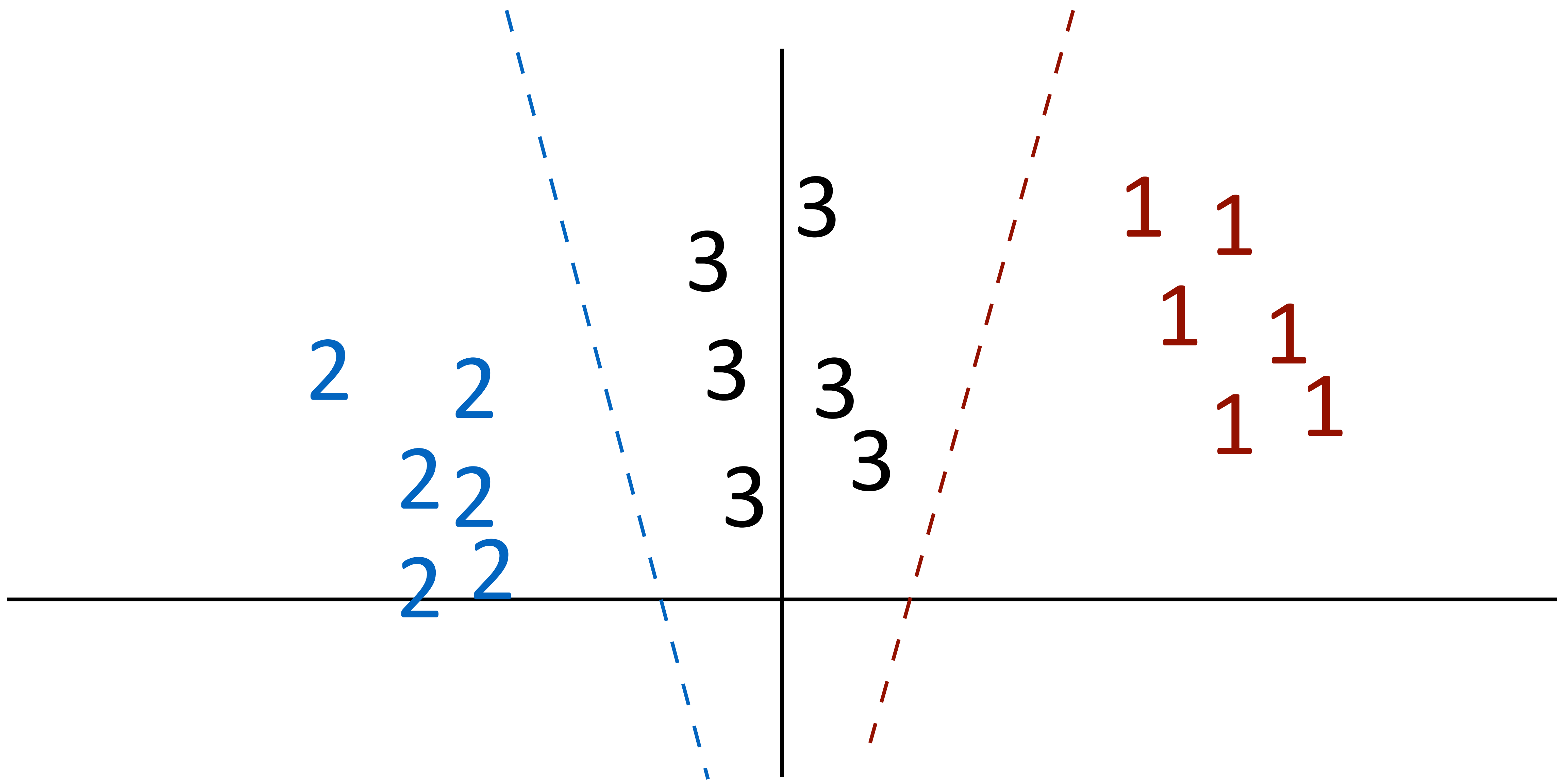

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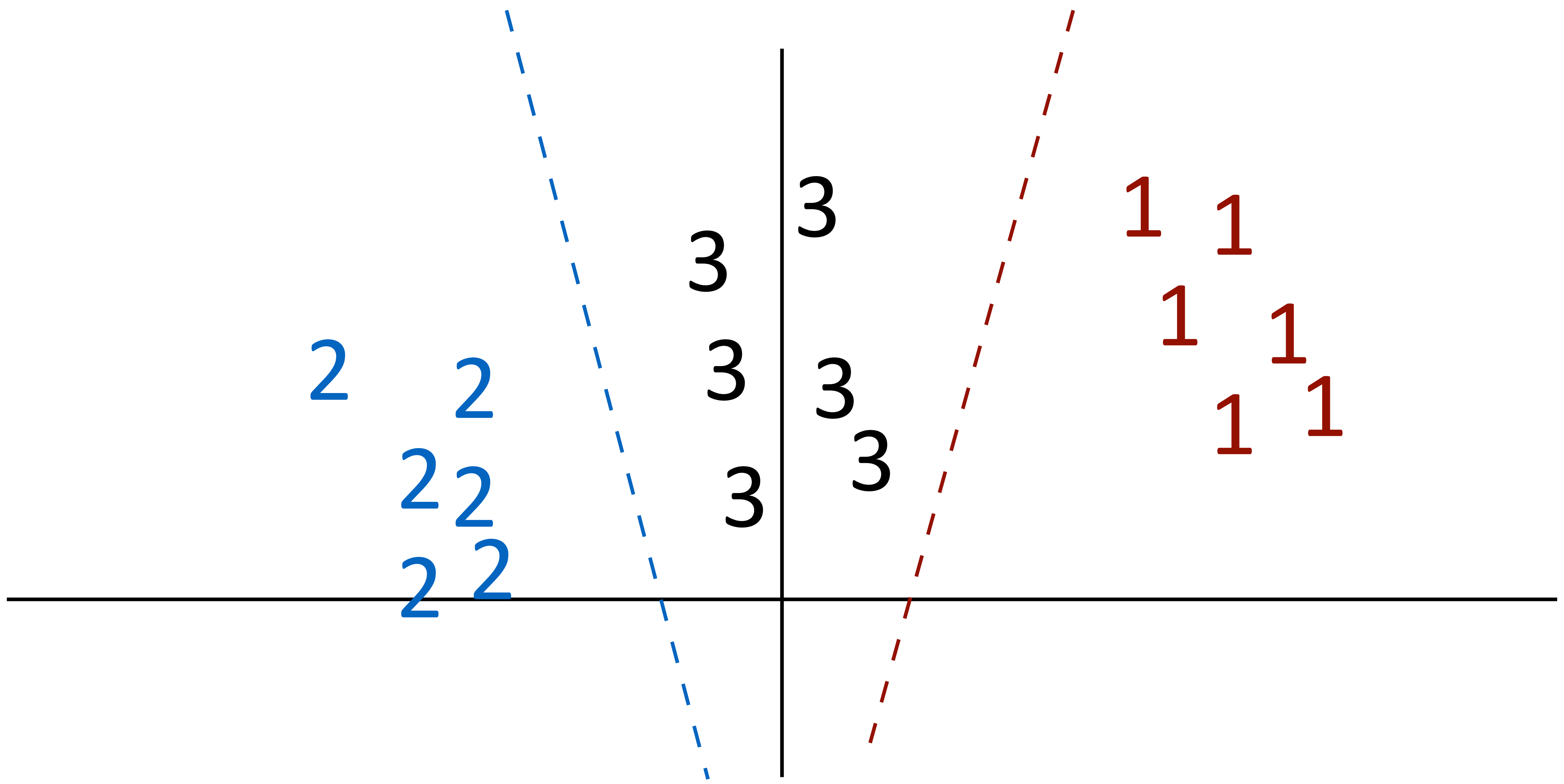


- Can separate 1 from 2+3 and 2 from 1+3 but not 3 from the others (with these features)

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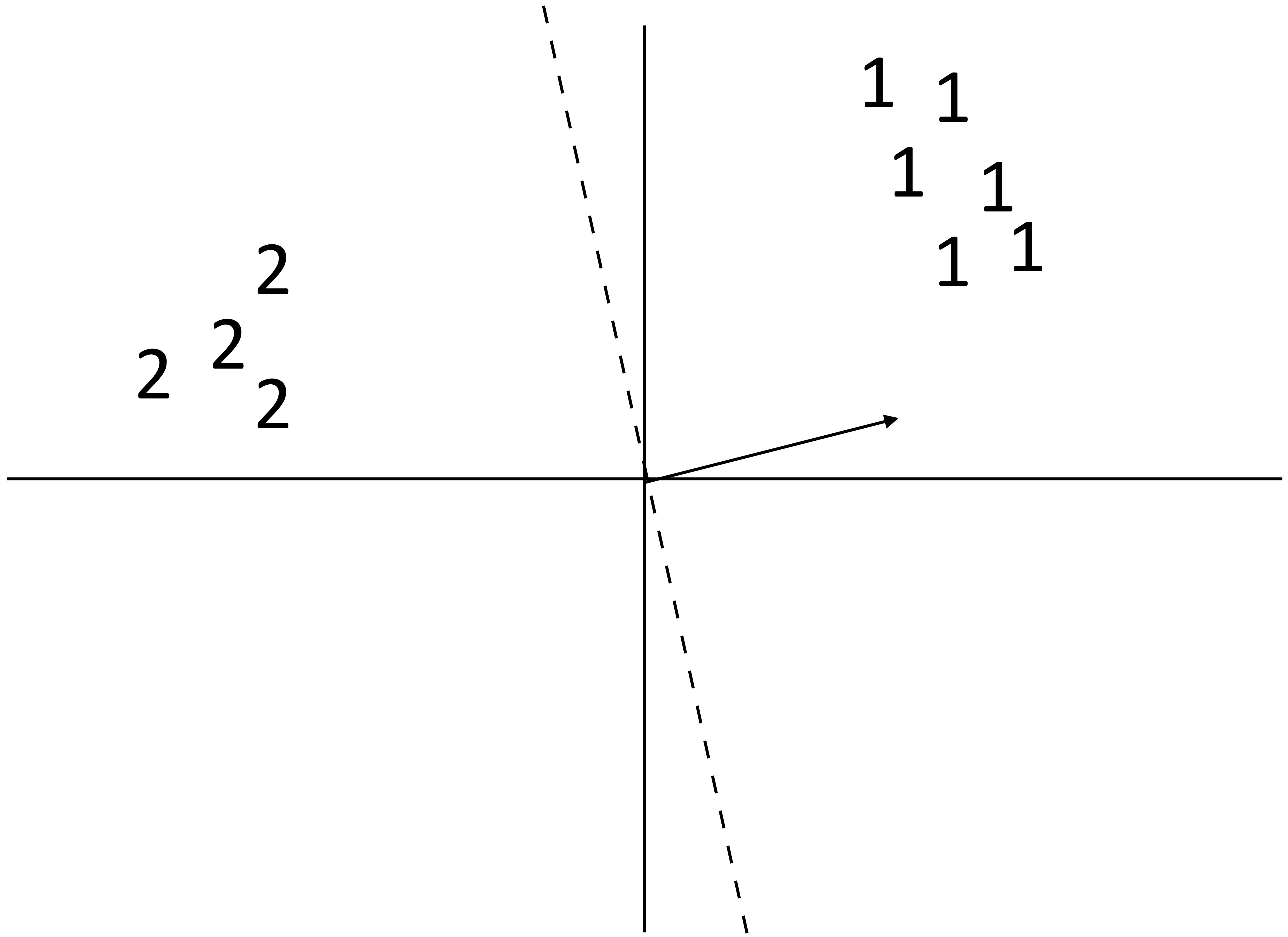

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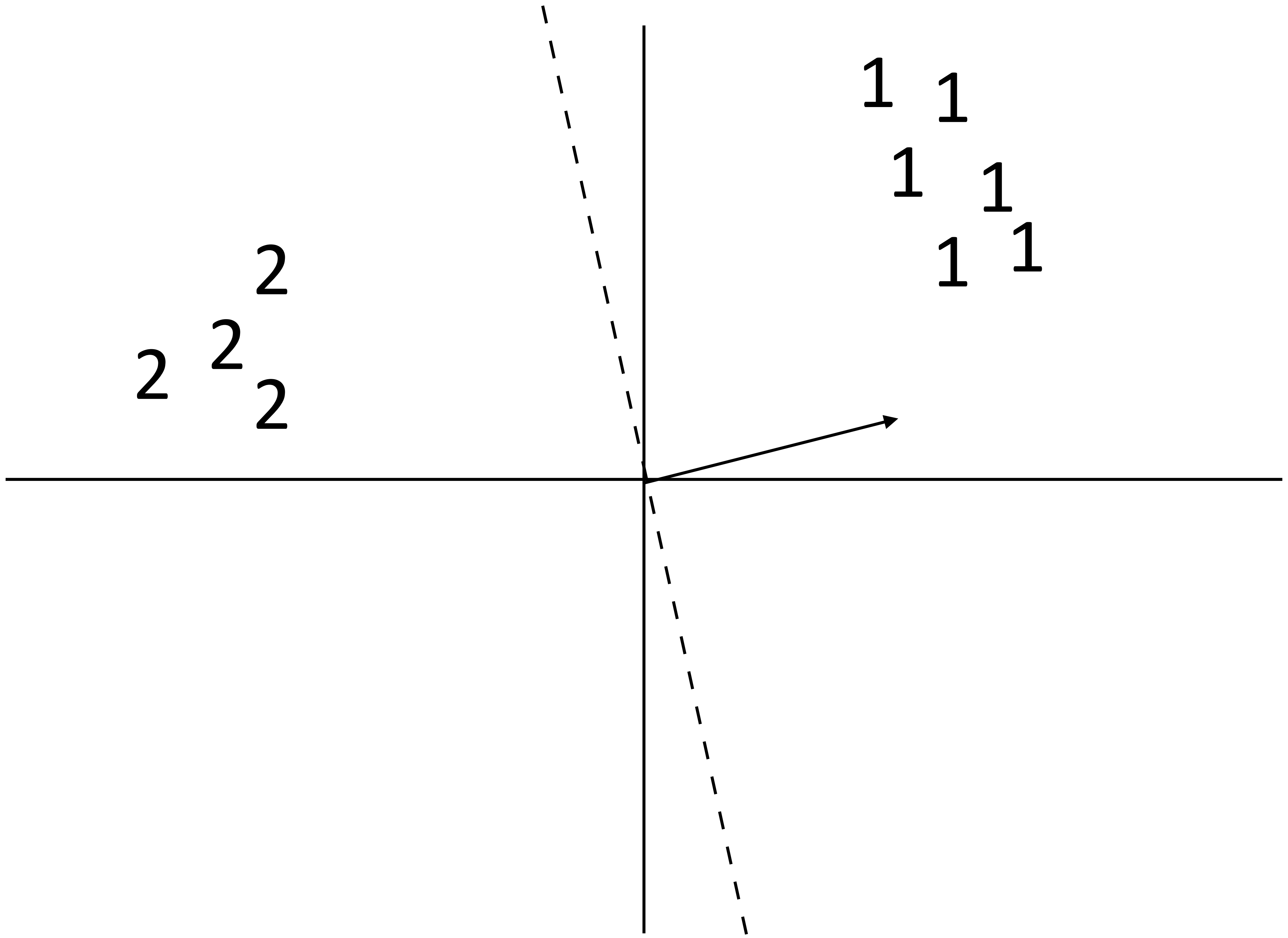
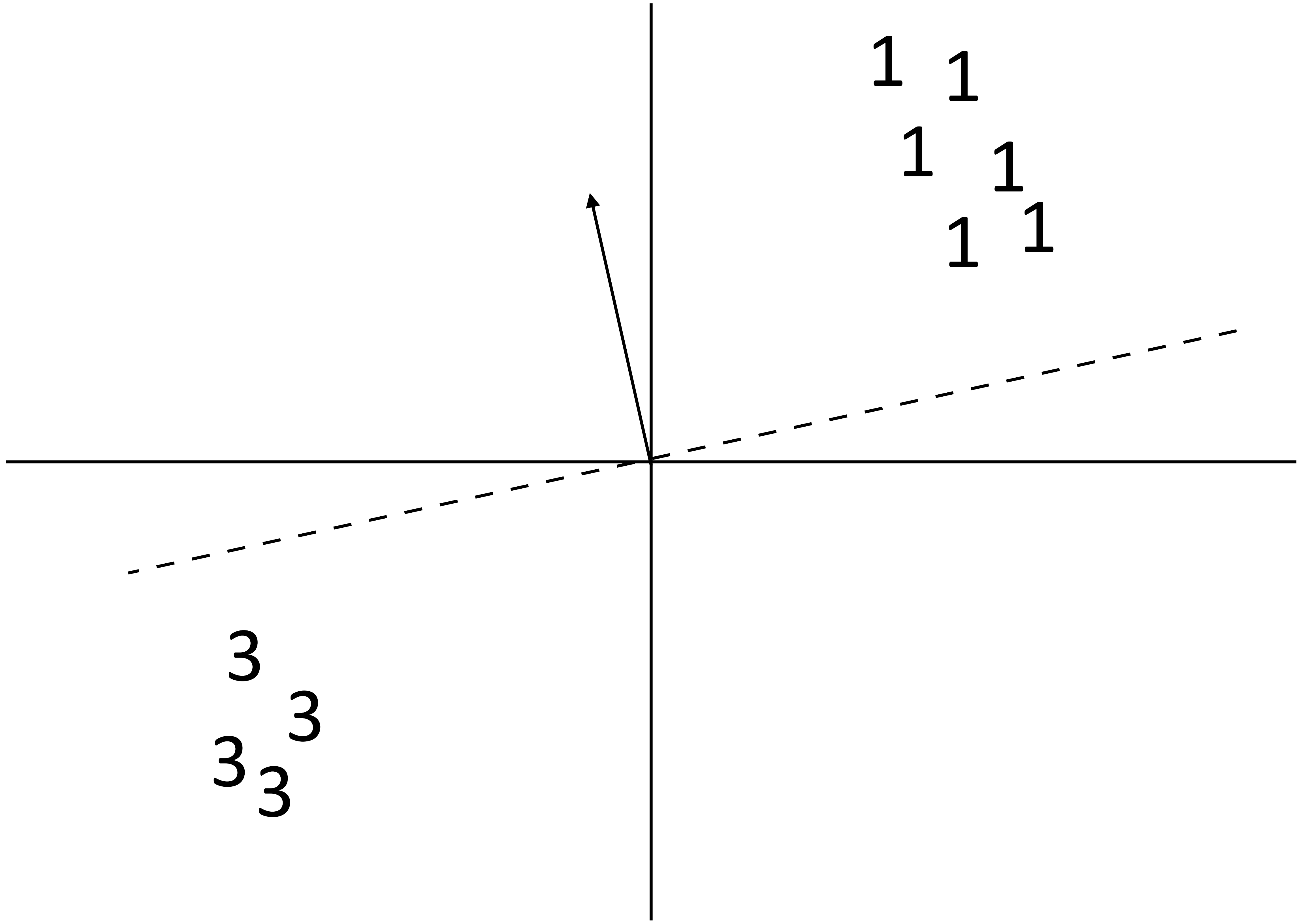
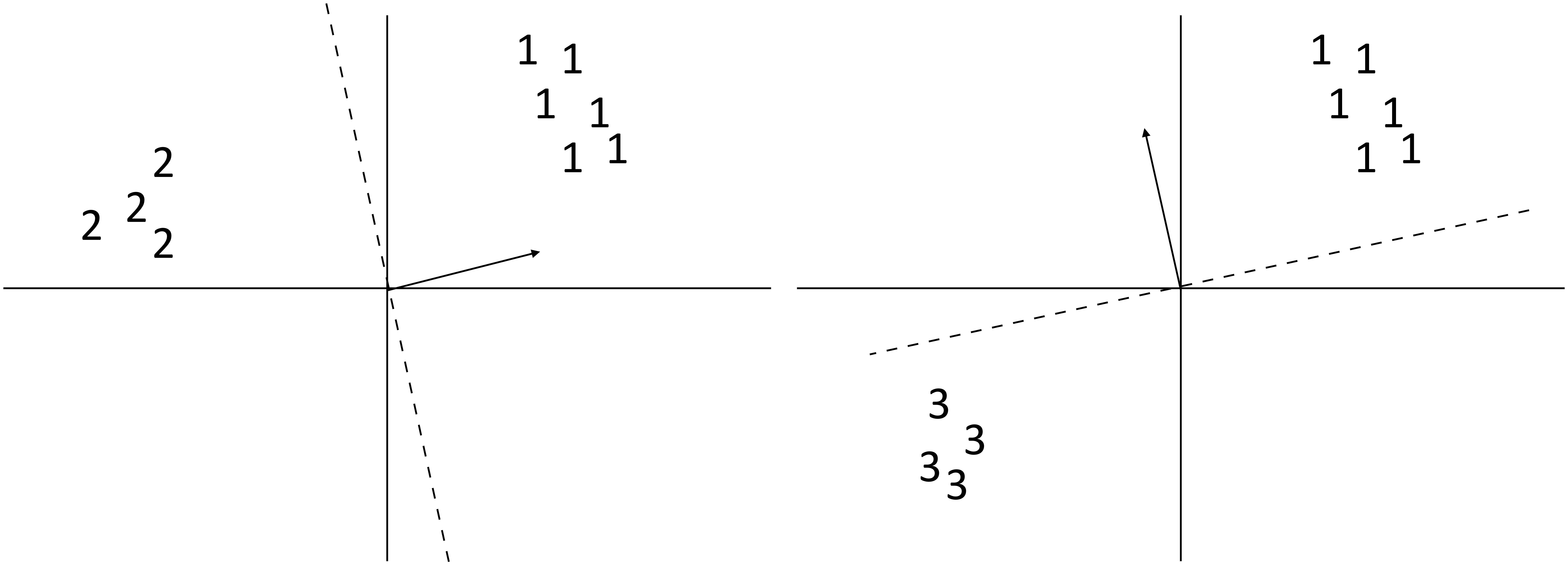


# Multiclass Classification

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



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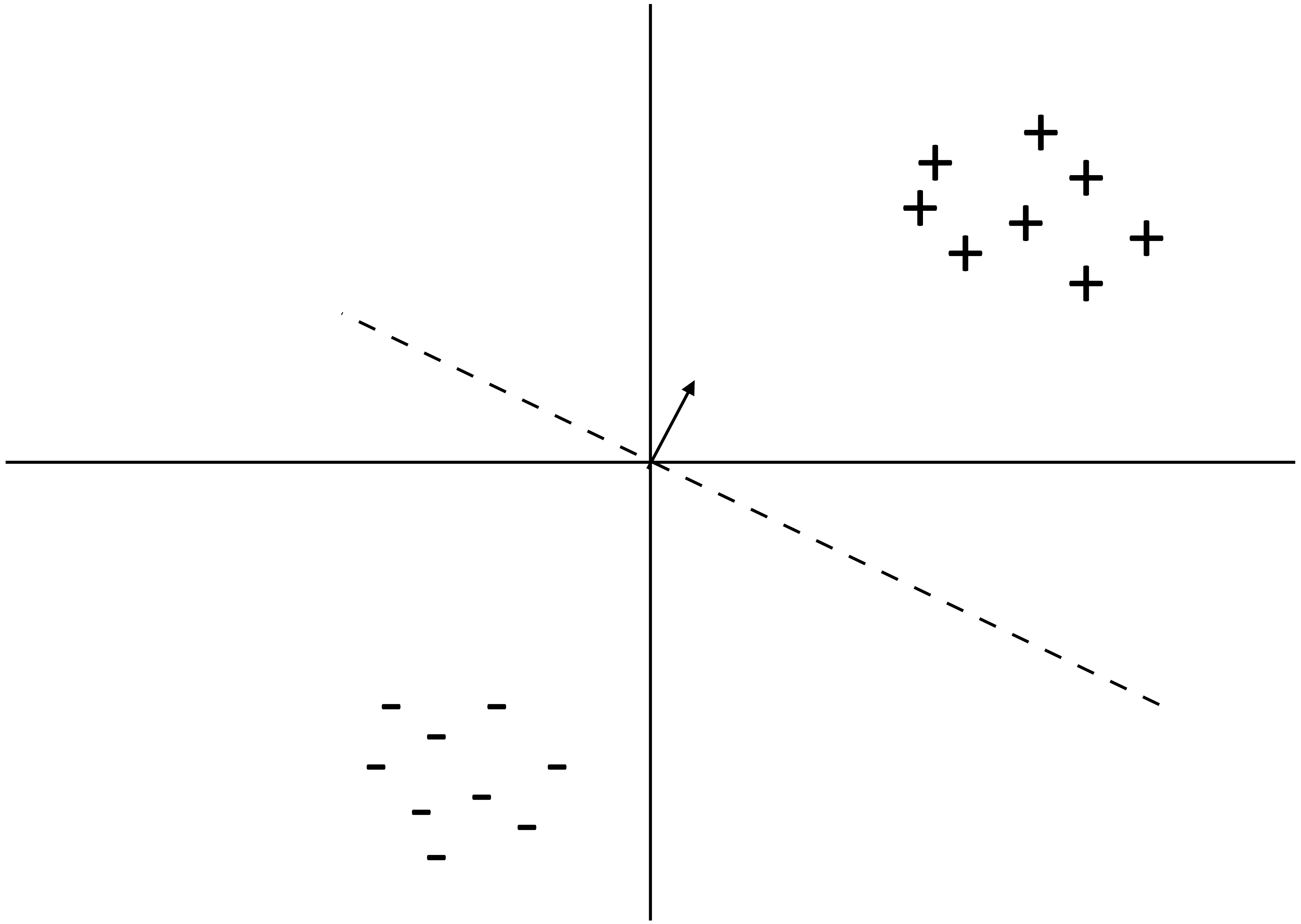


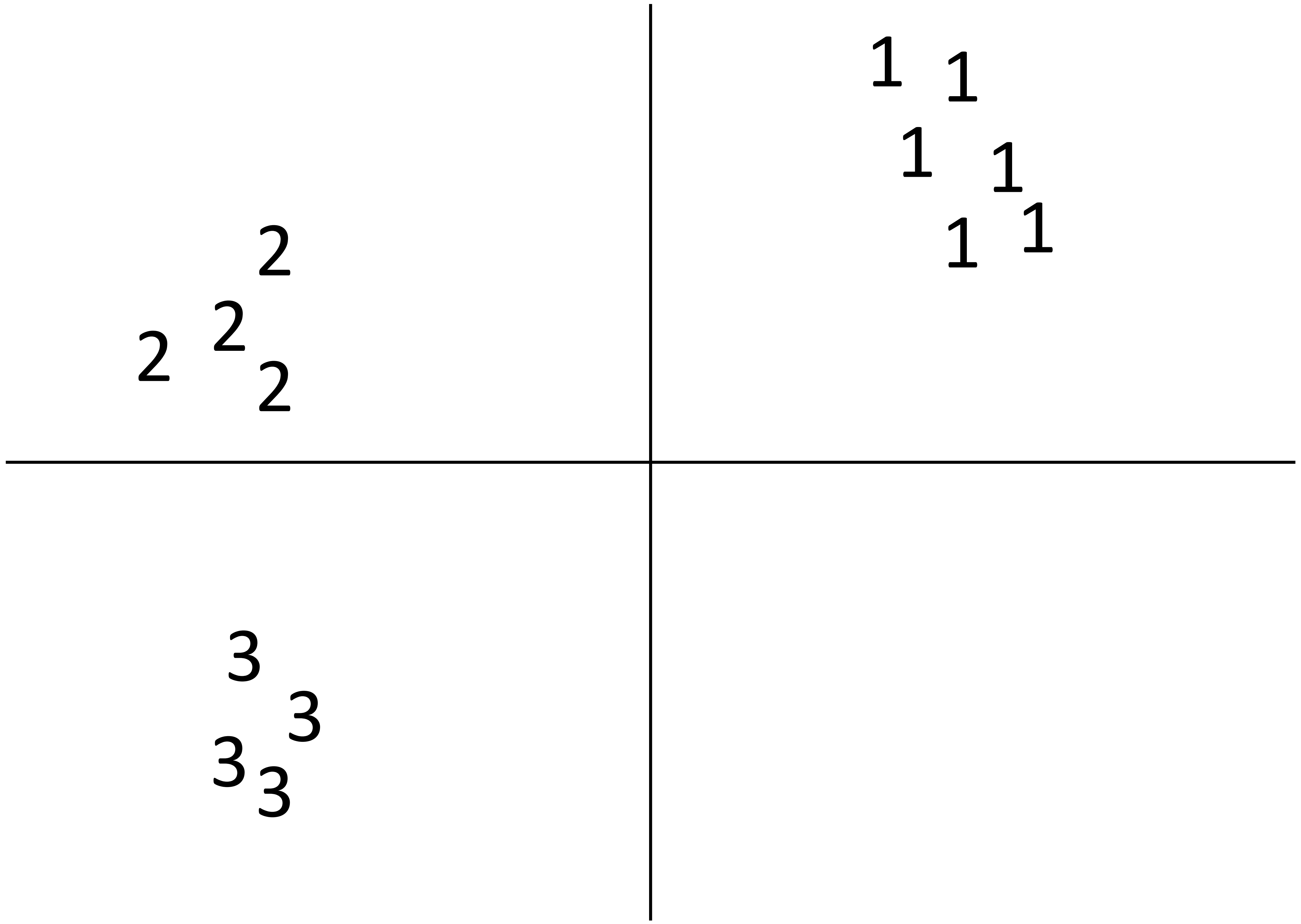

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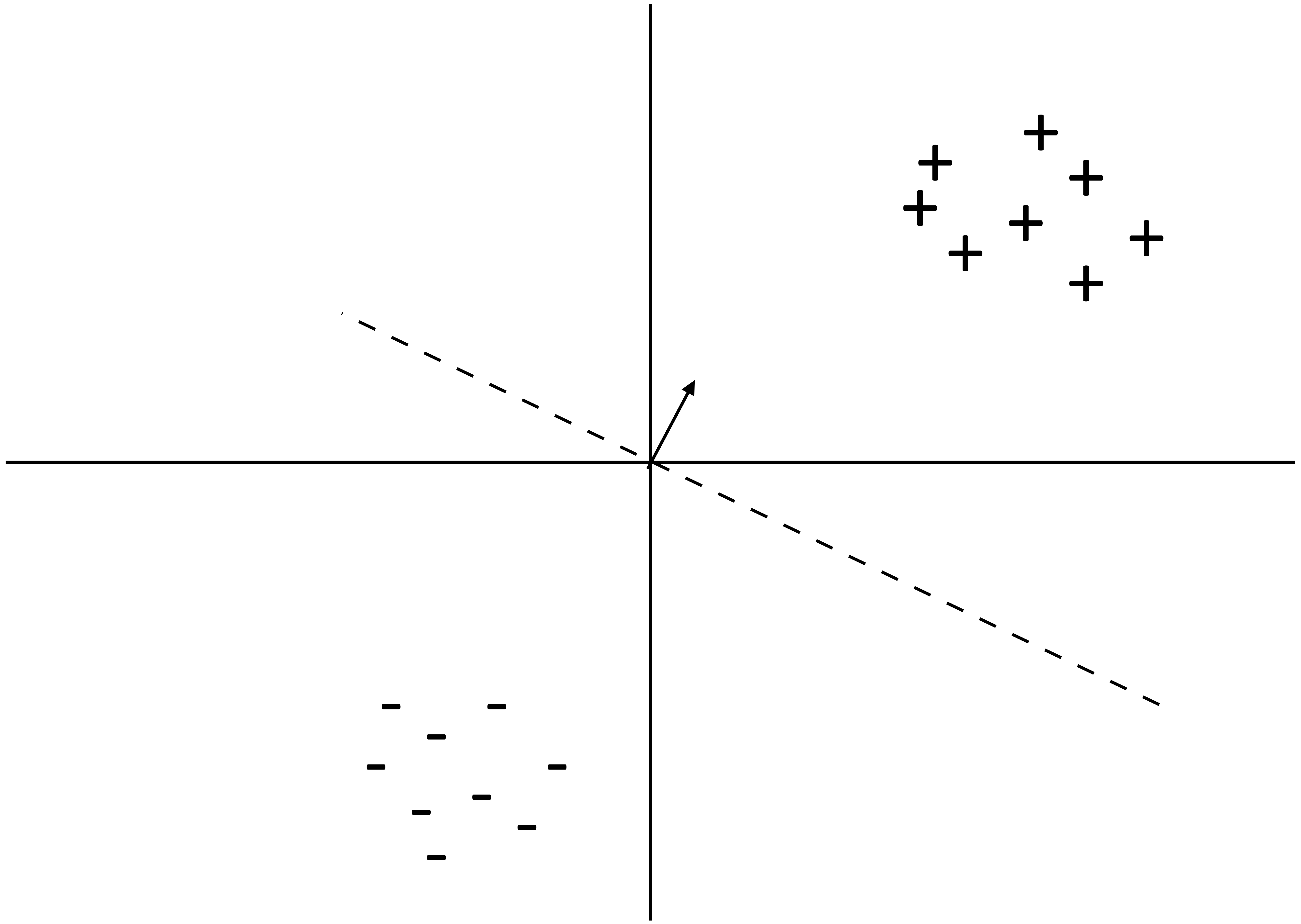

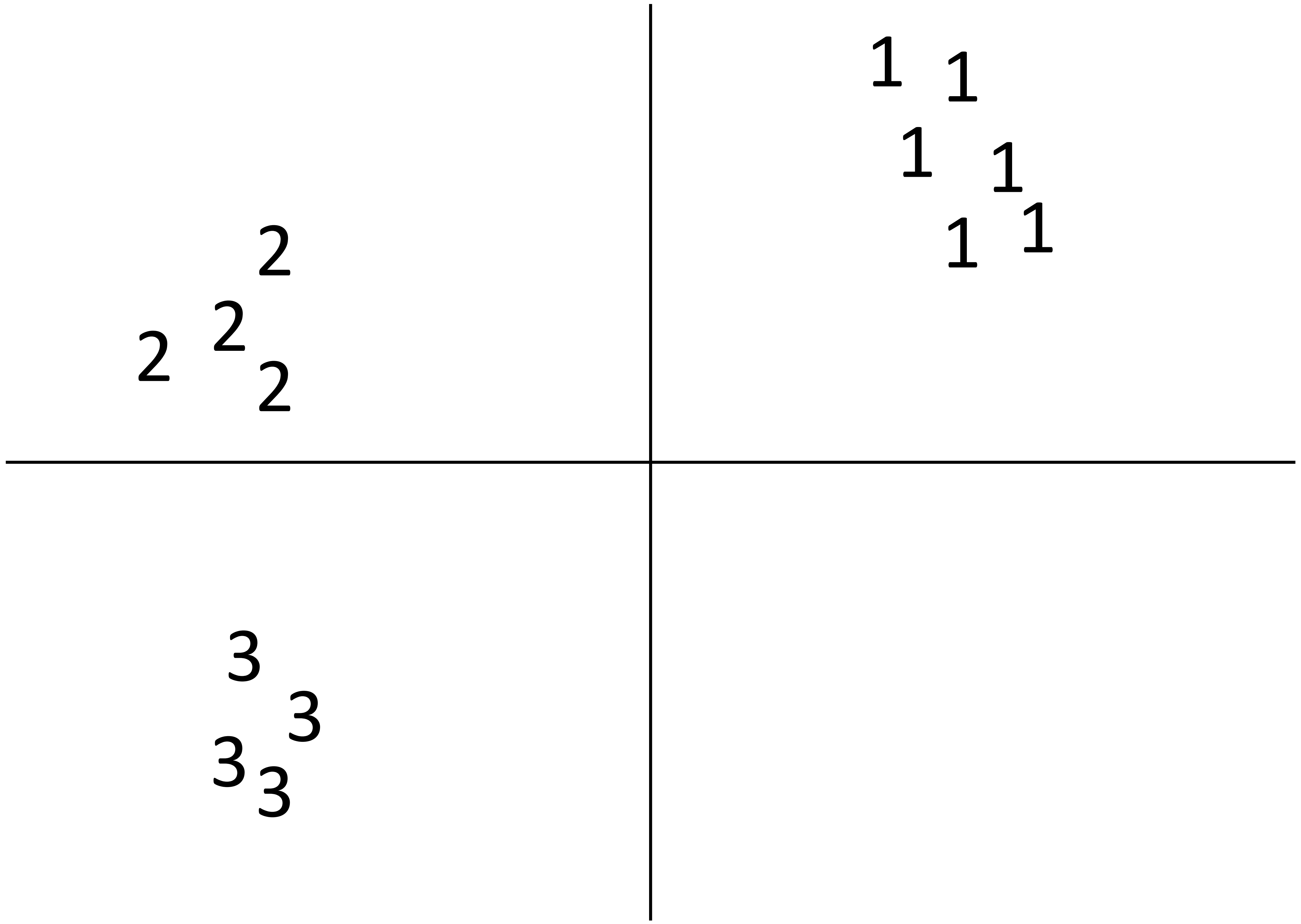

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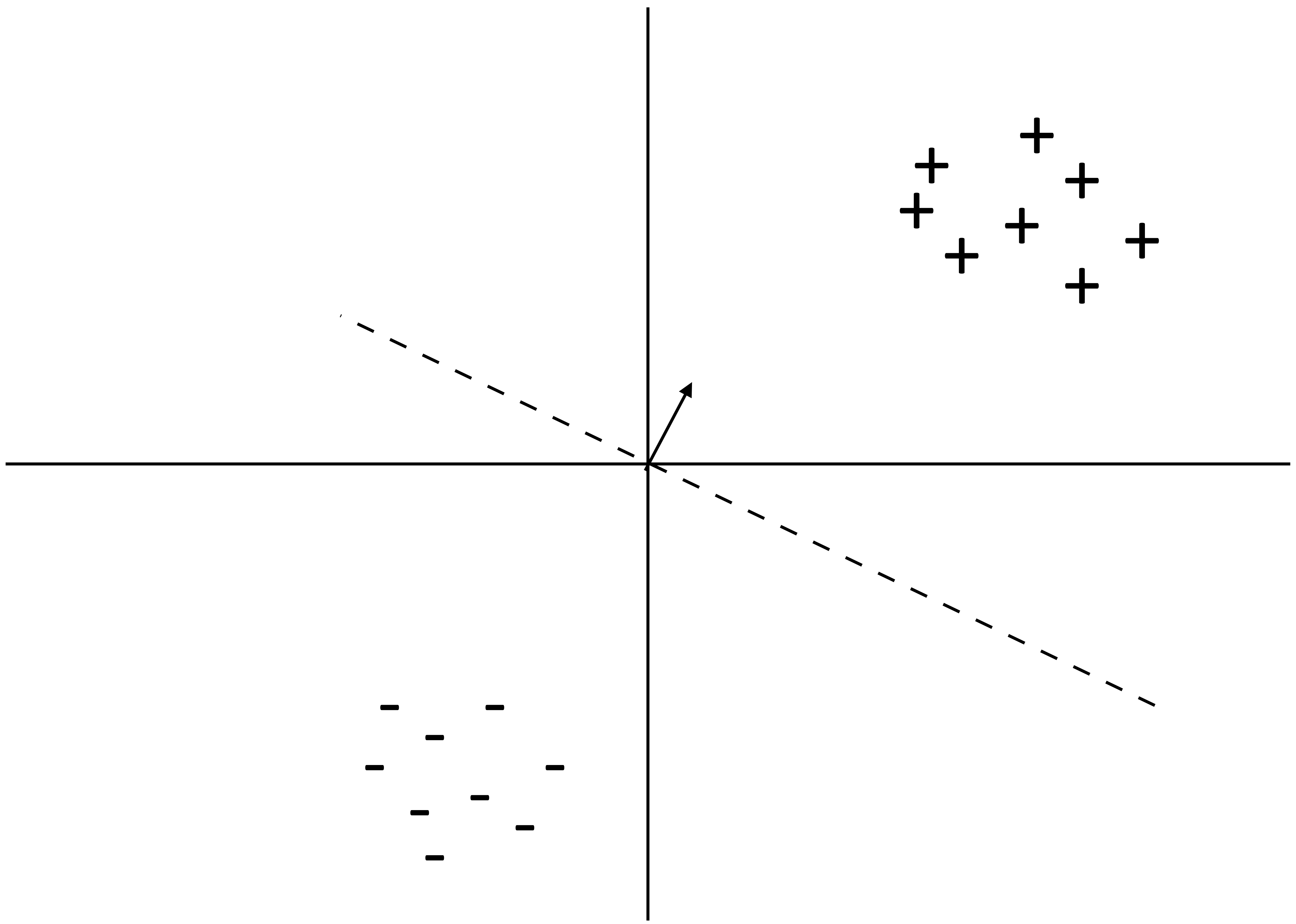


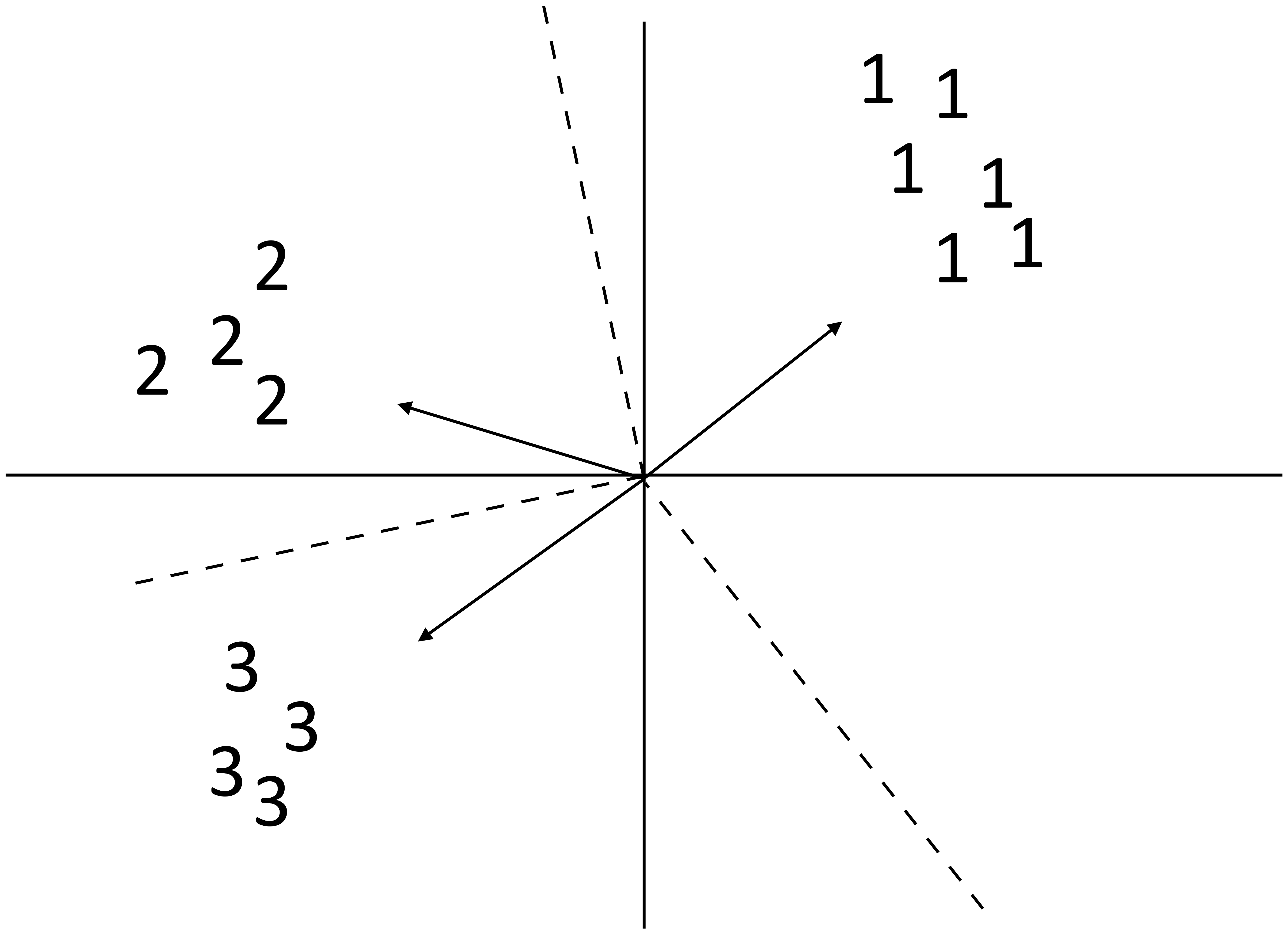

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  - The single weight vector approach will generalize to structured output spaces, whereas per-class weight vectors won't

# Feature Extraction

# Block Feature Vectors

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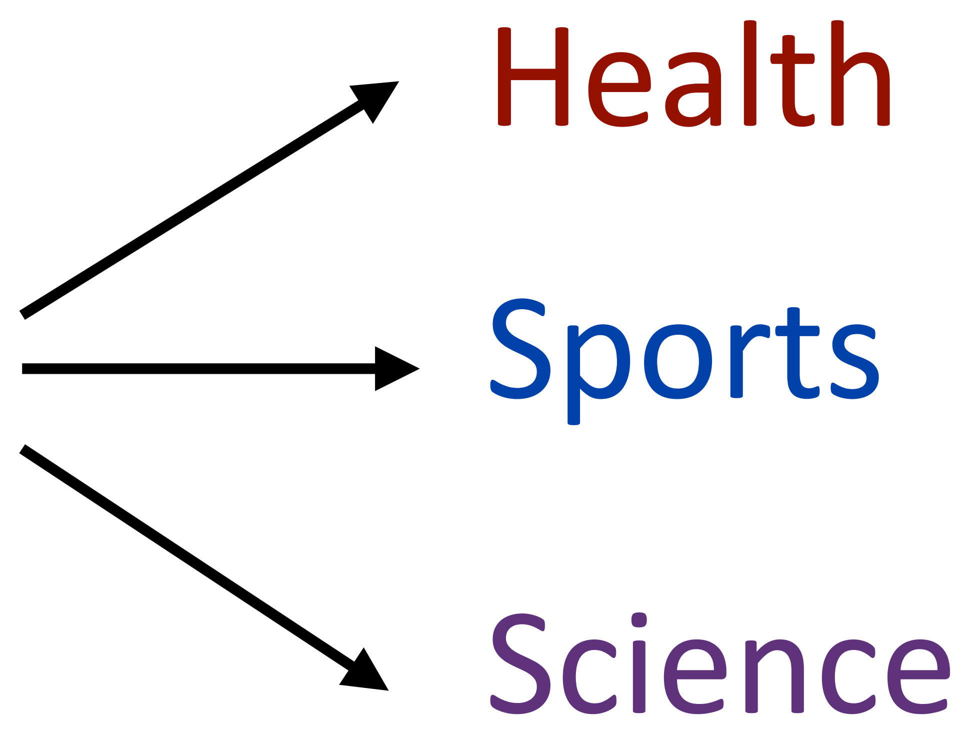

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*too many drug trials, too few patients*

Health

Sports

Science

- Base feature function:

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

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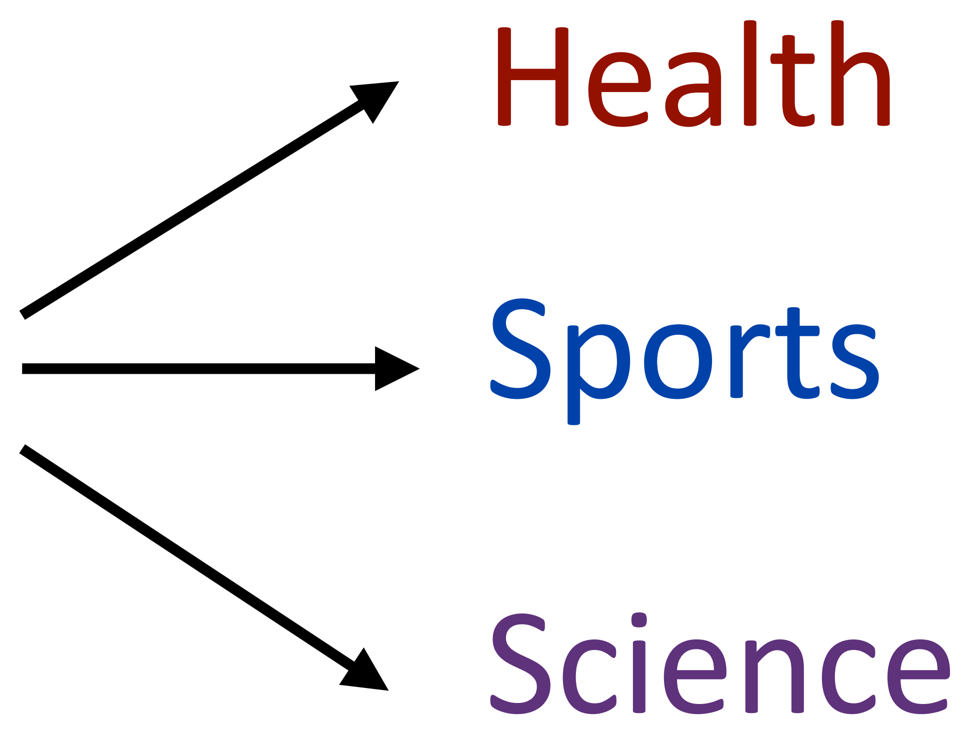


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feature vector blocks for each label

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

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I[contains *drug* & label = Health]

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- Equivalent to having three weight vectors in this case

# Making Decisions

*too many drug trials, too few patients* → Health / Sports / 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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$w^\top f(x, y)$ = Health: +4.4 Sports: -5.9 Science: -0.6

↖ 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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*f*(*x*, *y*=VBZ) = I[curr_word=*blocks* & tag = VBZ],
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I[next_word=*the* & tag = VBZ]
I[curr_suffix=*s* & tag = VBZ]

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

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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

# Multiclass Logistic Regression

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sum over output space to normalize

- Compare to binary:

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

# Multiclass Logistic Regression

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

sum over output space to normalize

- Compare to binary:

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

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

# Multiclass Logistic Regression

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

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

Softmax function

sum over output space to normalize

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

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Health: +2.2

Sports: +3.1

Science: -0.6

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

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

exp →

probabilities must be >= 0

| |
|---|
| 6.05 |
| 22.2 |
| 0.55 |

unnormalized probabilities

# Multiclass Logistic Regression

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

Softmax function

sum over output space to normalize

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

*too many drug trials, too few patients*

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

# 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

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

exp →

probabilities must be >= 0

6.05

22.2

0.55

unnormalized probabilities

normalize →

probabilities must sum to 1

0.21

0.77

0.02

probabilities

1.00

0.00

0.00

correct (gold) probabilities

# Multiclass Logistic Regression

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

Softmax function

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

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| $w^\top f(x,y)$ | exp → unnormalized probabilities (probabilities must be >= 0) | normalize → probabilities (probabilities must sum to 1) | compare ↔ correct (gold) probabilities |
|---|---|---|---|
| Health: +2.2 | 6.05 | 0.21 | 1.00 |
| Sports: +3.1 | 22.2 | 0.77 | 0.00 |
| Science: -0.6 | 0.55 | 0.02 | 0.00 |

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

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

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sum over output space to normalize

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| $w^\top f(x,y)$ | | probabilities must be >= 0 (unnormalized probabilities) | | probabilities must sum to 1 (probabilities) | | correct (gold) probabilities |
|---|---|---|---|---|---|---|
| Health: +2.2 | exp → | 6.05 | normalize → | 0.21 | log(0.21) = - 1.56 | 1.00 |
| Sports: +3.1 | | 22.2 | | 0.77 | ← compare → | 0.00 |
| Science: -0.6 | | 0.55 | | 0.02 | $\mathcal{L}(x_j, y_j^*) = \log P(y_j^*|x_j)$ | 0.00 |

# 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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sum over output space to normalize

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

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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

- 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

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

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

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- 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

# Training

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gold feature value

model's expectation of feature value

# Training

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

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gradient:

# Training

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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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update $w^\top$:

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

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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]

# 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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$f(x, y =$ 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]

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

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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

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

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

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

- 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

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

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

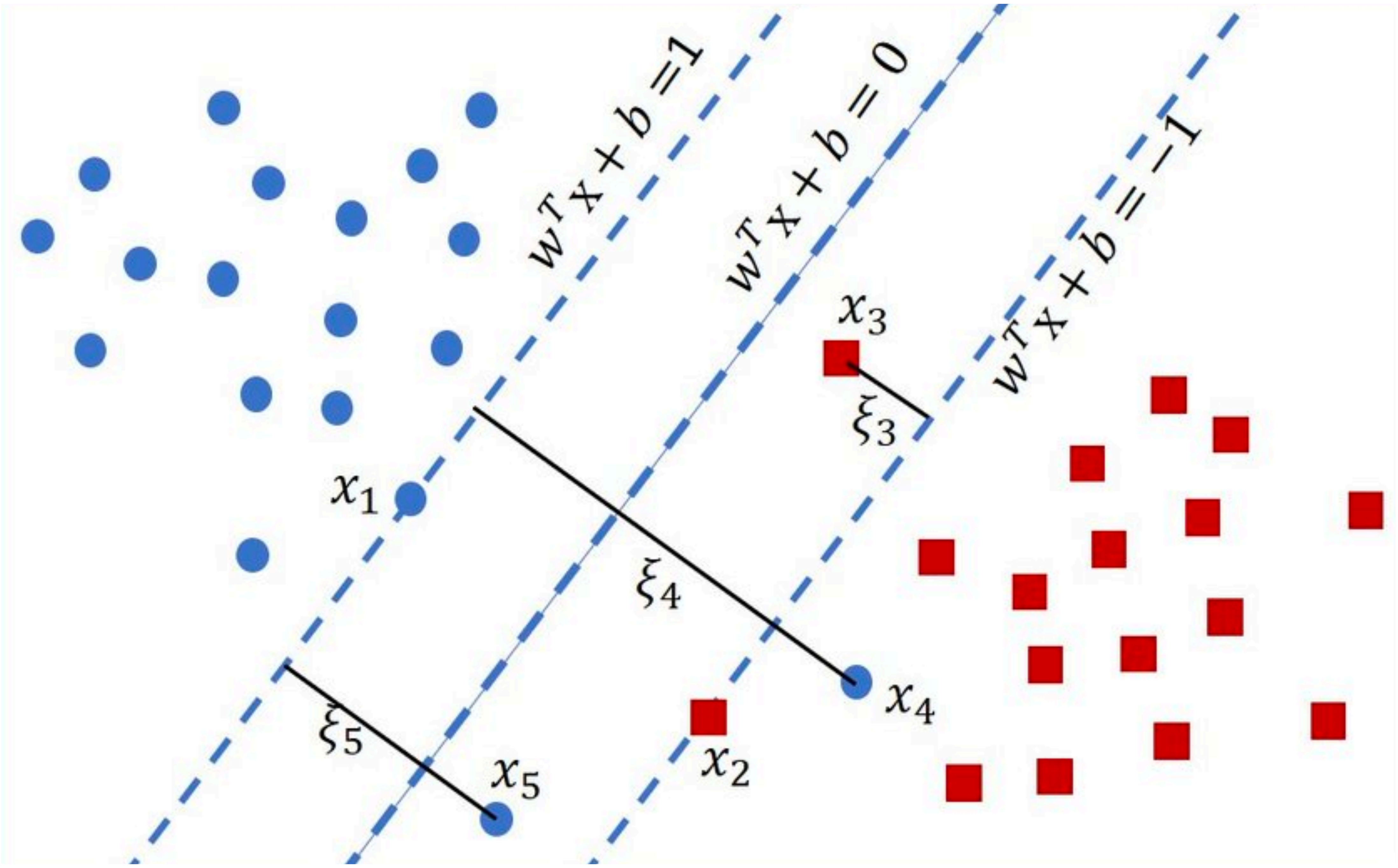


Image credit: Lang Van Tran

# Multiclass SVM

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

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

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

# Multiclass SVM

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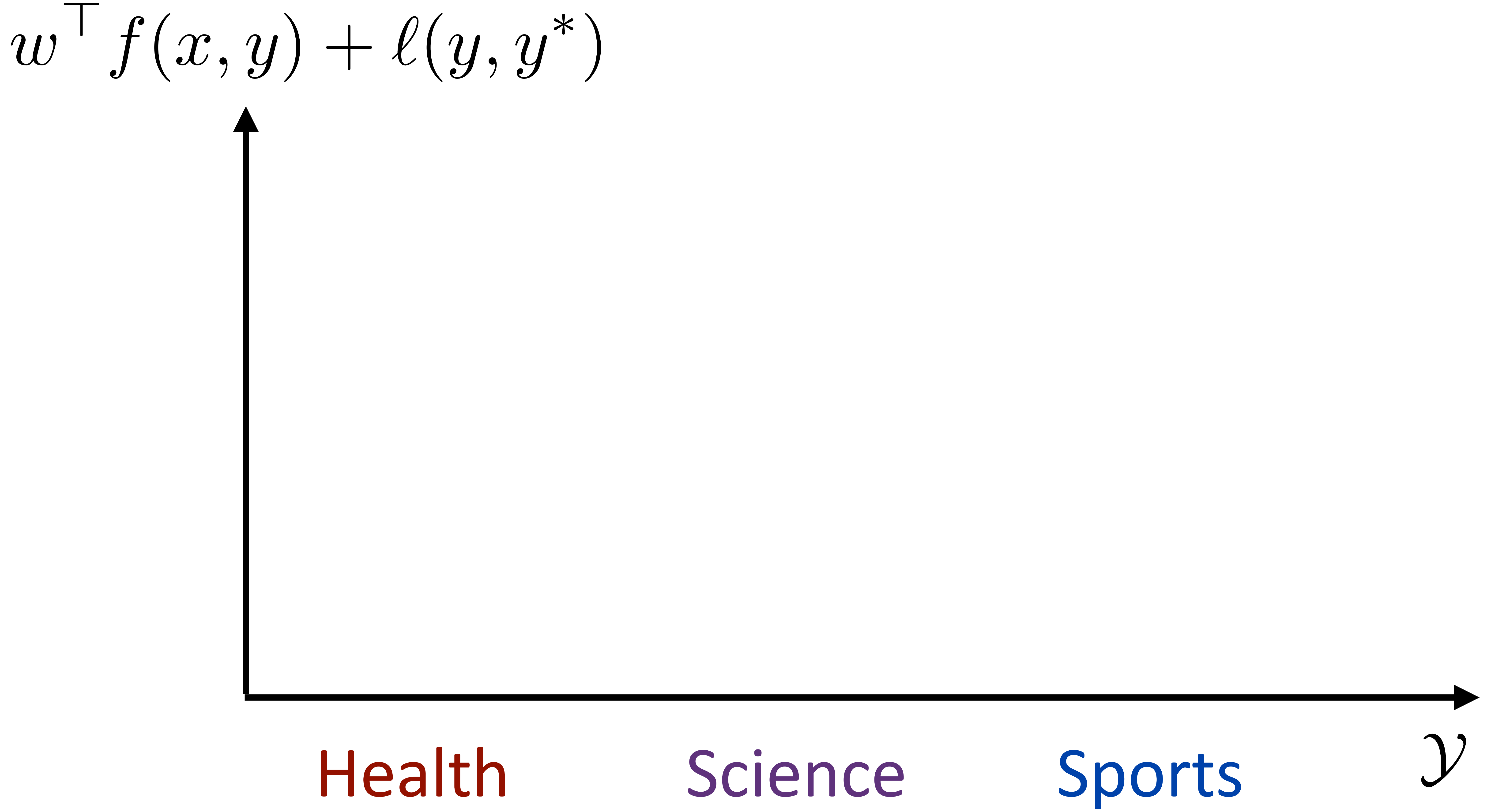

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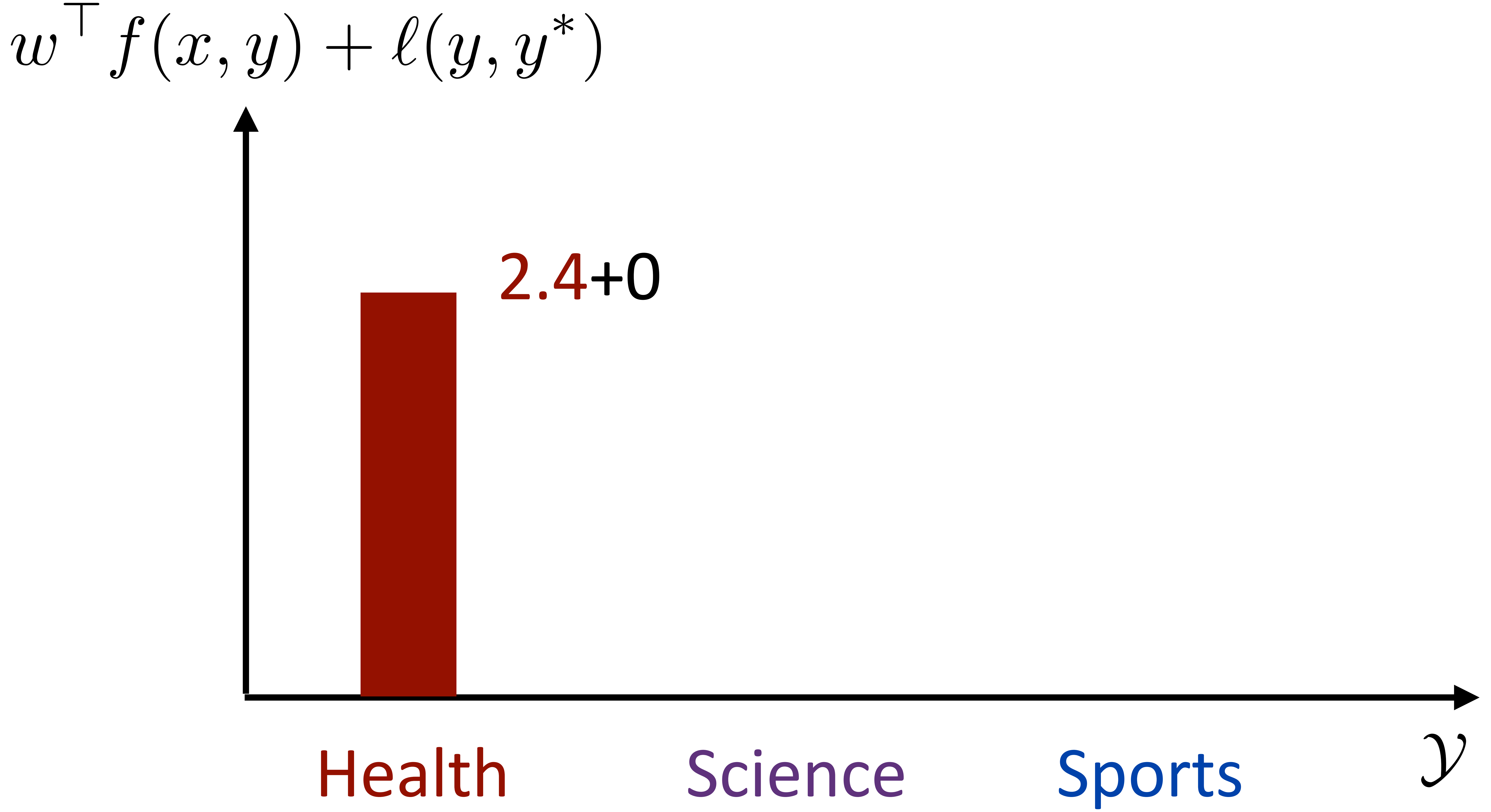

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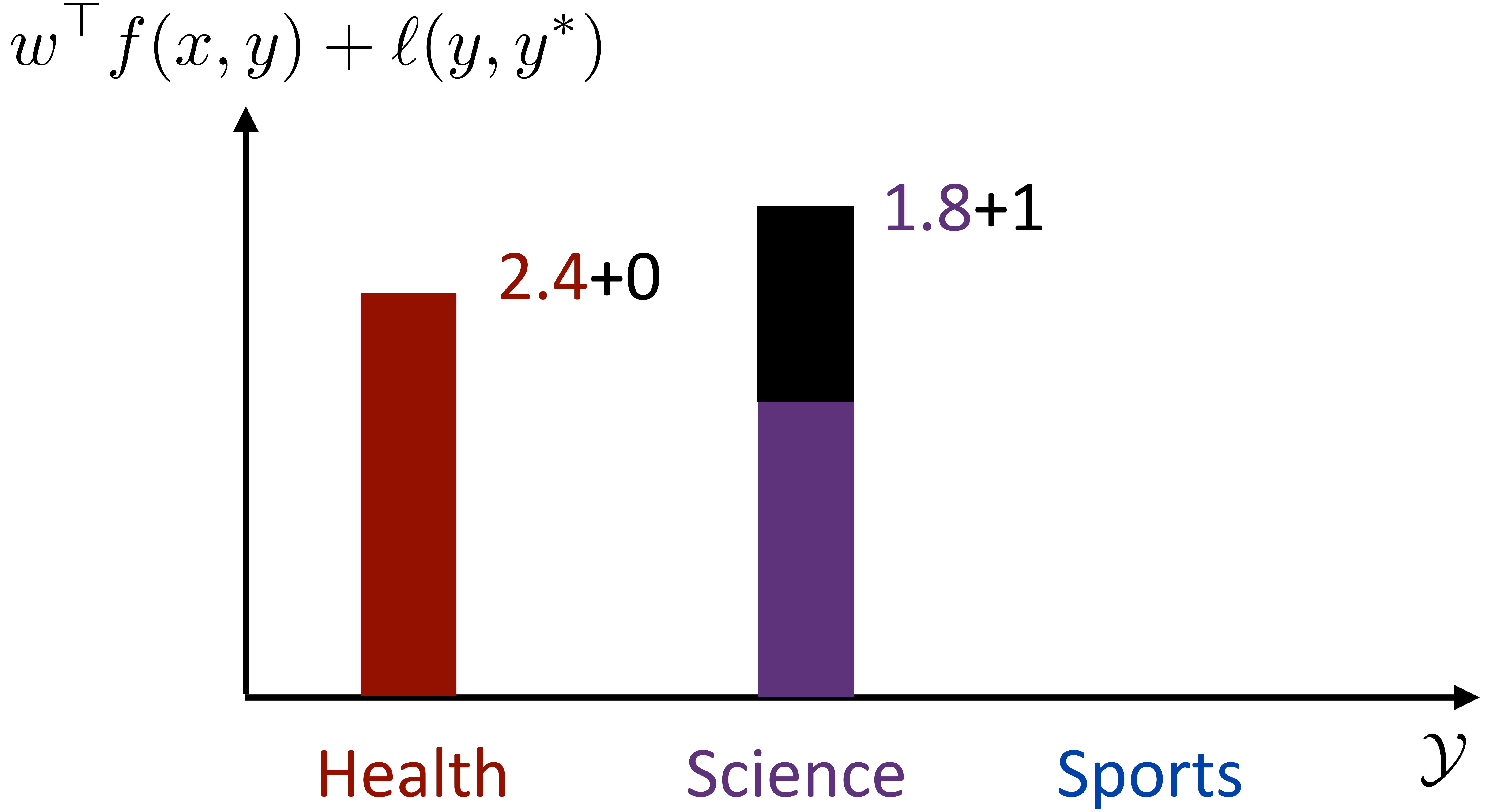

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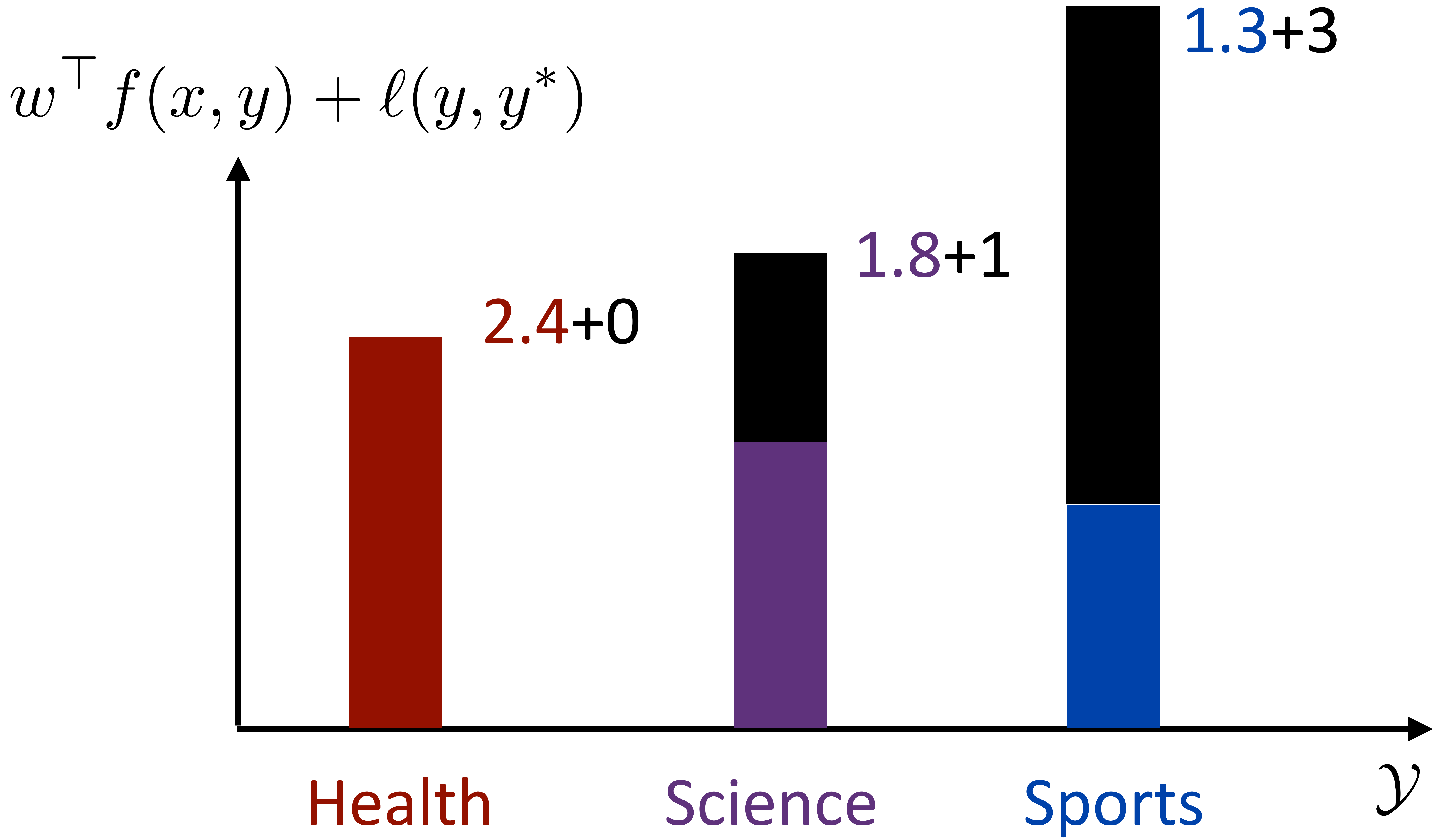

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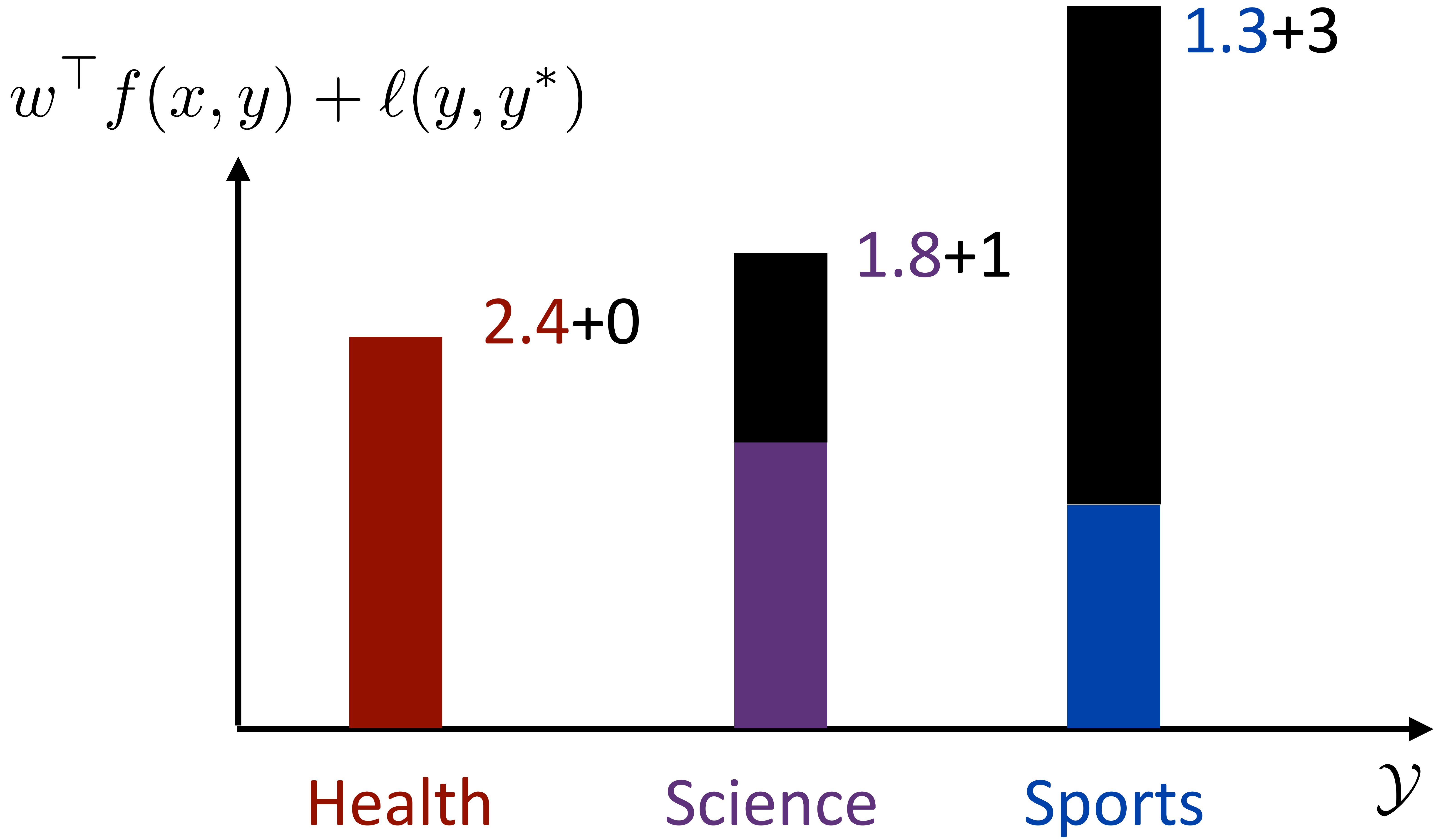


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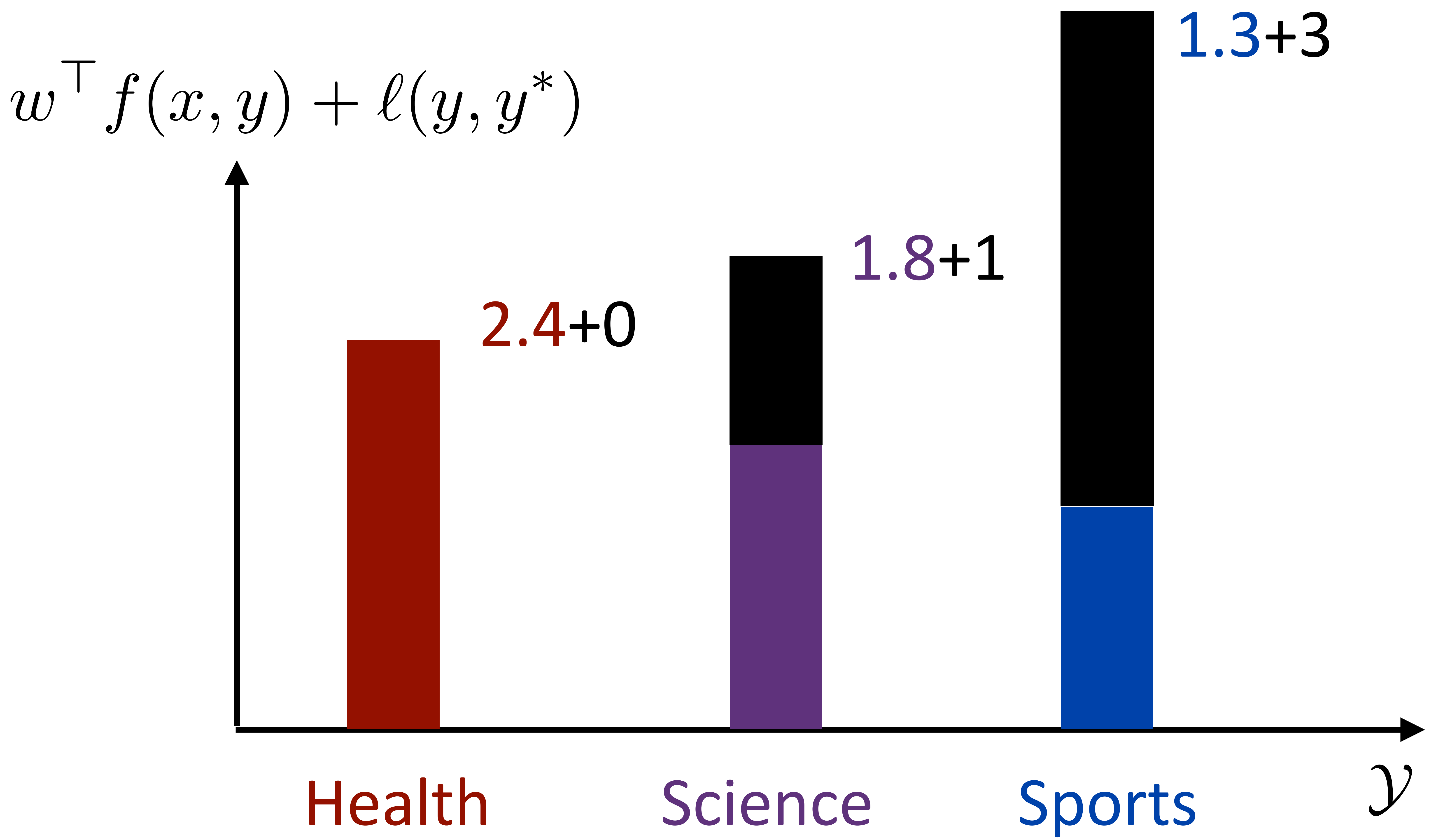


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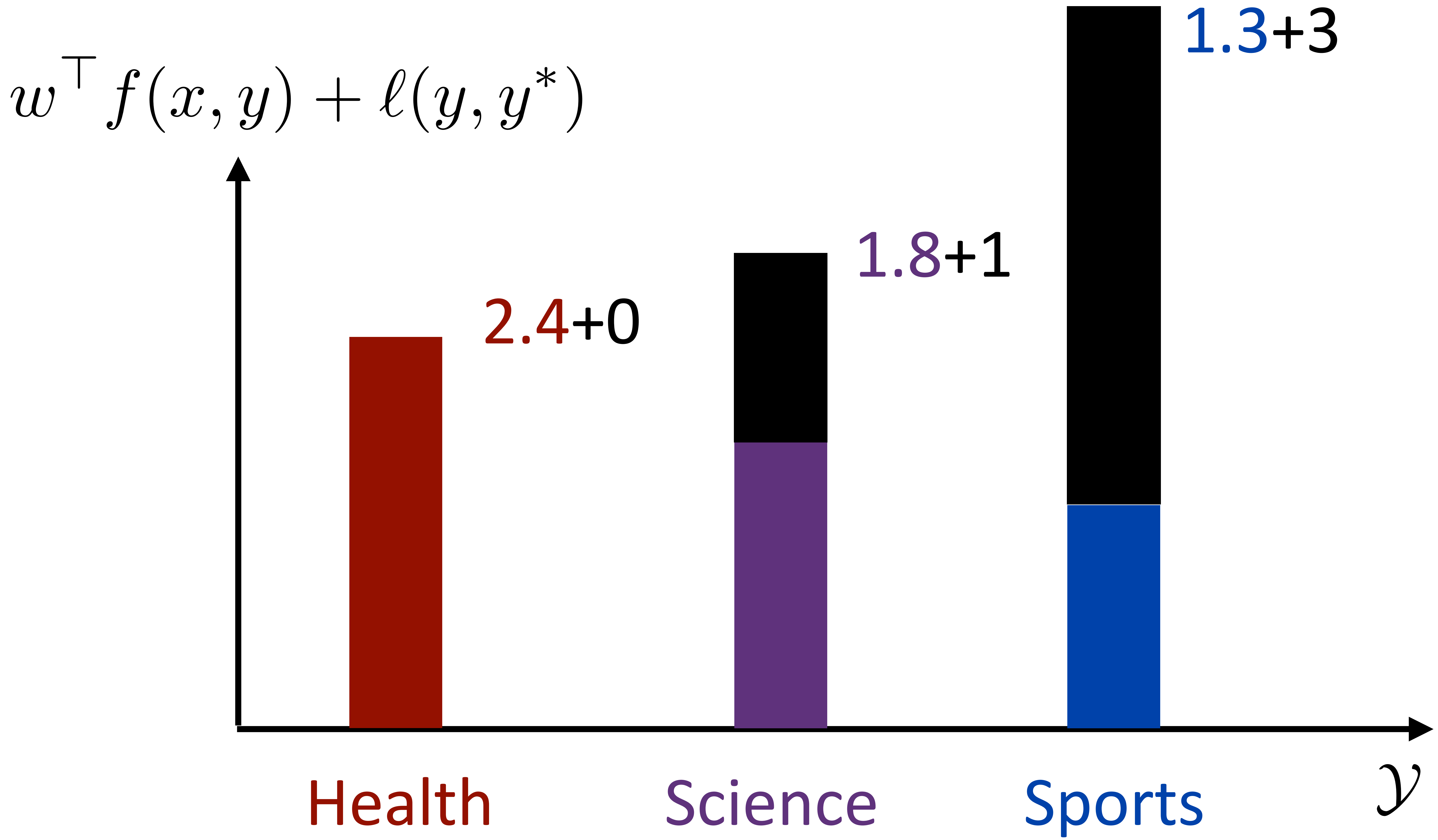


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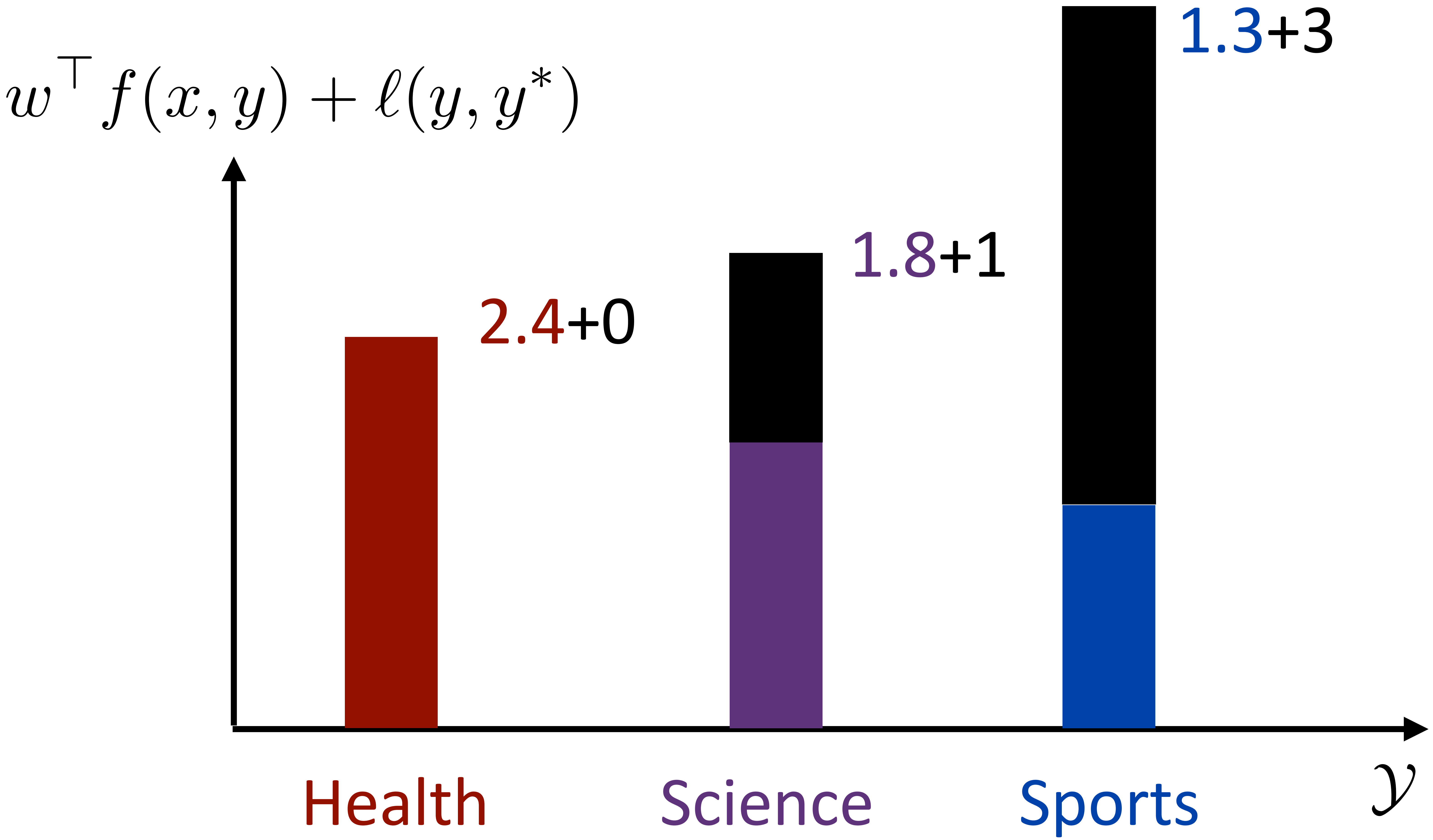


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- Perceptron would make no update here

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

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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

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

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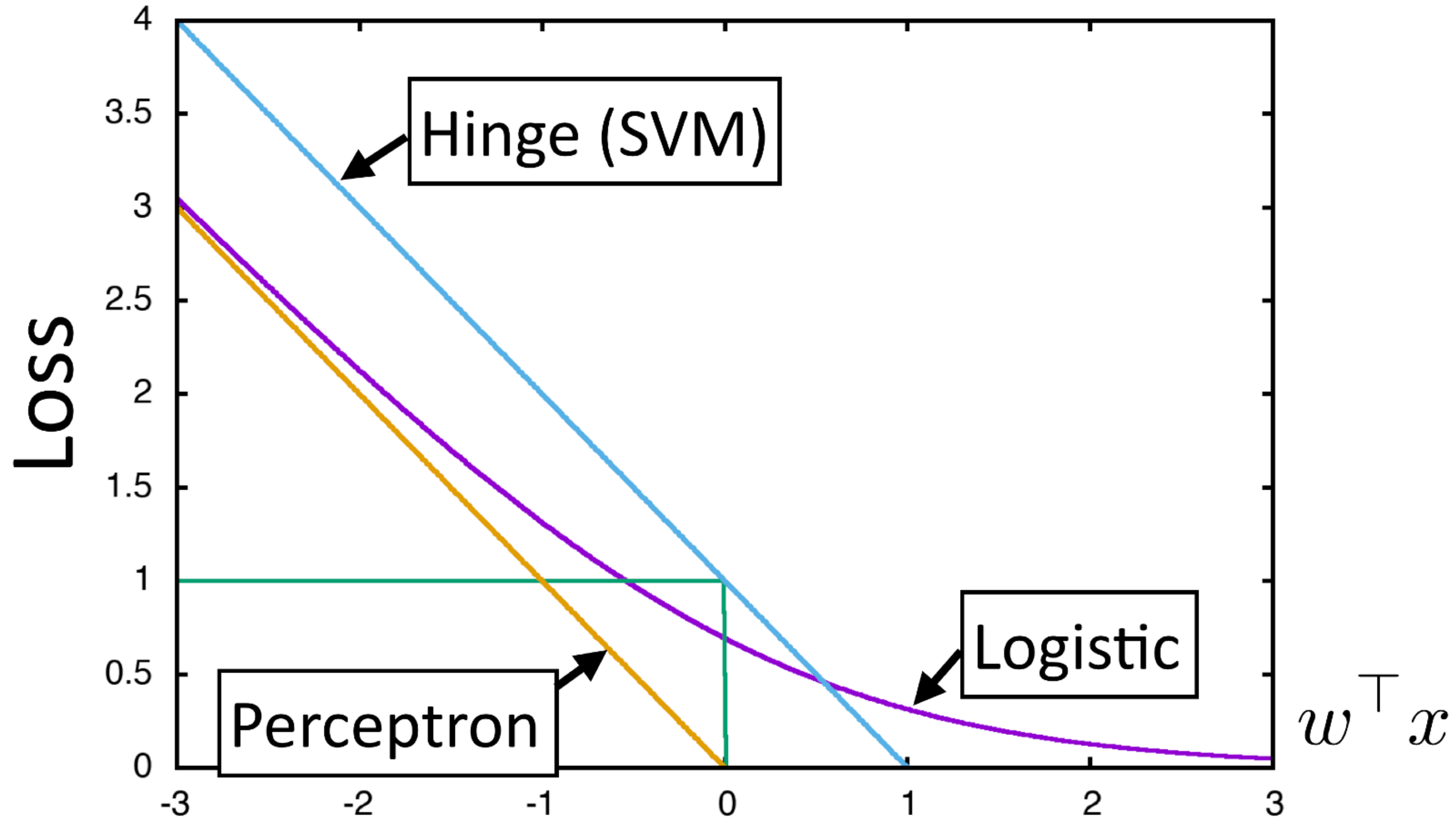

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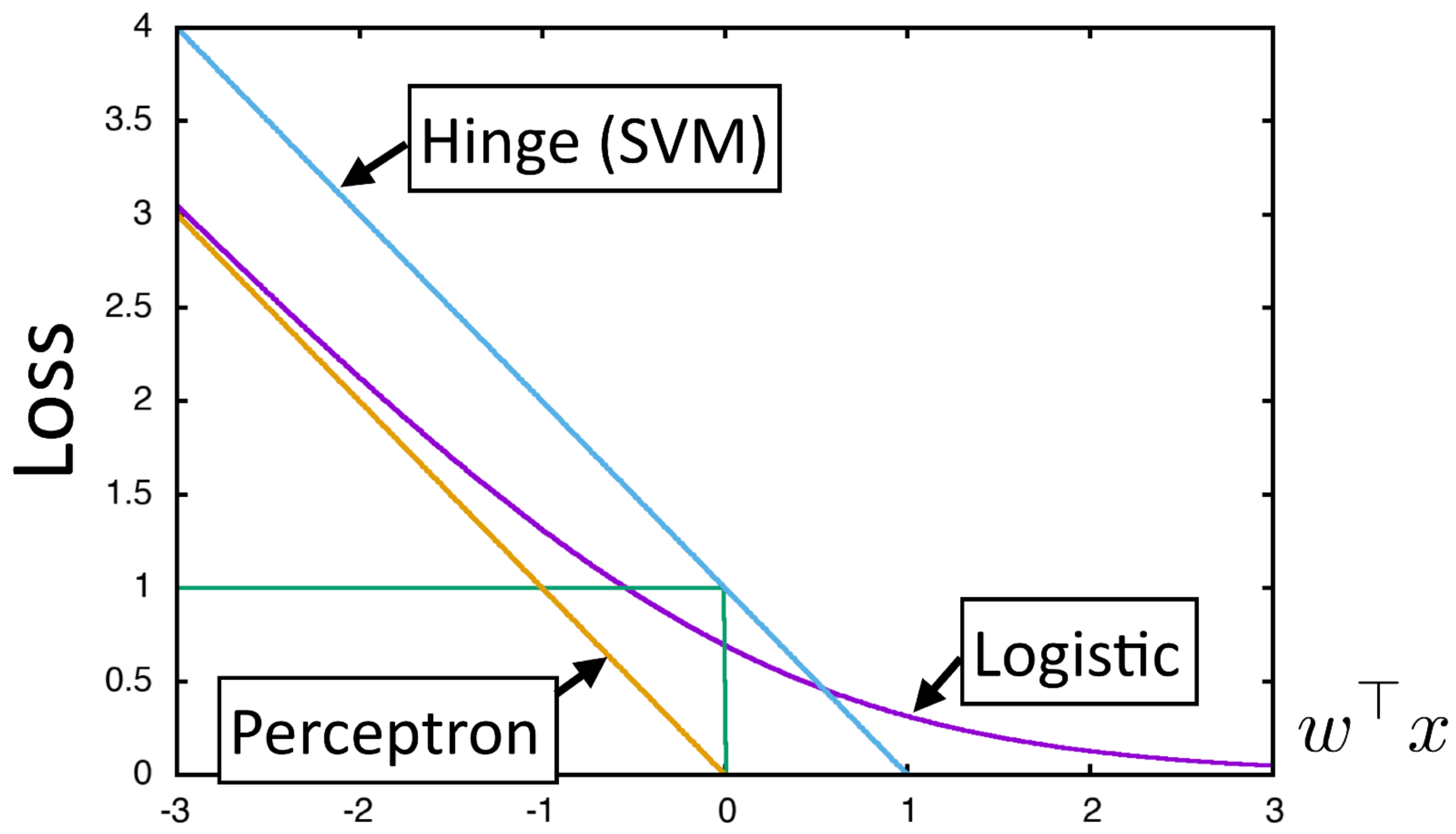


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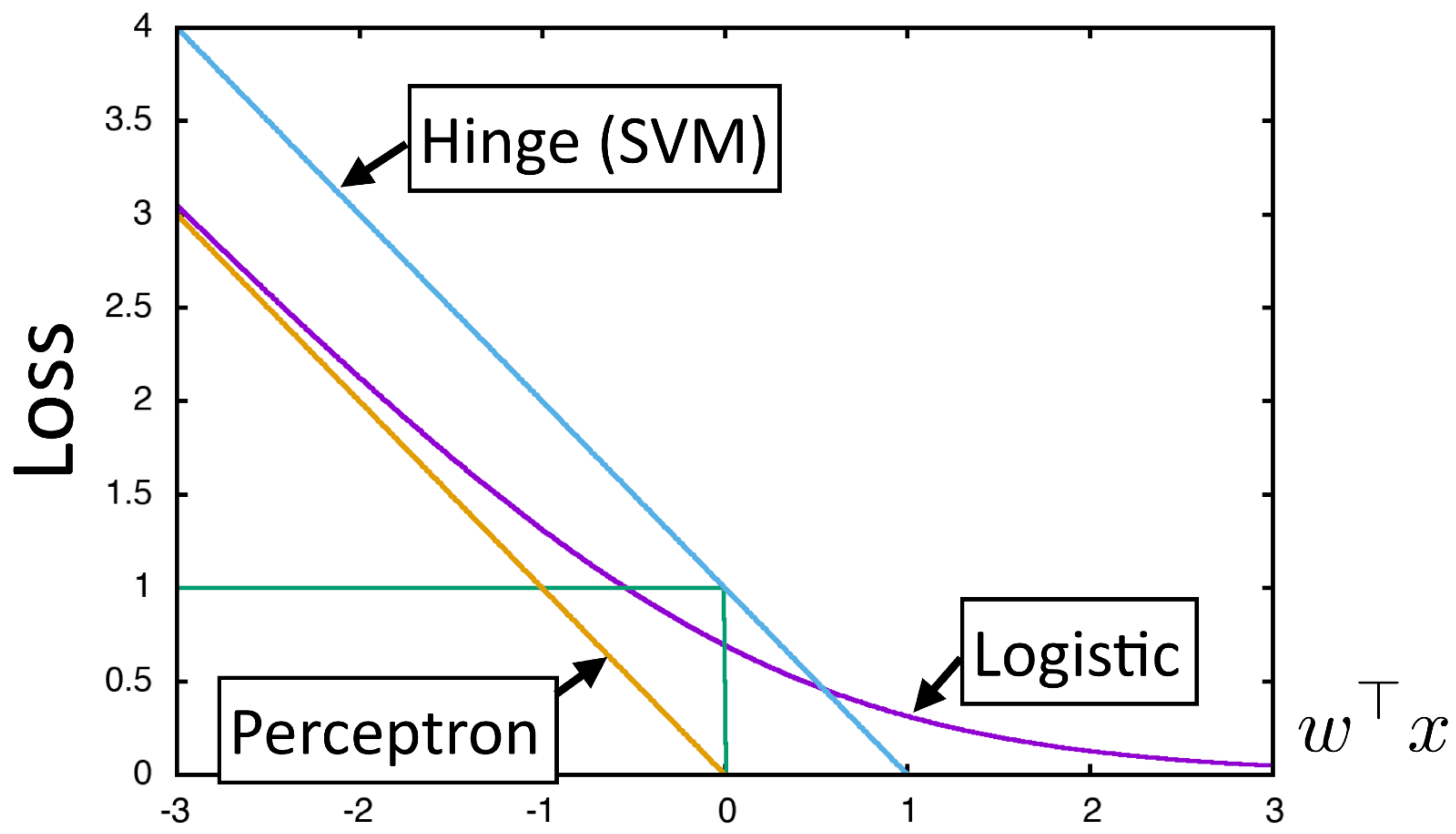


  - Inference: just maxes and simple expectations so far, but will get harder
  - Training: gradient descent?

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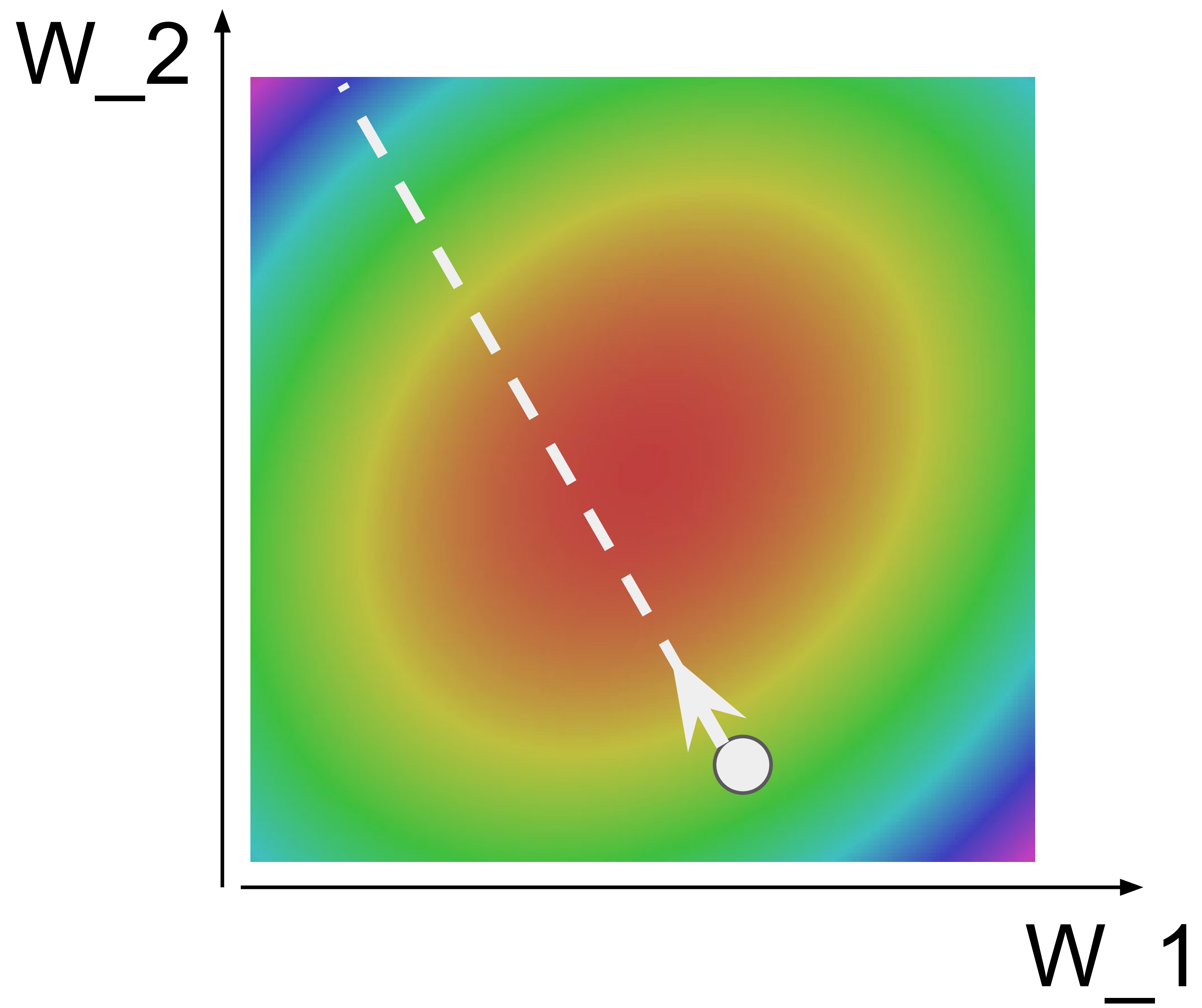
```
# Vanilla Gradient Descent

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



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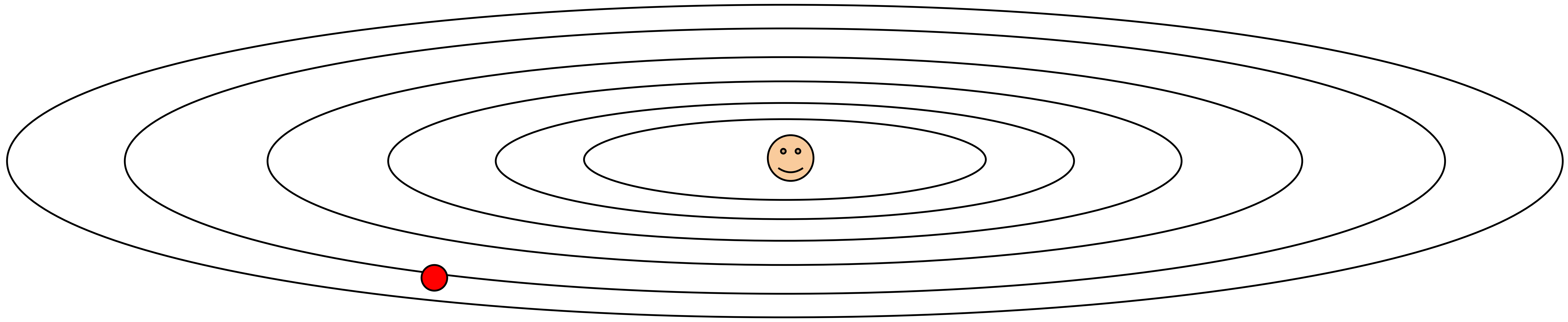

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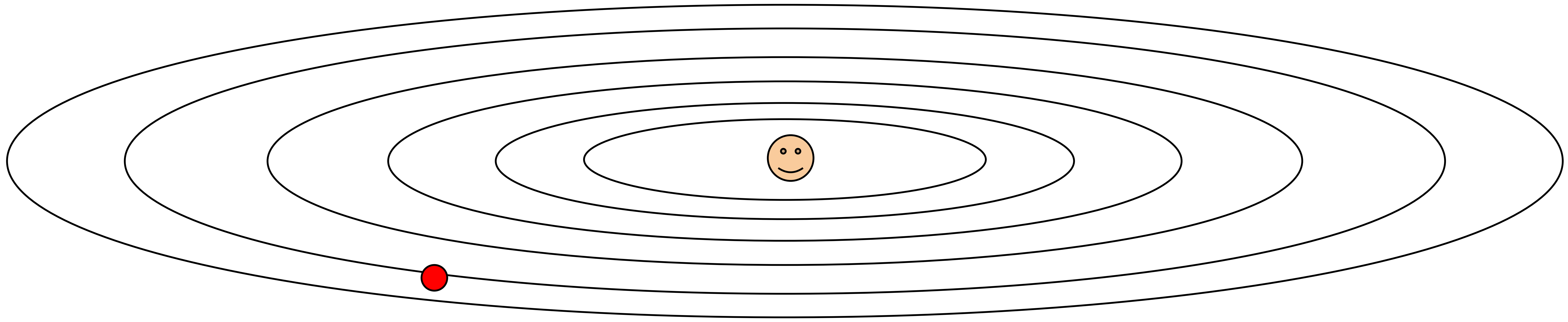

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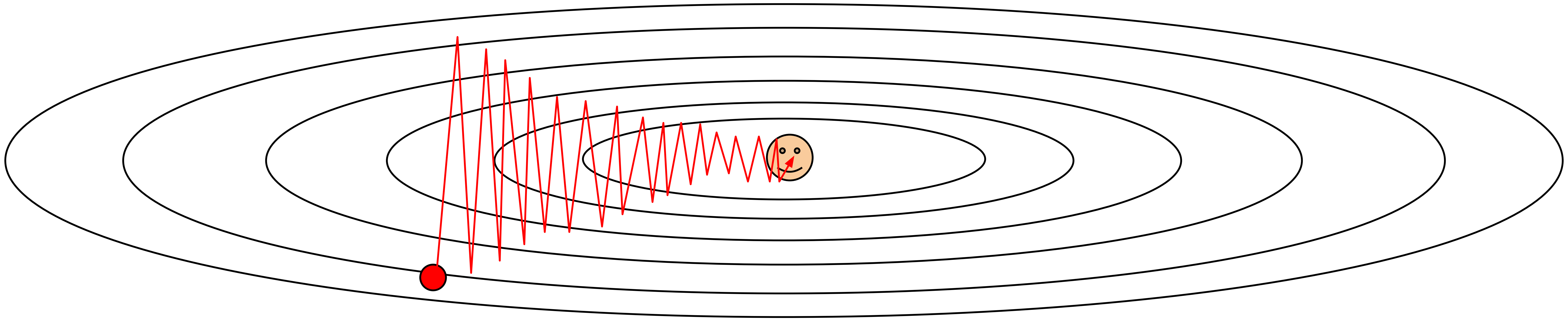

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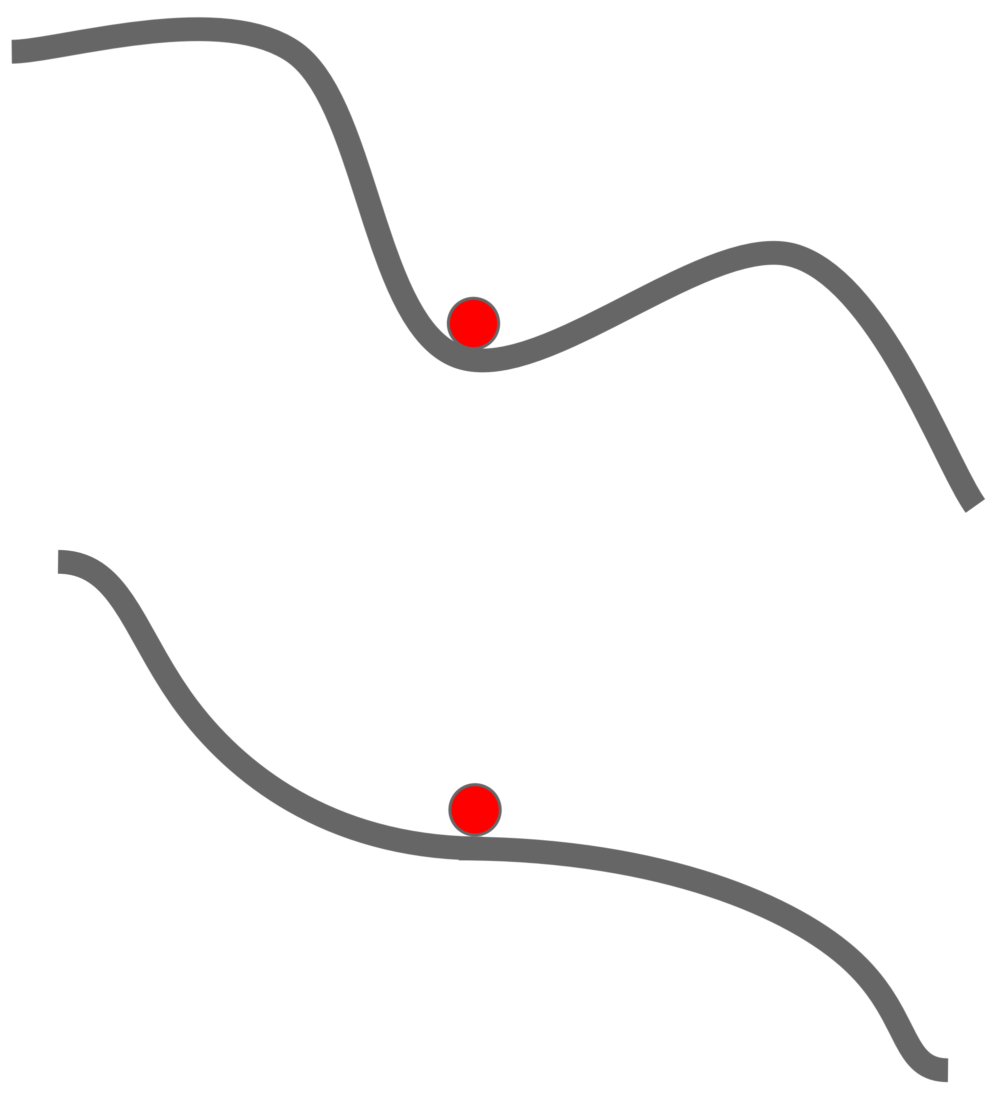

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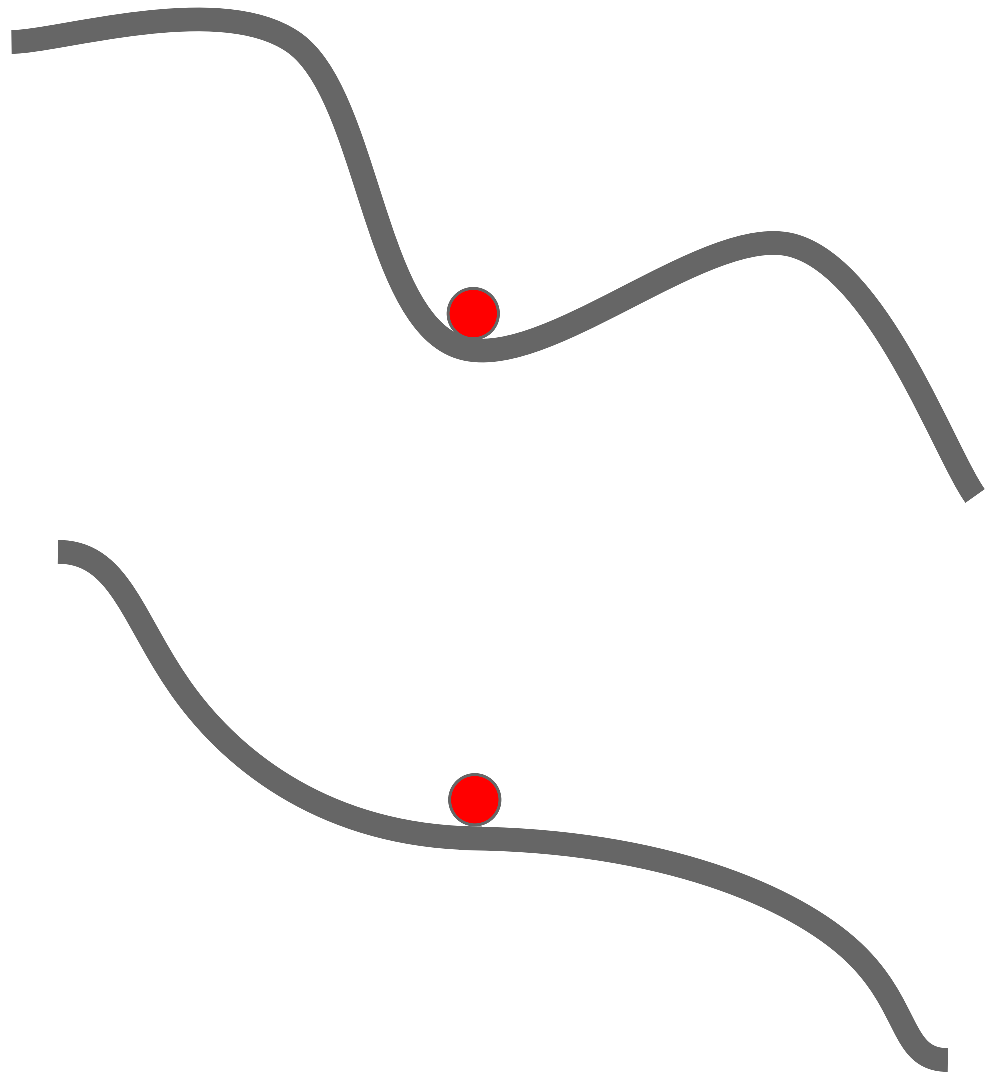

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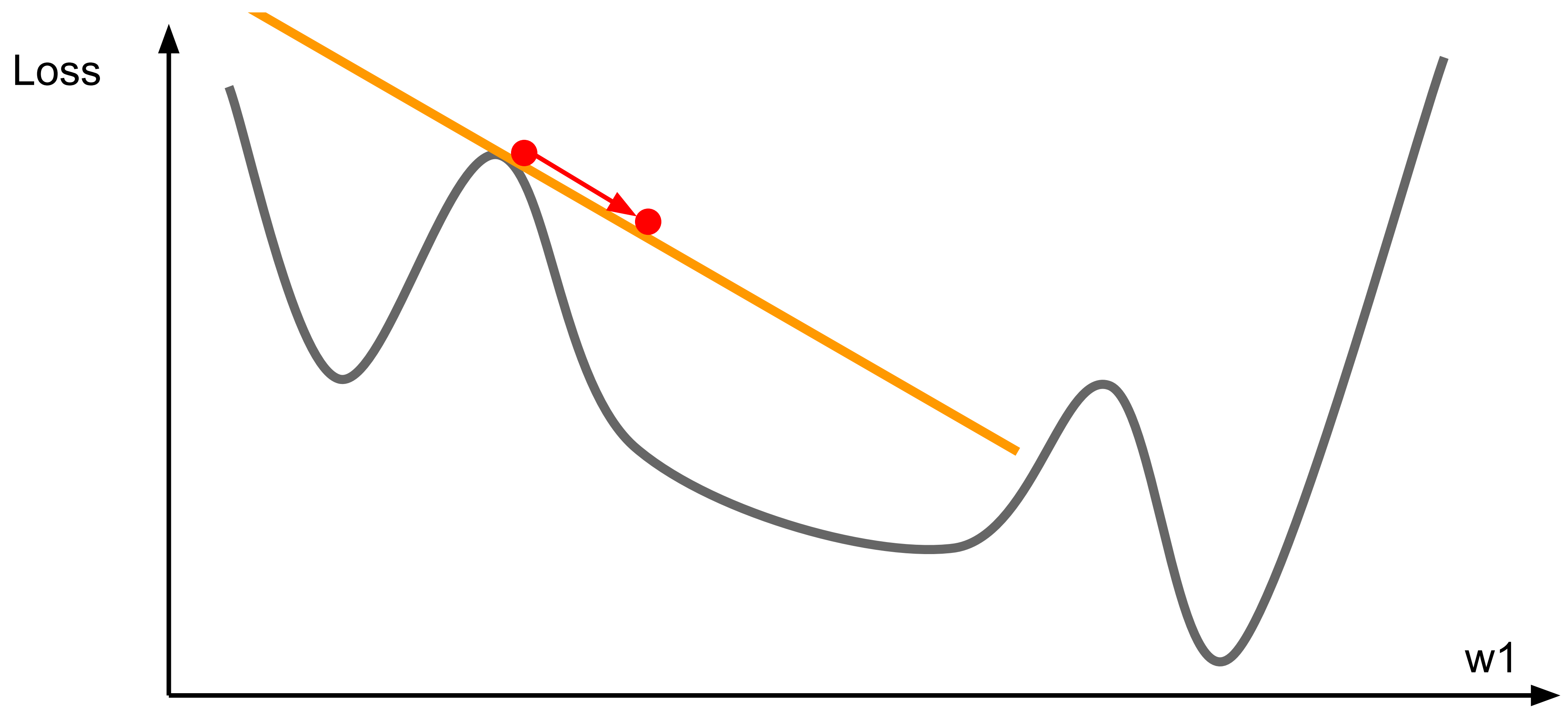


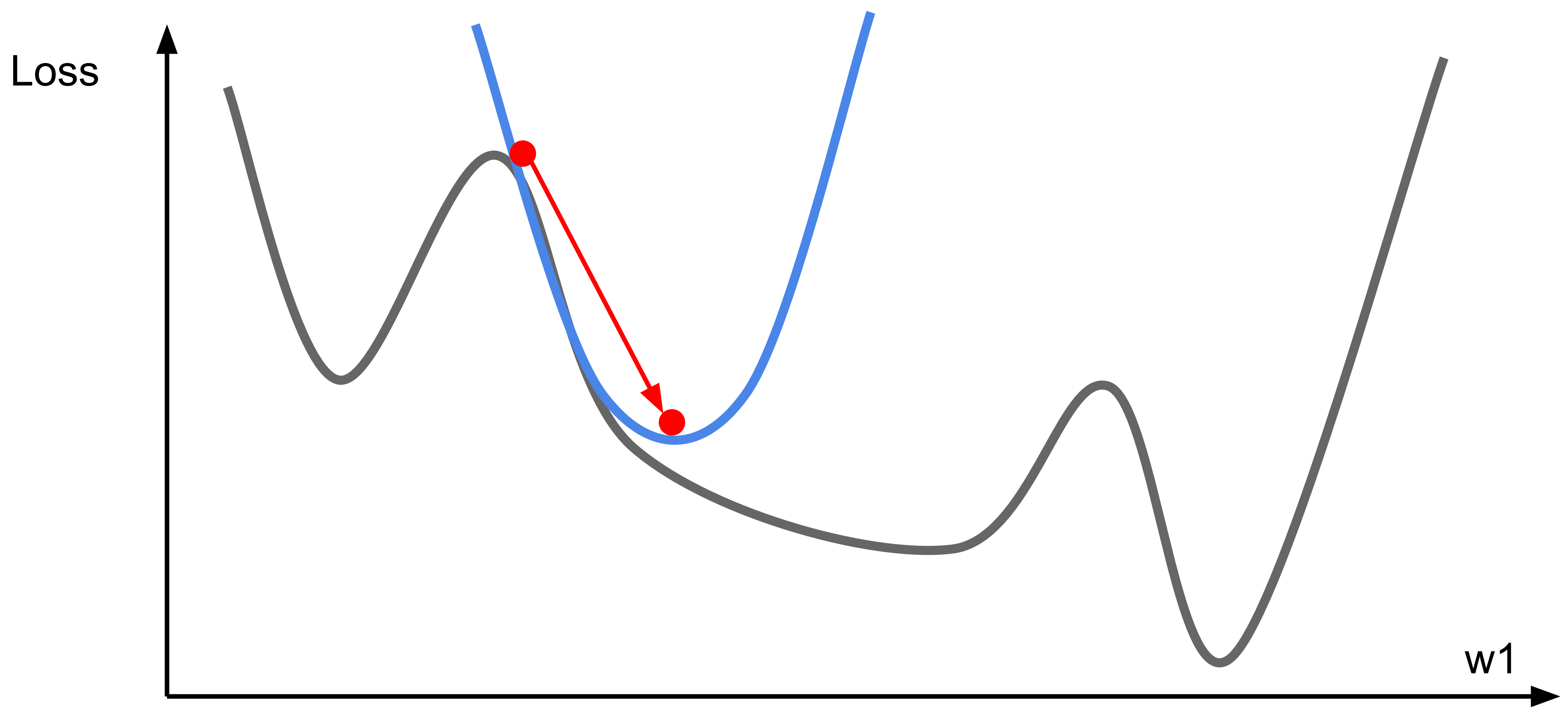

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  - Optimizes quadratic instantly

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# Optimization

- Stochastic gradient *ascent*

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

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

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

  - Second-order technique
  - Optimizes quadratic instantly

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

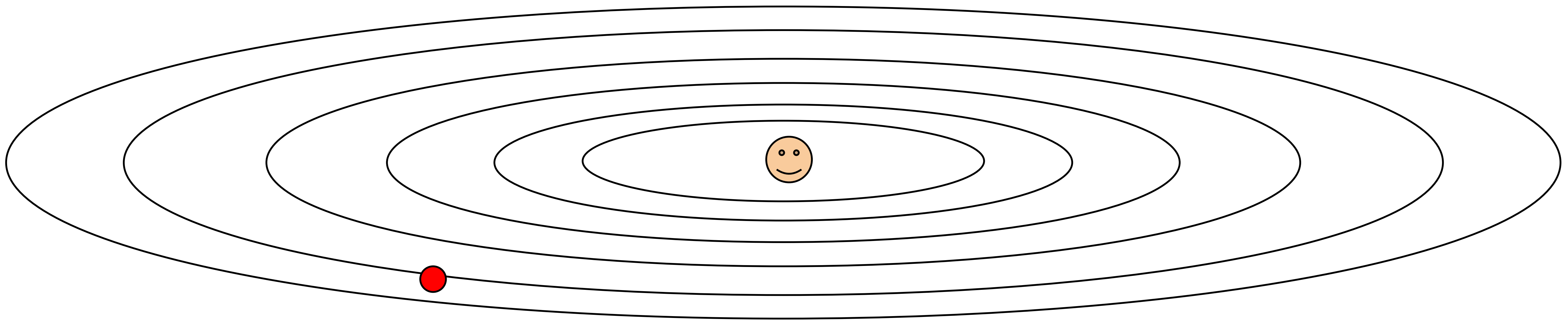
- Quasi-Newton methods: L-BFGS, etc. approximate inverse Hessian

# AdaGrad

- Optimized for problems with sparse features

- Per-parameter learning rate: smaller updates are made to parameters that get updated frequently

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



Duchi et al. (2011)

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

← (smoothed) sum of squared gradients from all updates

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- Other techniques for optimizing deep models — more later!

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