COS234:

Introduction To Machine Learning

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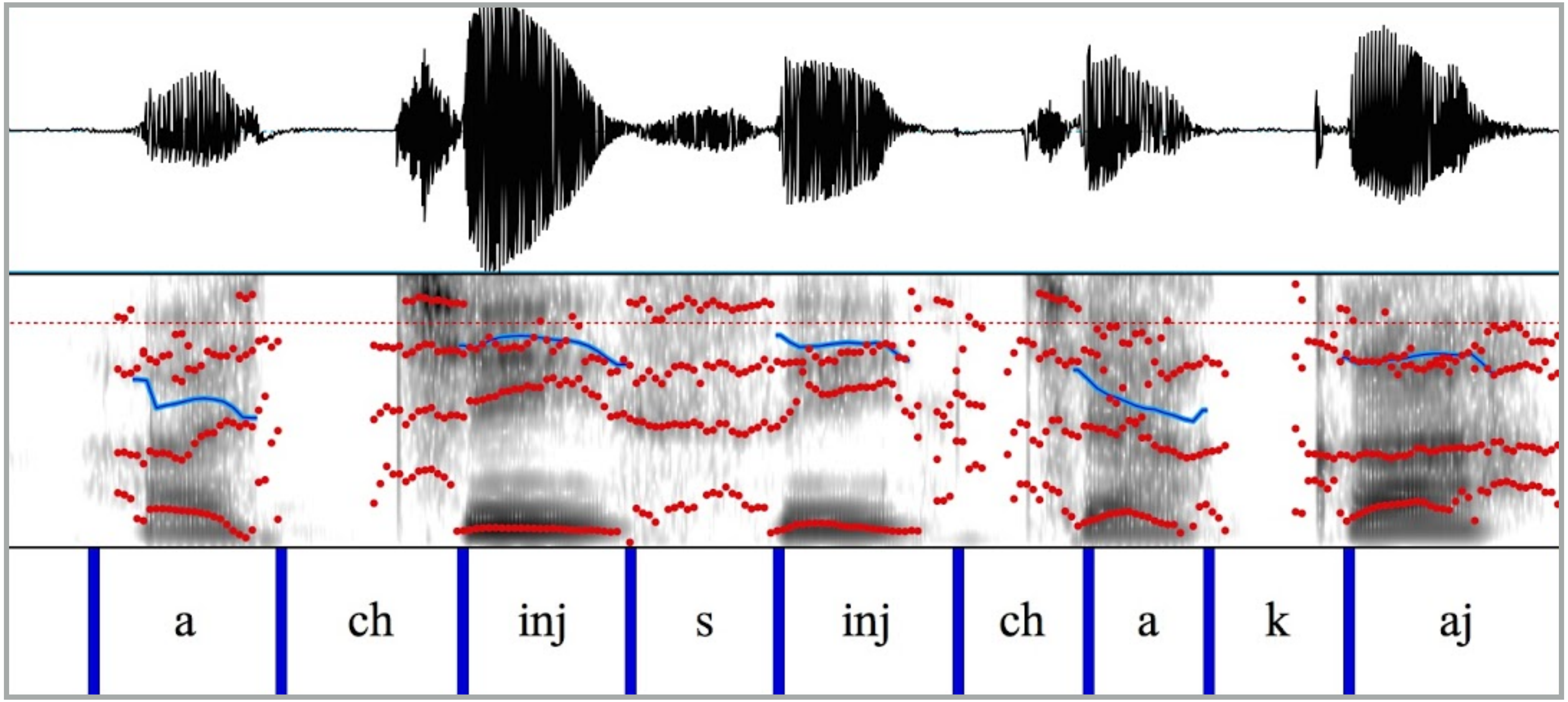
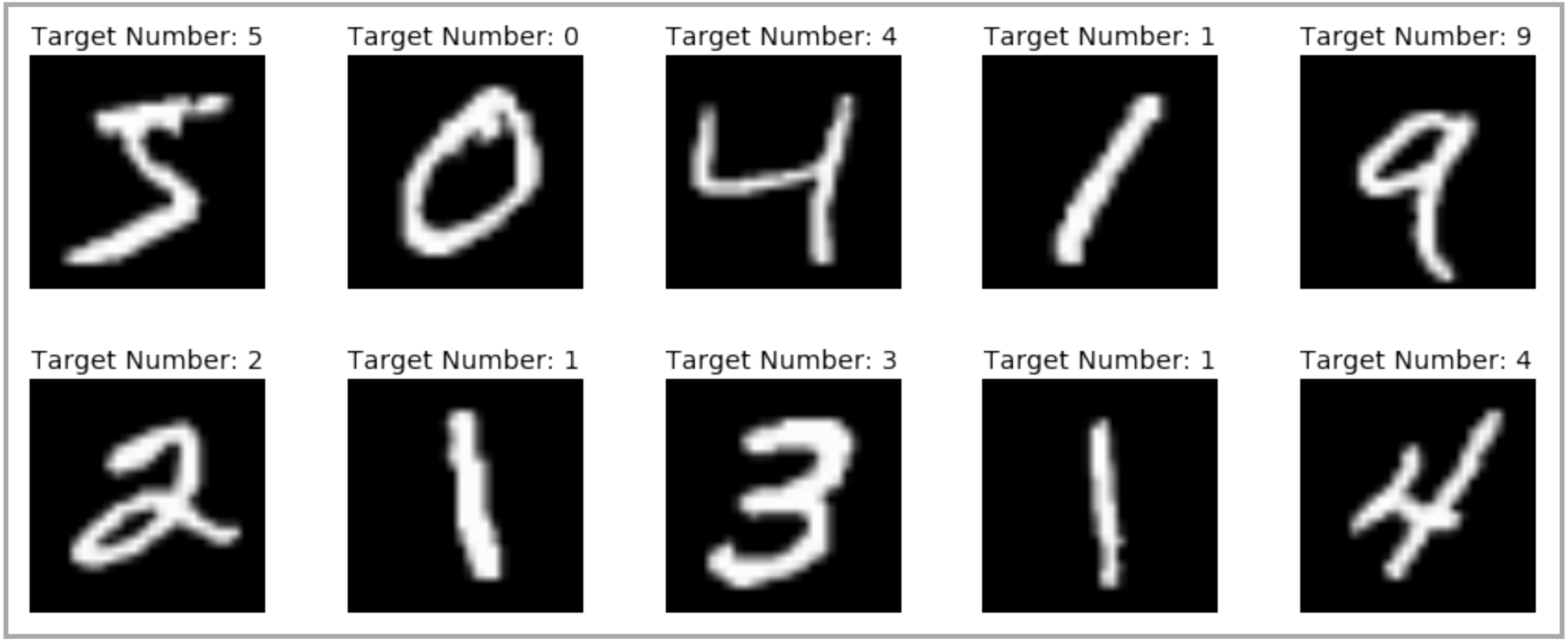
PRINCETON UNIVERSITY

Topic: Multiclass Learning

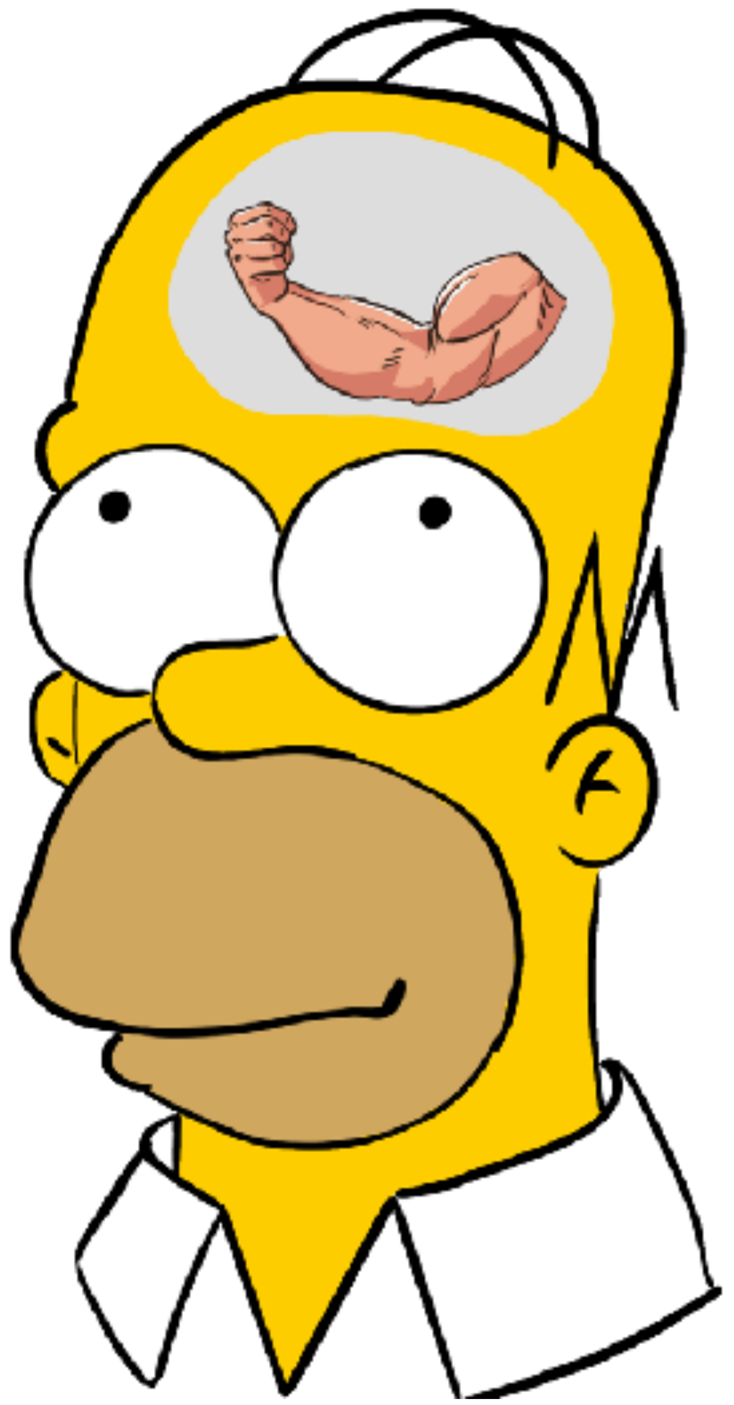
Phoneme Classification



Optical Character Recognition



Multiclass: Problem Setting



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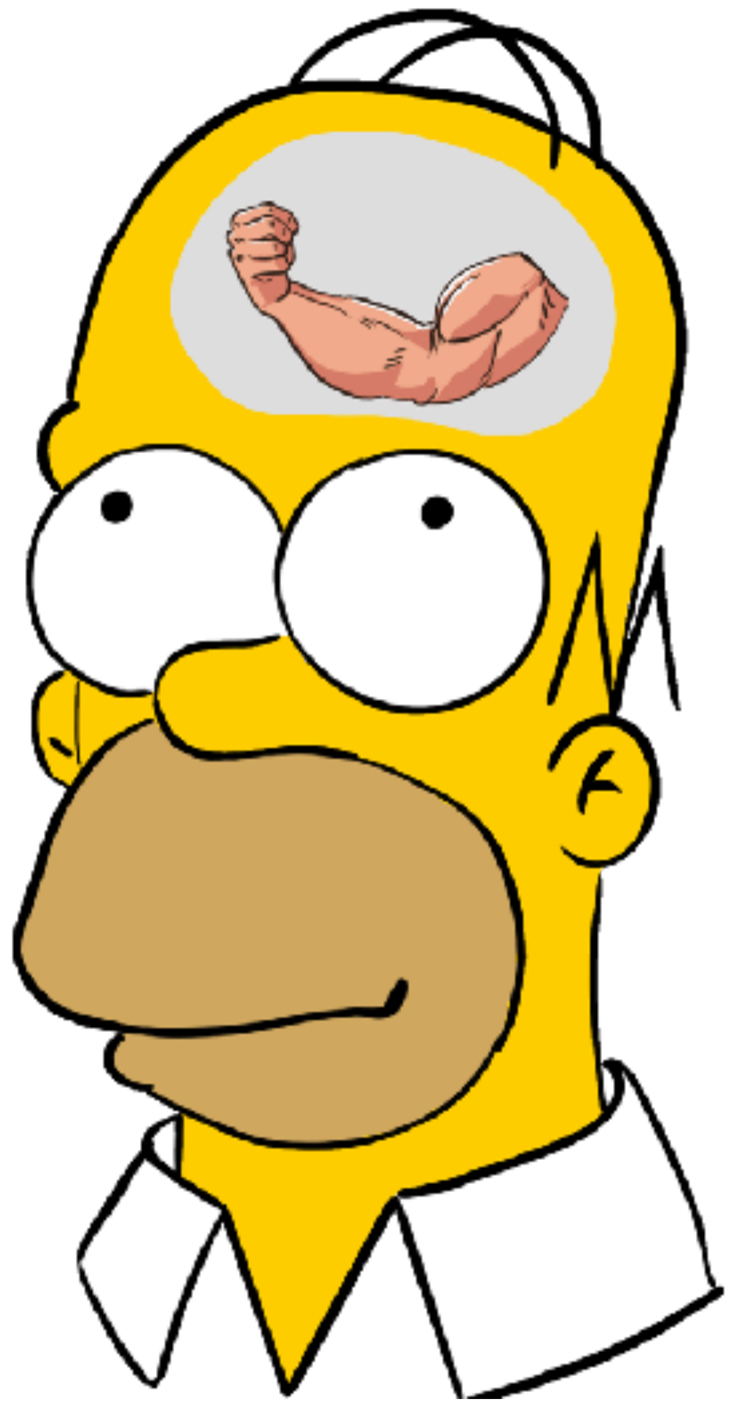
- Instances: $\mathbf{x} \in \mathbf{R}^d$



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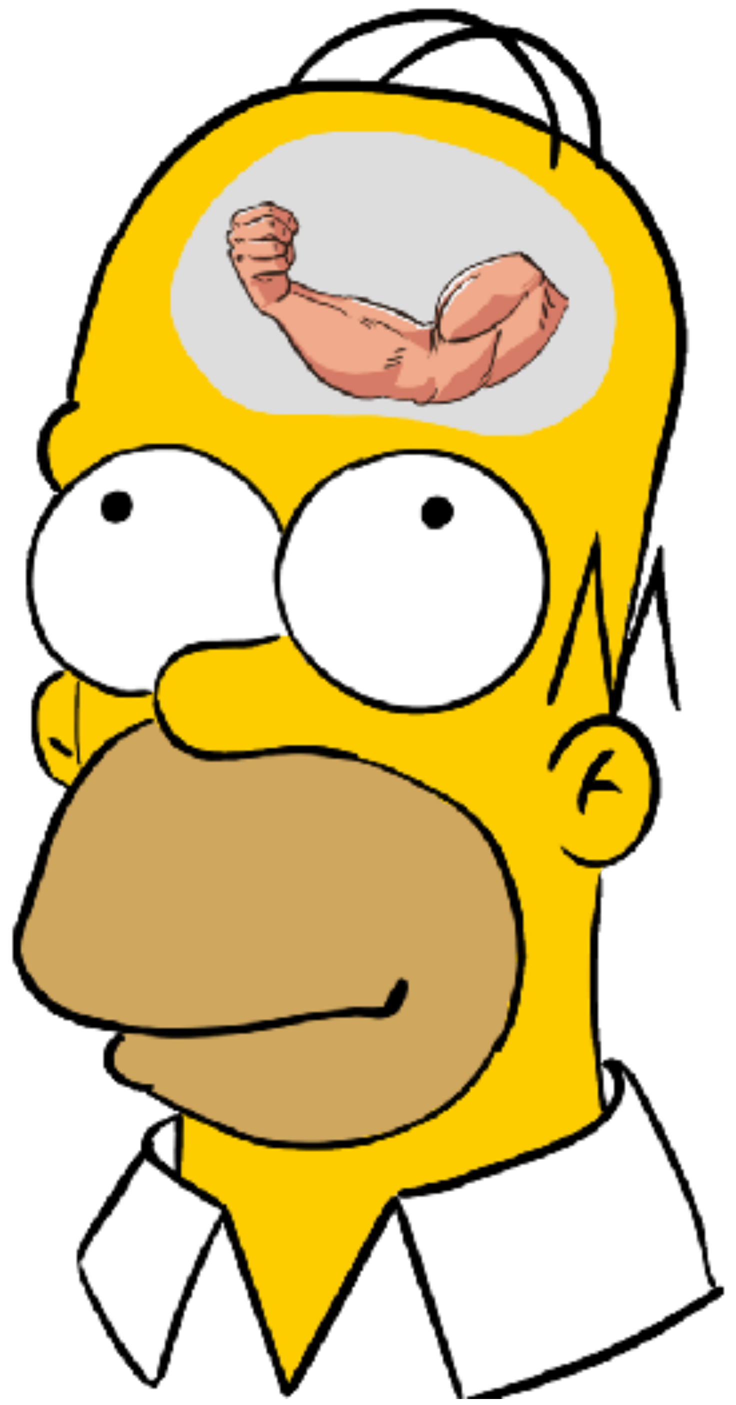

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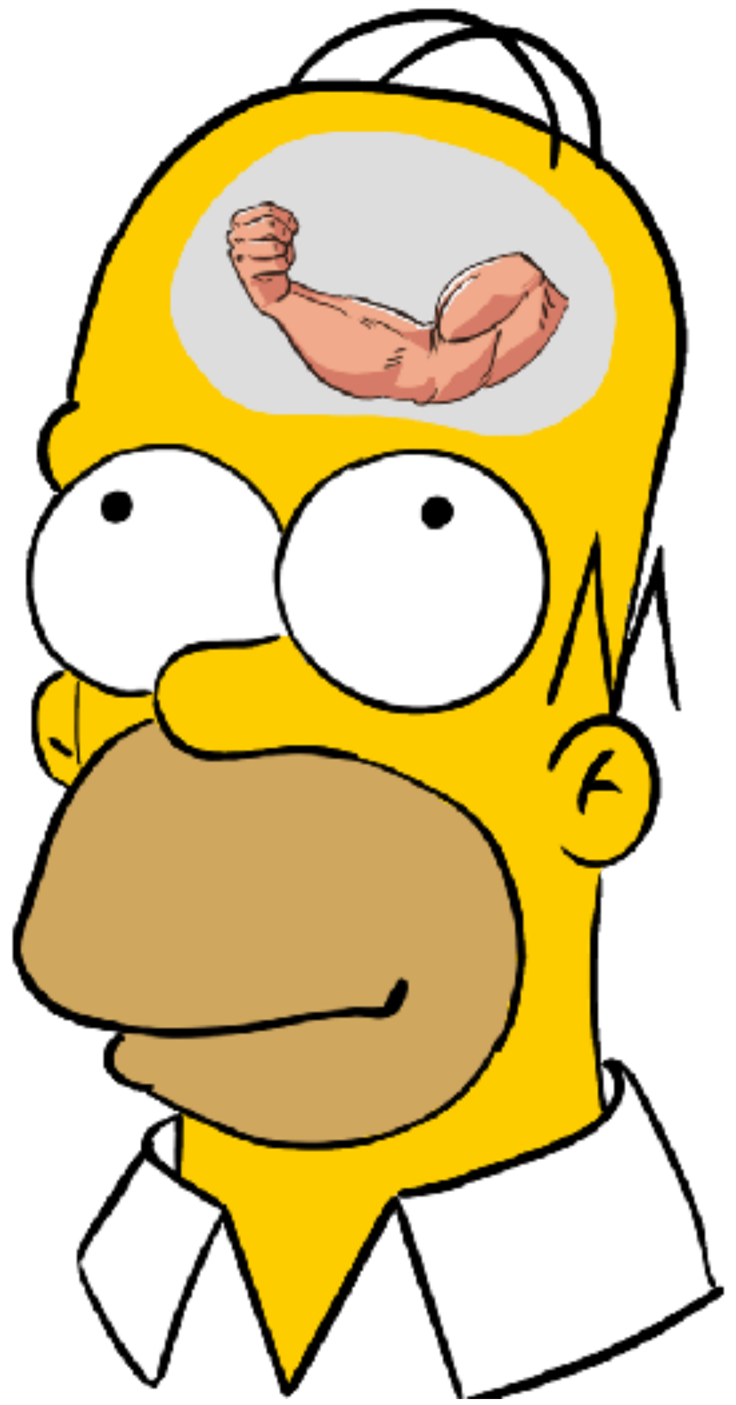

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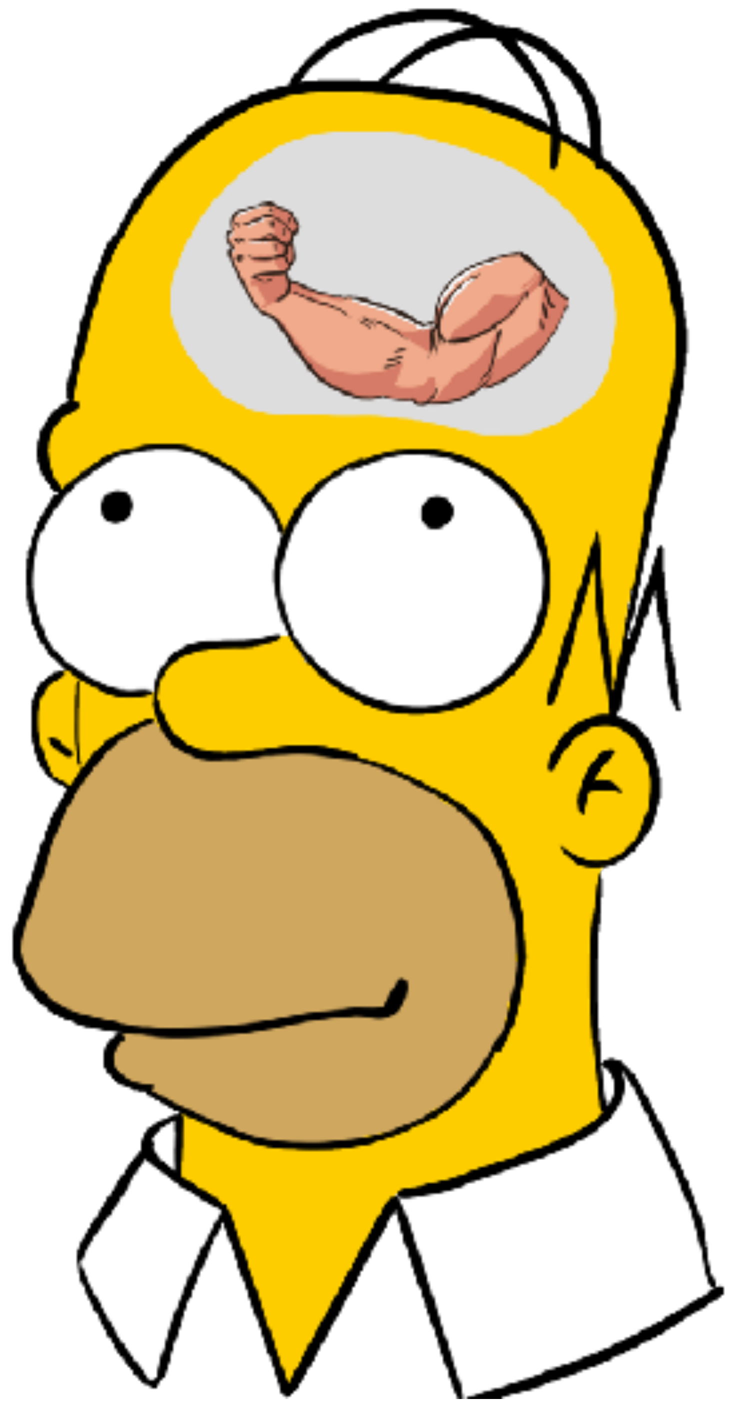

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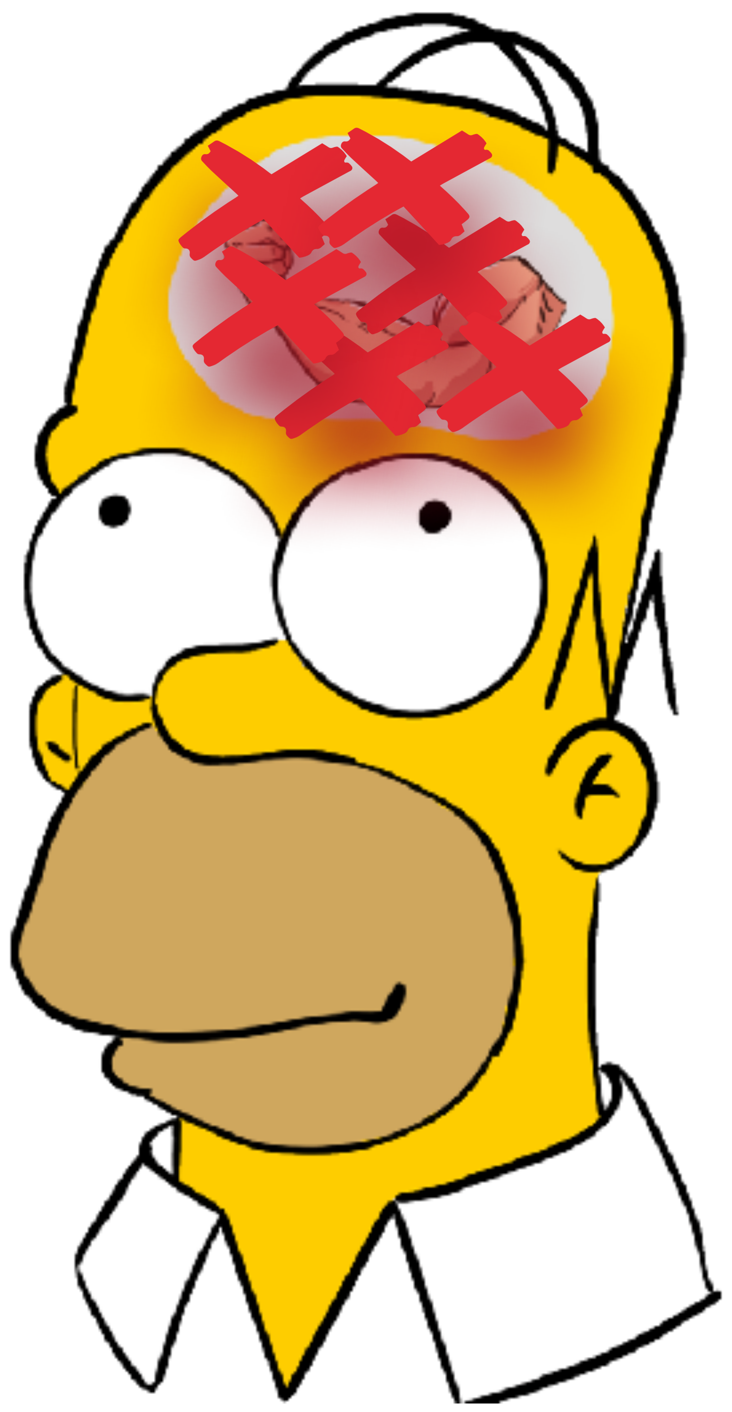

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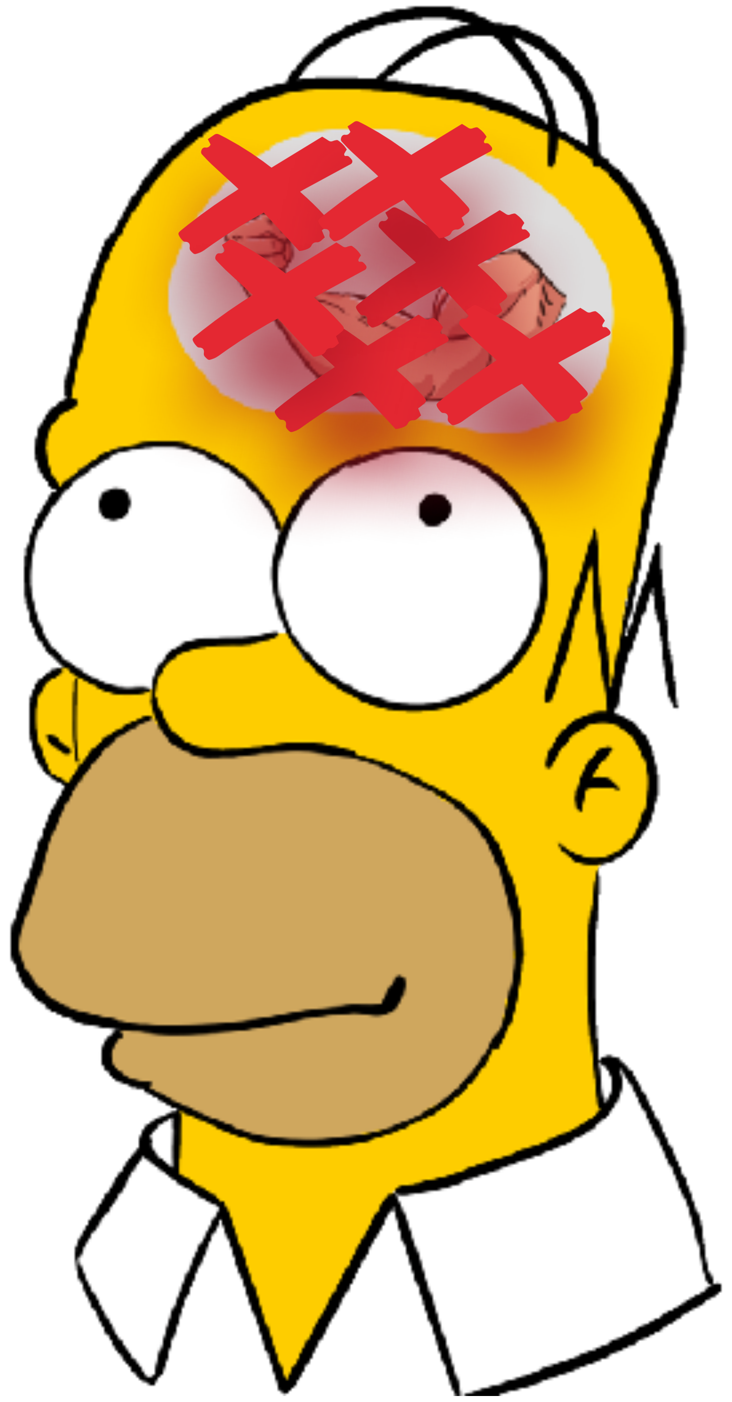
- As in binary case: minimizing prediction mistakes is NP-hard



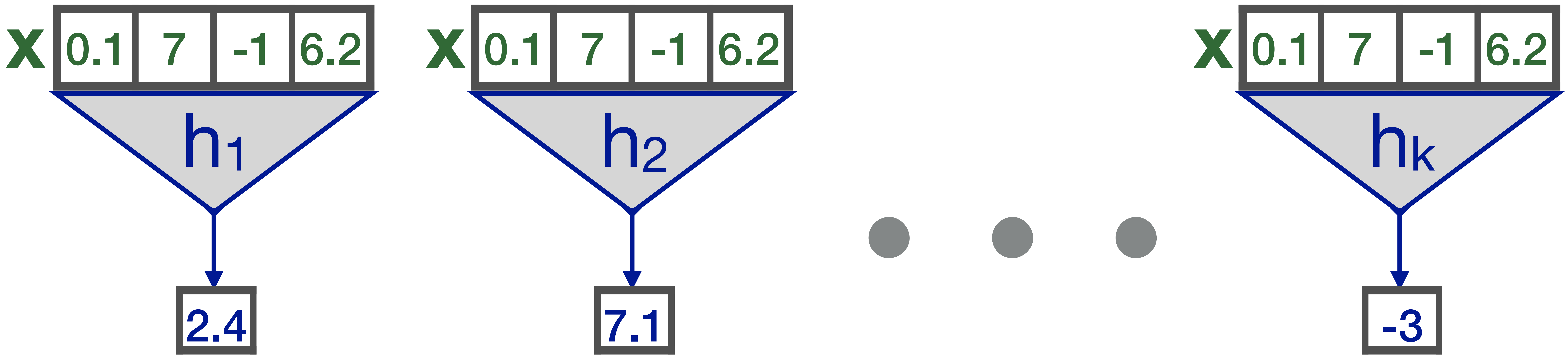
Prediction

I. Predictor h(**x**) can be a general function

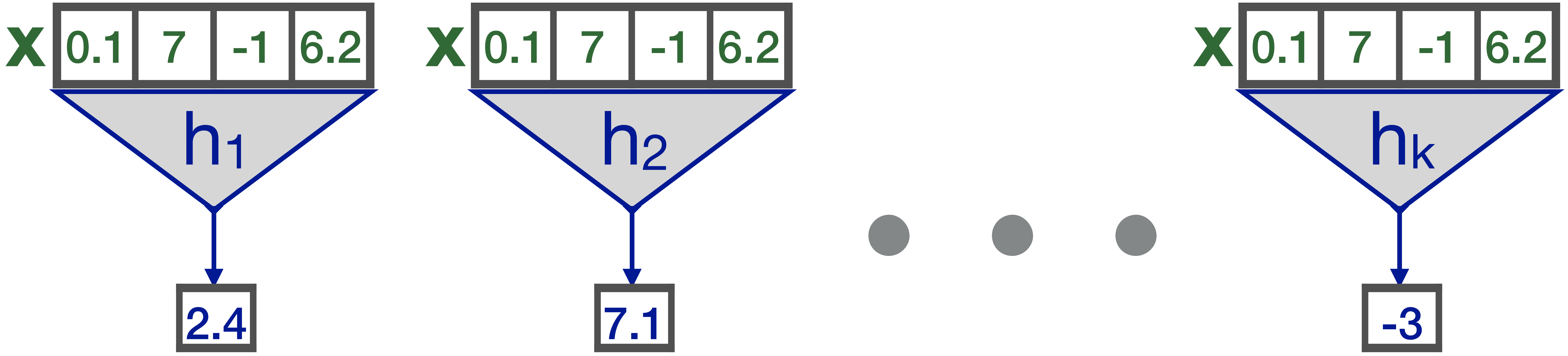
II. Need to express confidence in predicted class

Instead of $\mathbf{h} : \mathbf{R}^d \rightarrow [k]$ use $\mathbf{h} : \mathbf{R}^d \times [k] \rightarrow \mathbf{R}$:

where h(**x**,*c*) confidence that label of **x** is *c*



Winner Takes All



Predicted class: $\hat{y} = \arg\max_j \mathrm{h}_j(\mathbf{x})$

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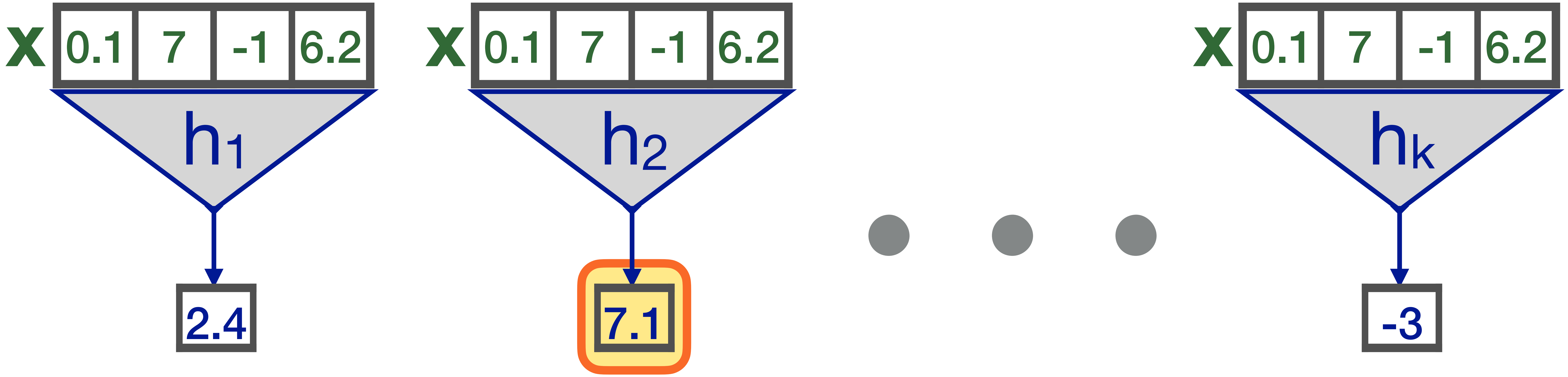

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Linear Multiclass Predictors

Linear predictor for class j : $h_j(\mathbf{x})$ is $\mathbf{w}_j \cdot \mathbf{x}$

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Construct matrix W of size k × d whose j'th row is $\mathbf{w}_j$

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Predicted scores: $\mathbf{z} = W\mathbf{x}$

$$\mathbf{z} = \begin{bmatrix} W_{11} & \cdots & W_{1d} \\ \vdots & \cdots & \vdots \\ W_{k1} & \cdots & W_{kd} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

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Predicted label: $\hat{y} = \arg\max_{j=1}^{k} z_j$

One vs. Rest (One vs. All)

- Learn **k** binary linear predictors
- **j**'th predictor distinguishes **j**'th class from the rest
- Learning scheme:

I. Transform $S \mapsto S_1, S_2, \ldots, S_k$ where $S_j = \left\{ \left(\mathbf{x}_i, (-1)^{\mathbf{1}[y_i \neq j]} \right) \right\}_{i=1}^{m}$

II. For j = 1,...,k learn a linear classifier $\mathbf{w}_j$ from S_j

- Inference: $\hat{y} = \arg\max_{j=1}^{k} z_j = \arg\max_{j=1}^{k} \mathbf{w}_j \cdot \mathbf{x}$

Example

Original training set: $S = \{(\mathbf{x}_1, 2), (\mathbf{x}_2, 4), (\mathbf{x}_3, 2), (\mathbf{x}_4, 3), (\mathbf{x}_5, 1)\}$

Results in four binary-labeled datasets:

S_1	S_2	S_3	S_4
$(\mathbf{x}_1, -)$	$(\mathbf{x}_1, +)$	$(\mathbf{x}_1, -)$	$(\mathbf{x}_1, -)$
$(\mathbf{x}_2, -)$	$(\mathbf{x}_2, -)$	$(\mathbf{x}_2, -)$	$(\mathbf{x}_2, +)$
$(\mathbf{x}_3, -)$	$(\mathbf{x}_3, +)$	$(\mathbf{x}_3, -)$	$(\mathbf{x}_3, -)$
$(\mathbf{x}_4, -)$	$(\mathbf{x}_4, -)$	$(\mathbf{x}_4, +)$	$(\mathbf{x}_4, -)$
$(\mathbf{x}_5, +)$	$(\mathbf{x}_5, -)$	$(\mathbf{x}_5, -)$	$(\mathbf{x}_5, -)$

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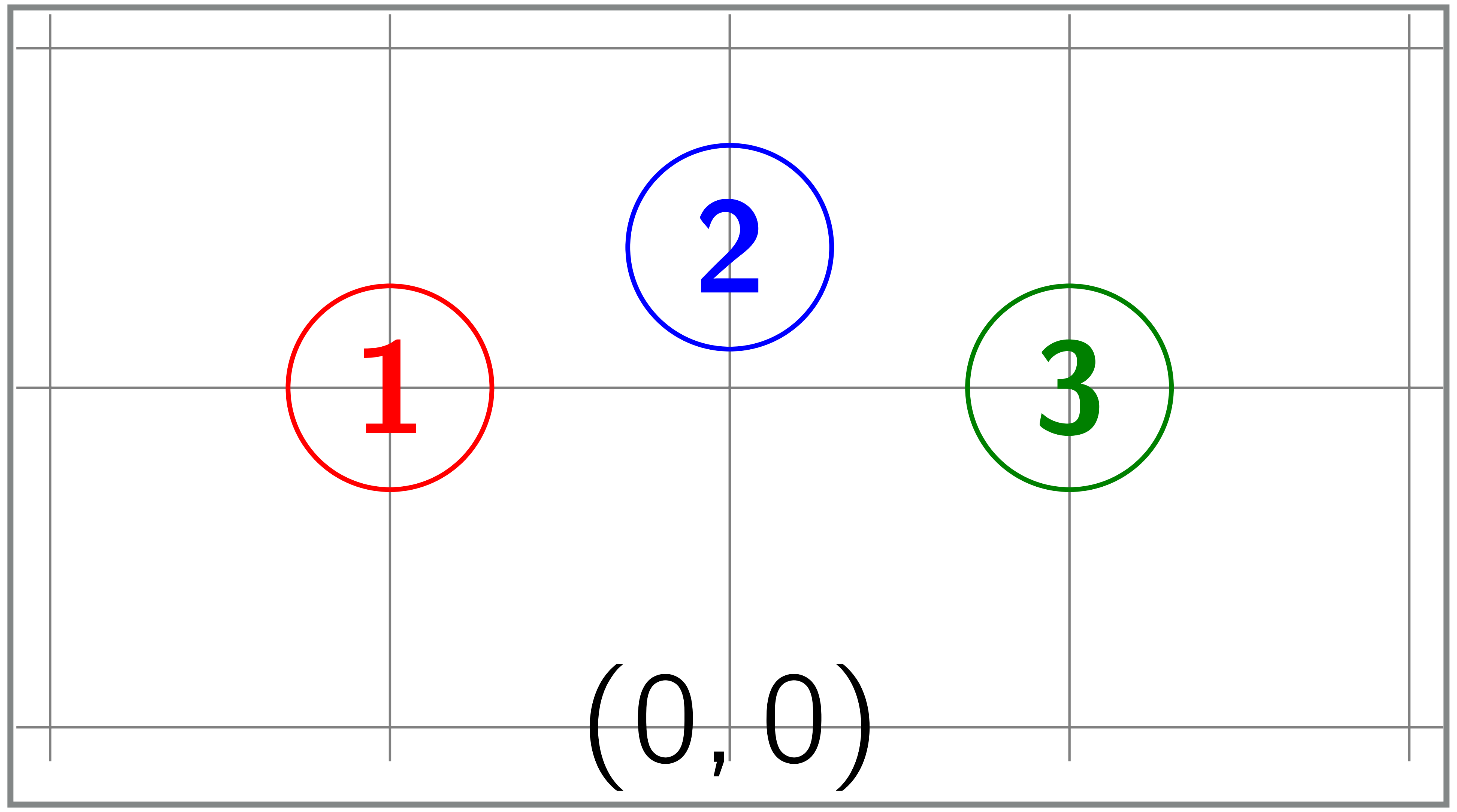
OvA would fail for setting:



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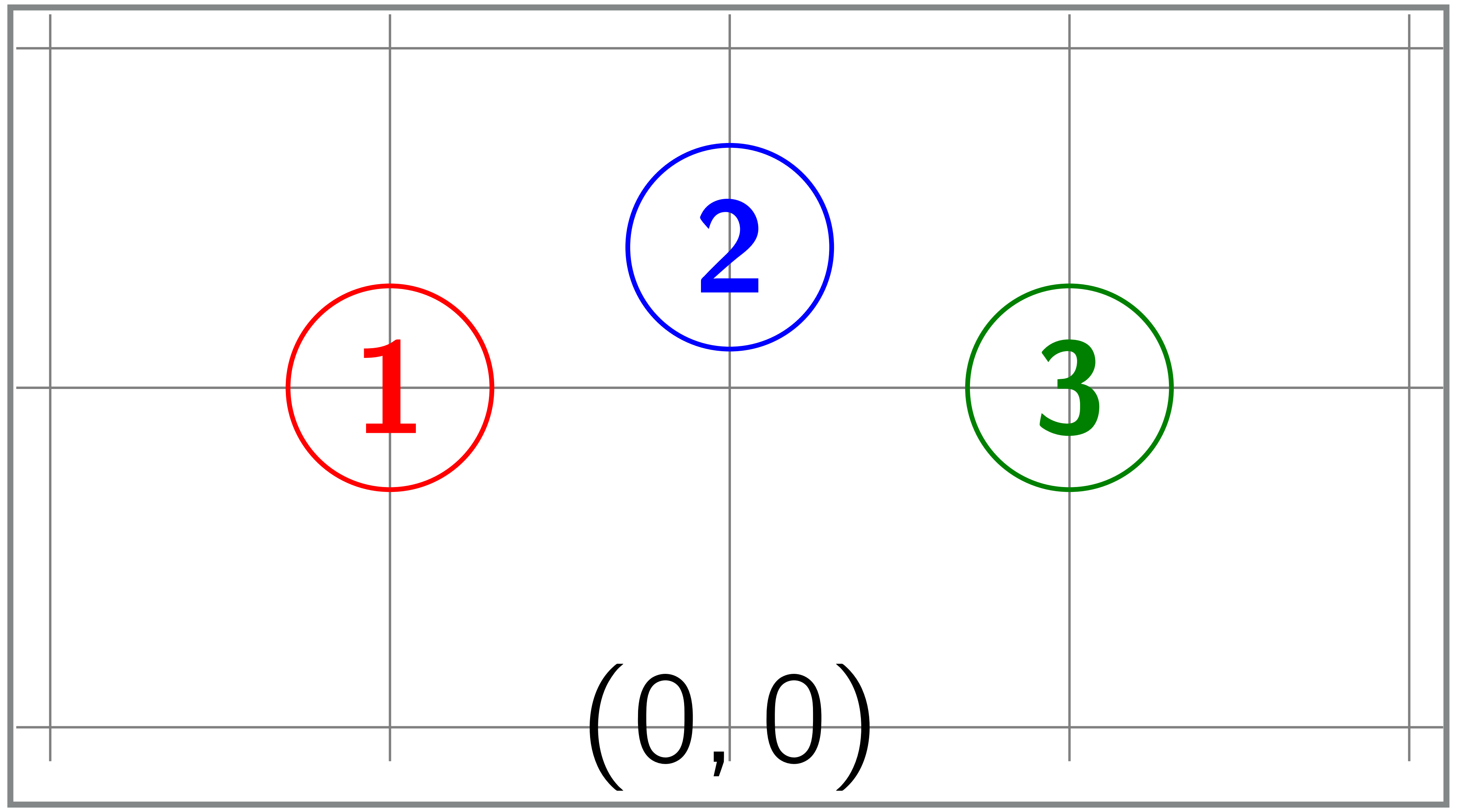


While data is linearly separable using:

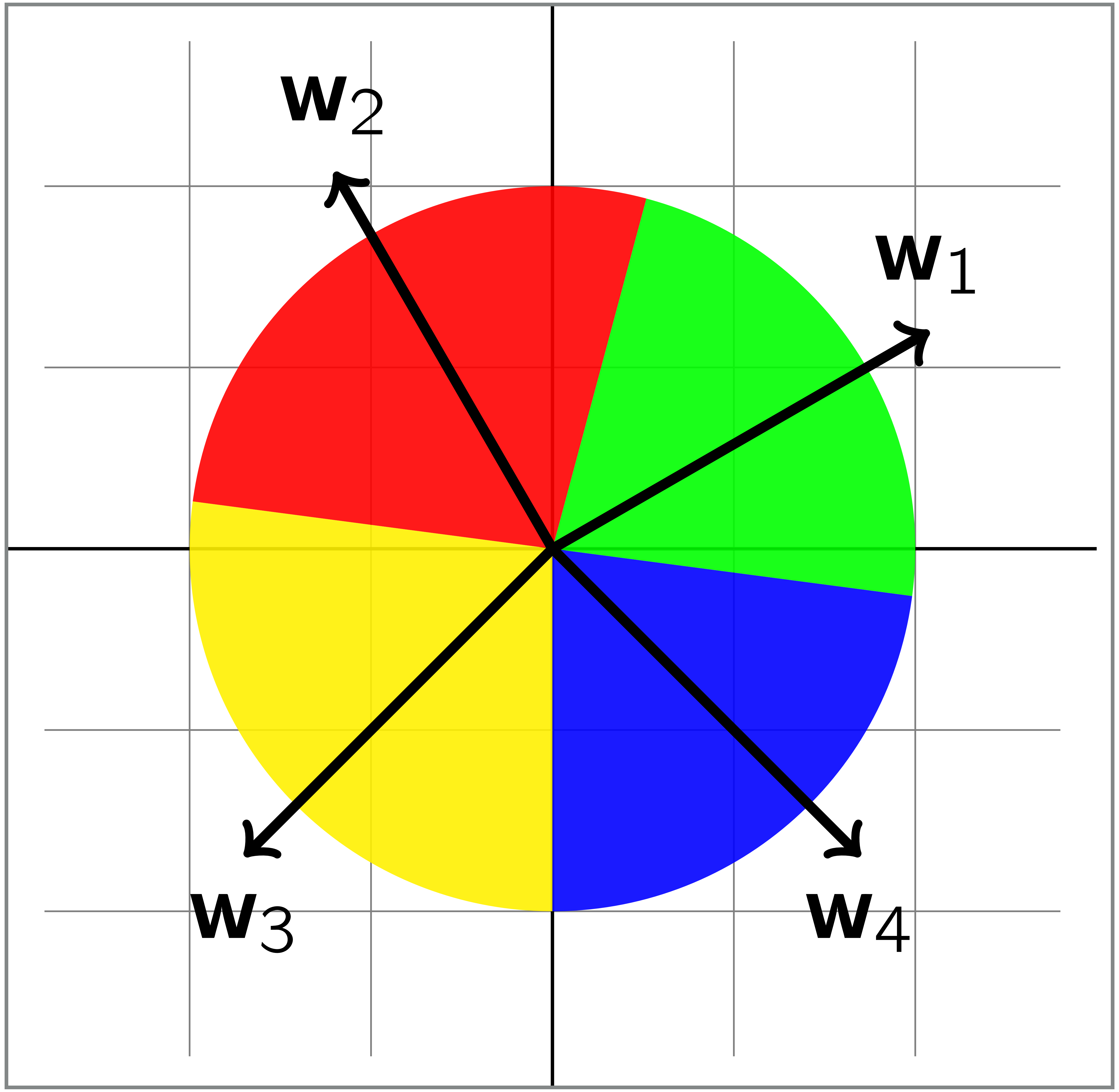
$$W = \begin{bmatrix} -1 & 1 \\ 0 & \sqrt{2} \\ 1 & 1 \end{bmatrix}$$

Multiclass Margin

$$W = \begin{bmatrix} -\mathbf{w}_1- \\ -\mathbf{w}_2- \\ -\mathbf{w}_3- \\ -\mathbf{w}_4- \end{bmatrix} \in \mathbf{R}^{4x2}$$

Assume : $\|\mathbf{w}_j\| = 1 \quad \|\mathbf{x}\| = 1$

$$\measuredangle(\mathbf{w}, \mathbf{x}) = \cos^{-1}(\mathbf{w} \cdot \mathbf{x})$$



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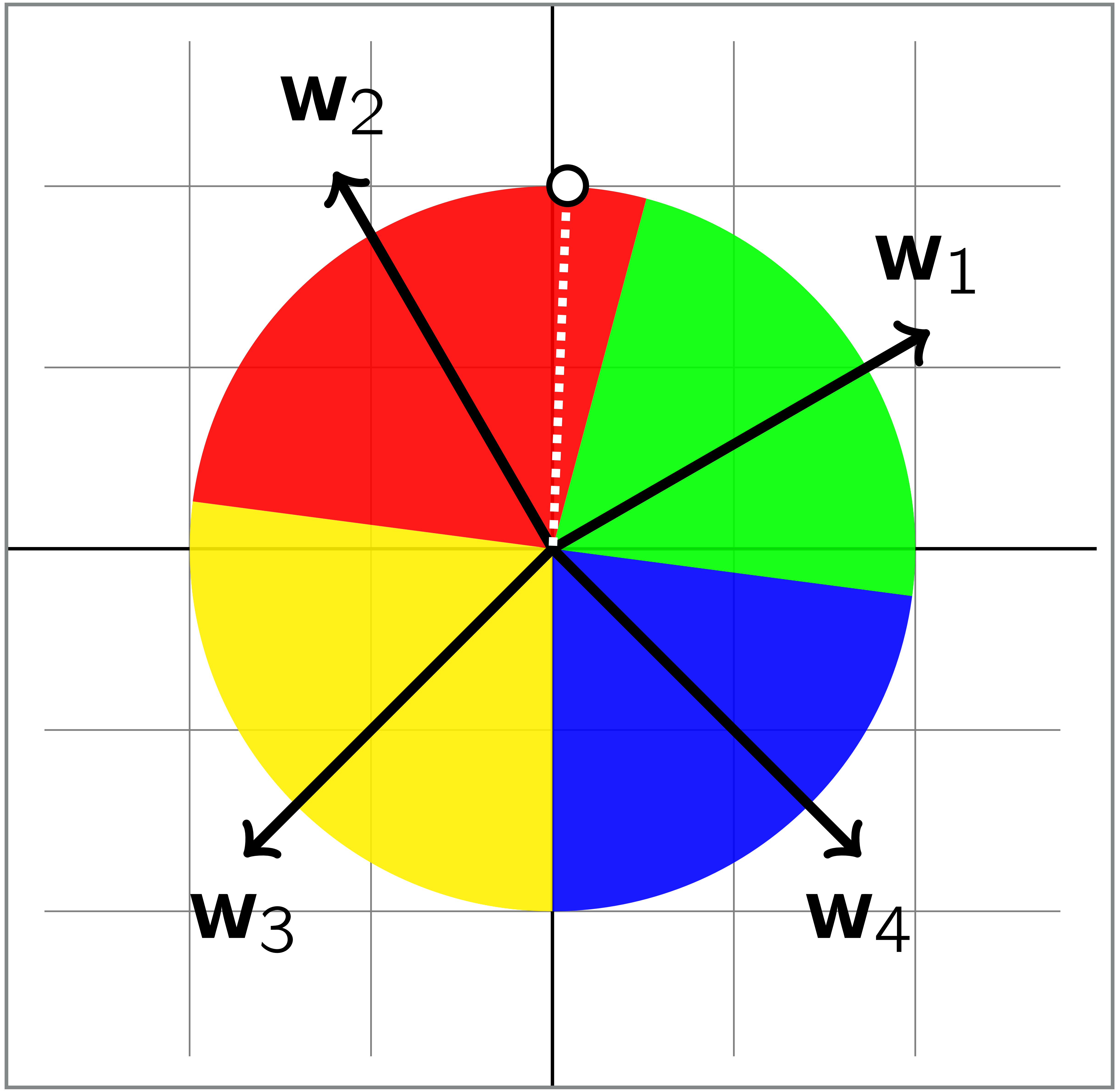

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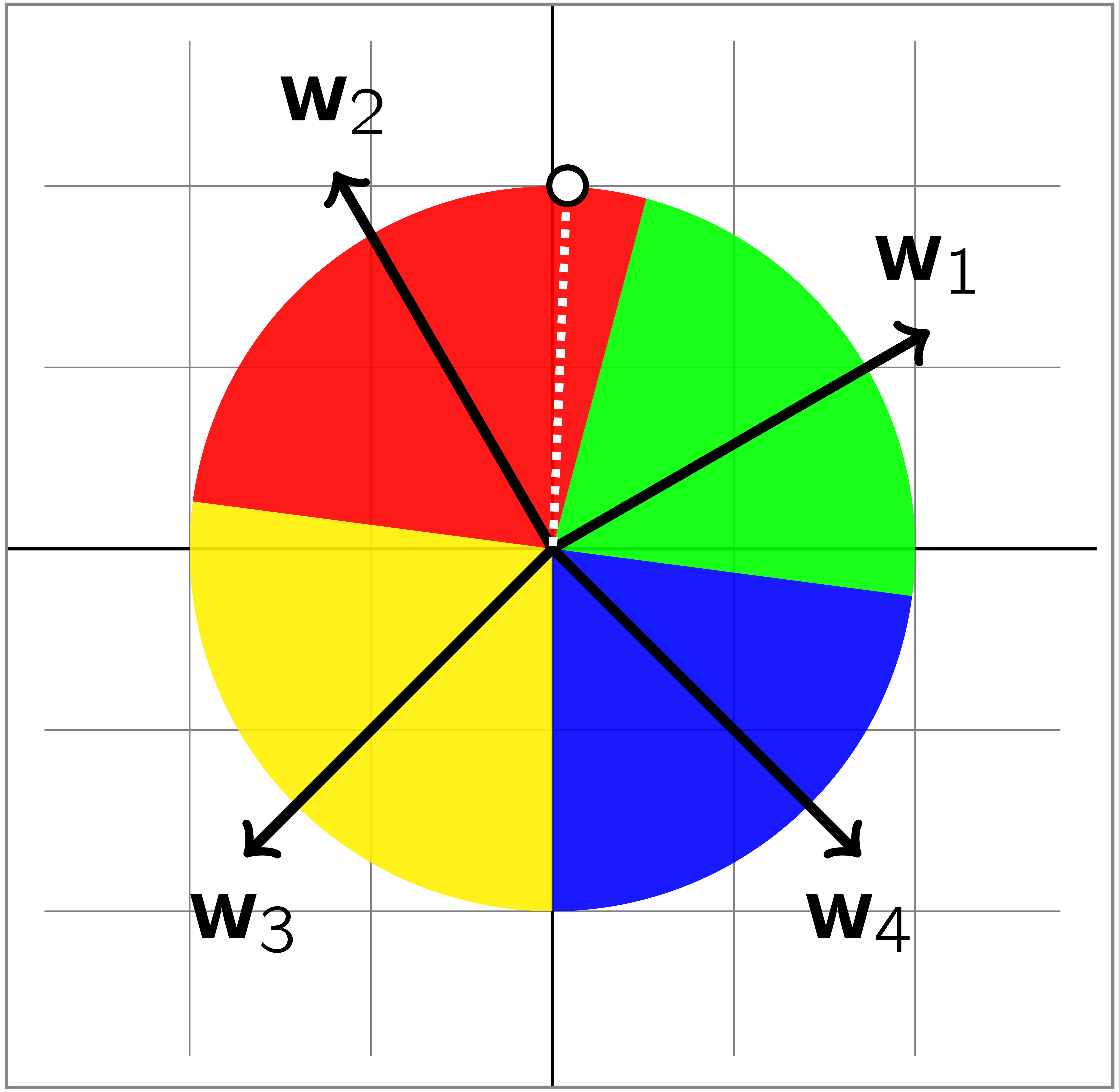

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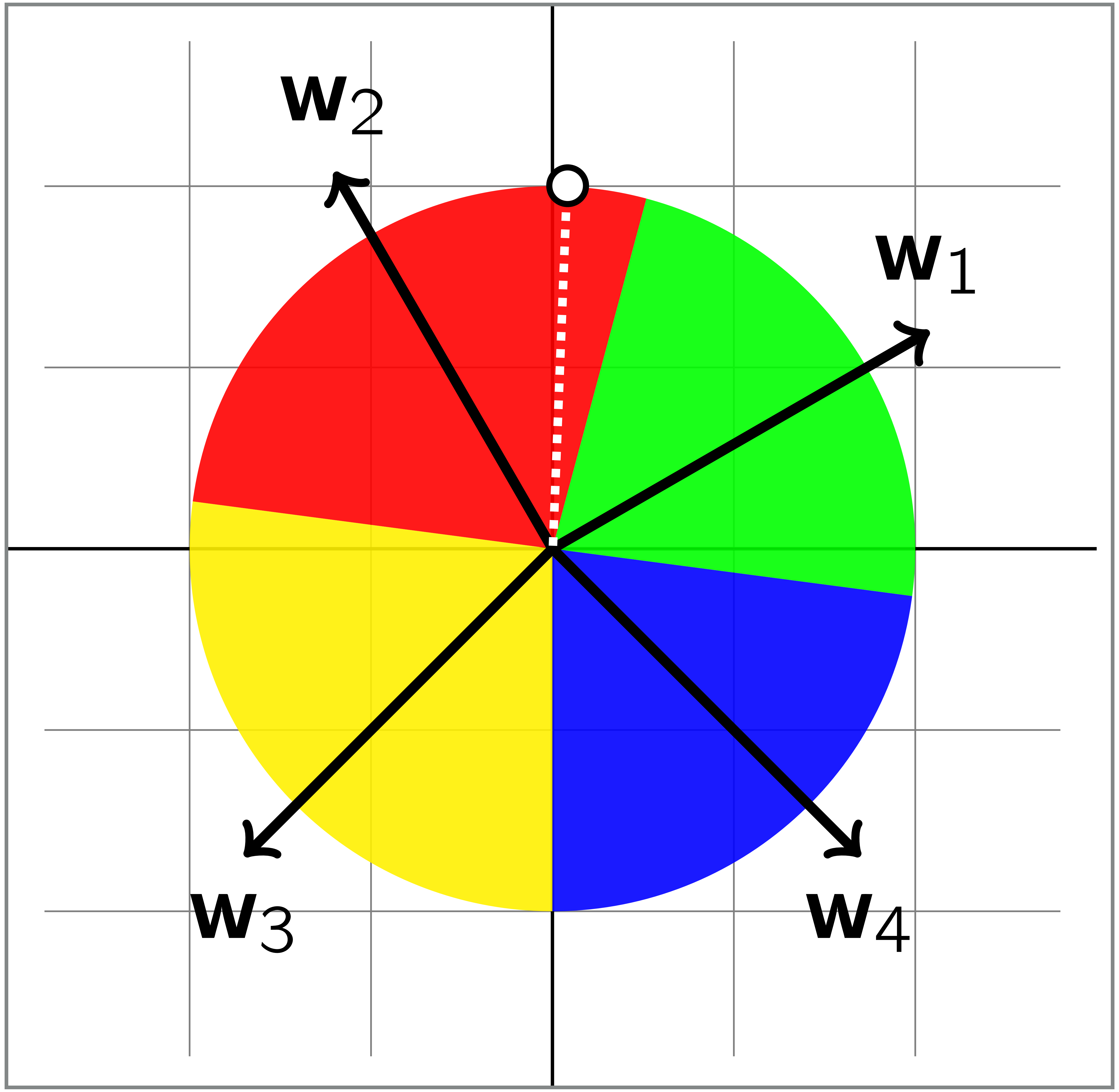

Multiclass Margin

For general vectors impose:

$$(\mathbf{x}, \mathrm{y}) \quad \Rightarrow \quad \forall \mathrm{j} \neq \mathrm{y} : \ \mathbf{w}_{\mathrm{y}} \cdot \mathbf{x} > \mathbf{w}_{\mathrm{j}} \cdot \mathbf{x}$$

In matrix-vector format:

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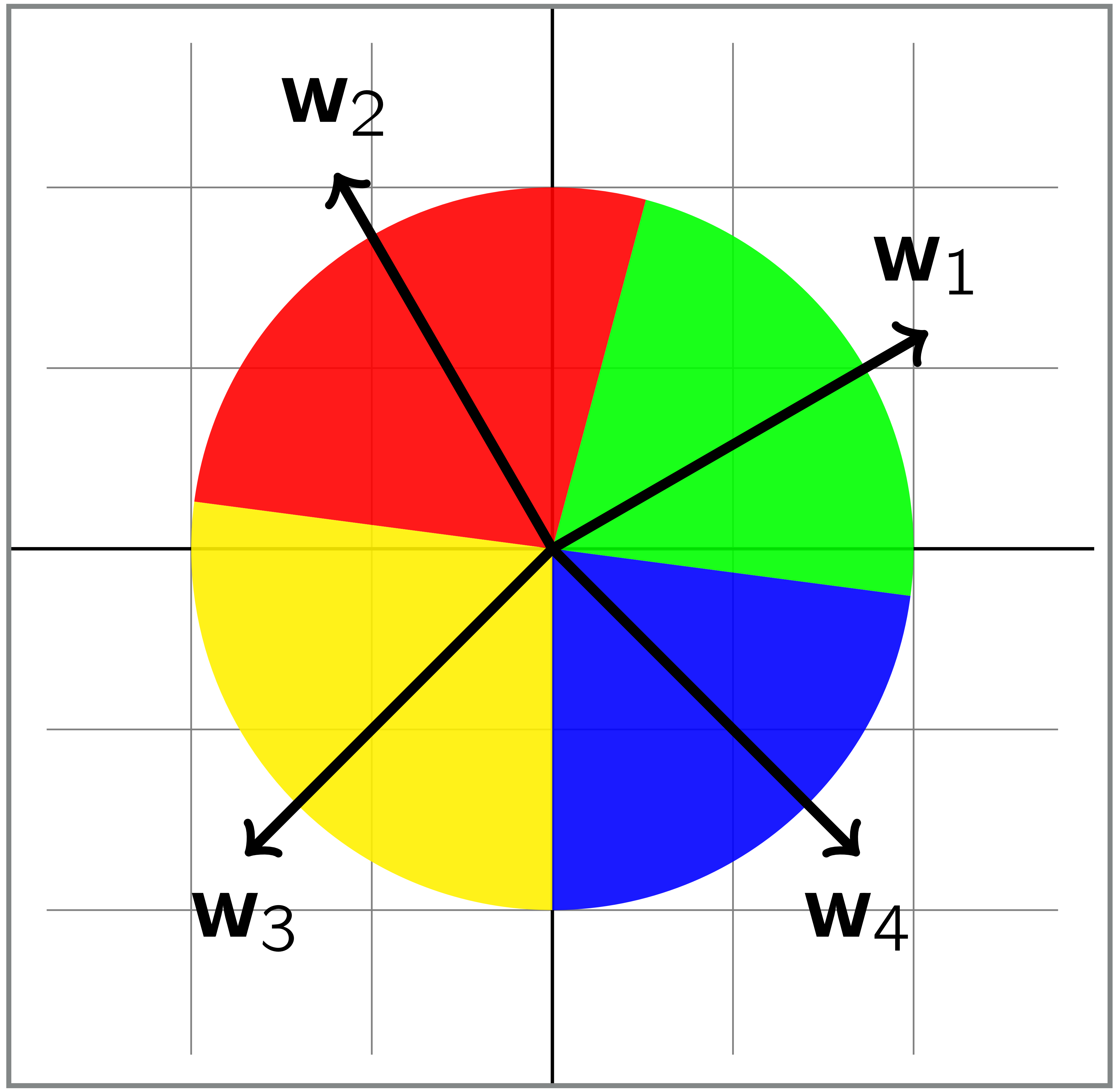


Margin Loss

Predicted class: $\hat{y}(\mathbf{z}) = \arg\max_{j=1}^{k} z_j$

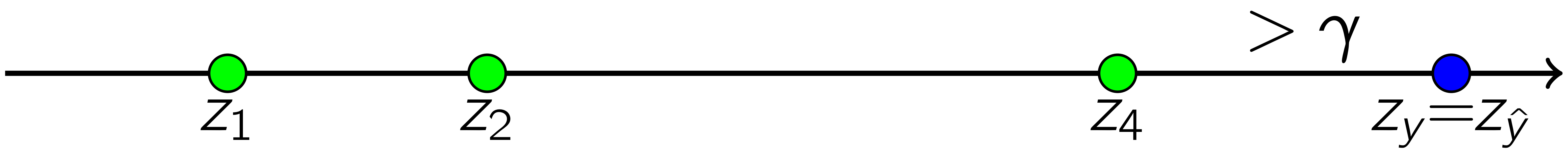
Classification error:

$$\ell^{MC}(\mathbf{z}) = \mathbf{1}\left[\hat{y}(\mathbf{z}) \neq y\right]$$

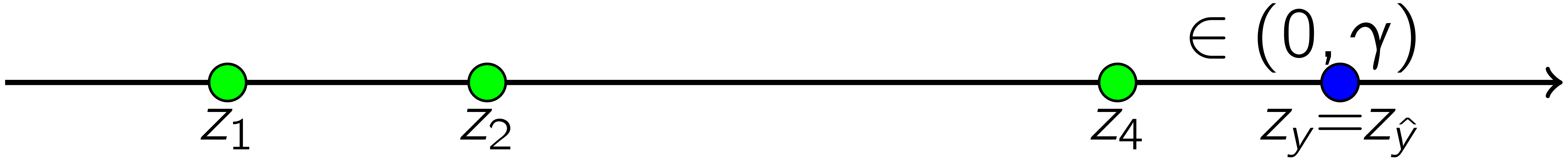
Max-Margin Loss is difference in scores + penalty γ:

$$\ell^{MM}(\mathbf{z}) = \left[\gamma + \max_{j \neq y} z_j - z_y\right]_+ \qquad \text{where} \quad [z]_+ = \max\{0, z\}$$

Margin great than $\gamma \;\Rightarrow\; \ell^{\mathrm{MC}} = \ell^{\mathrm{MM}} = 0$



Margin $\in (0, \gamma) \;\Rightarrow\; \ell^{\mathrm{MC}} = 0$ but $\ell^{\mathrm{MM}} \geq 0$



Margin $< 0 \;\Rightarrow\; \ell^{\mathrm{MC}} = 1$ and $\ell^{\mathrm{MM}} \geq \gamma$

Convexity of Max-Margin Loss*

Inner product $\mathbf{w_j} \cdot \mathbf{x}$ is linear in $\mathbf{w_j}$ $\Rightarrow$ $\mathbf{w_j} \cdot \mathbf{x}$ convex in $\mathbf{w_j}$ (and concave)

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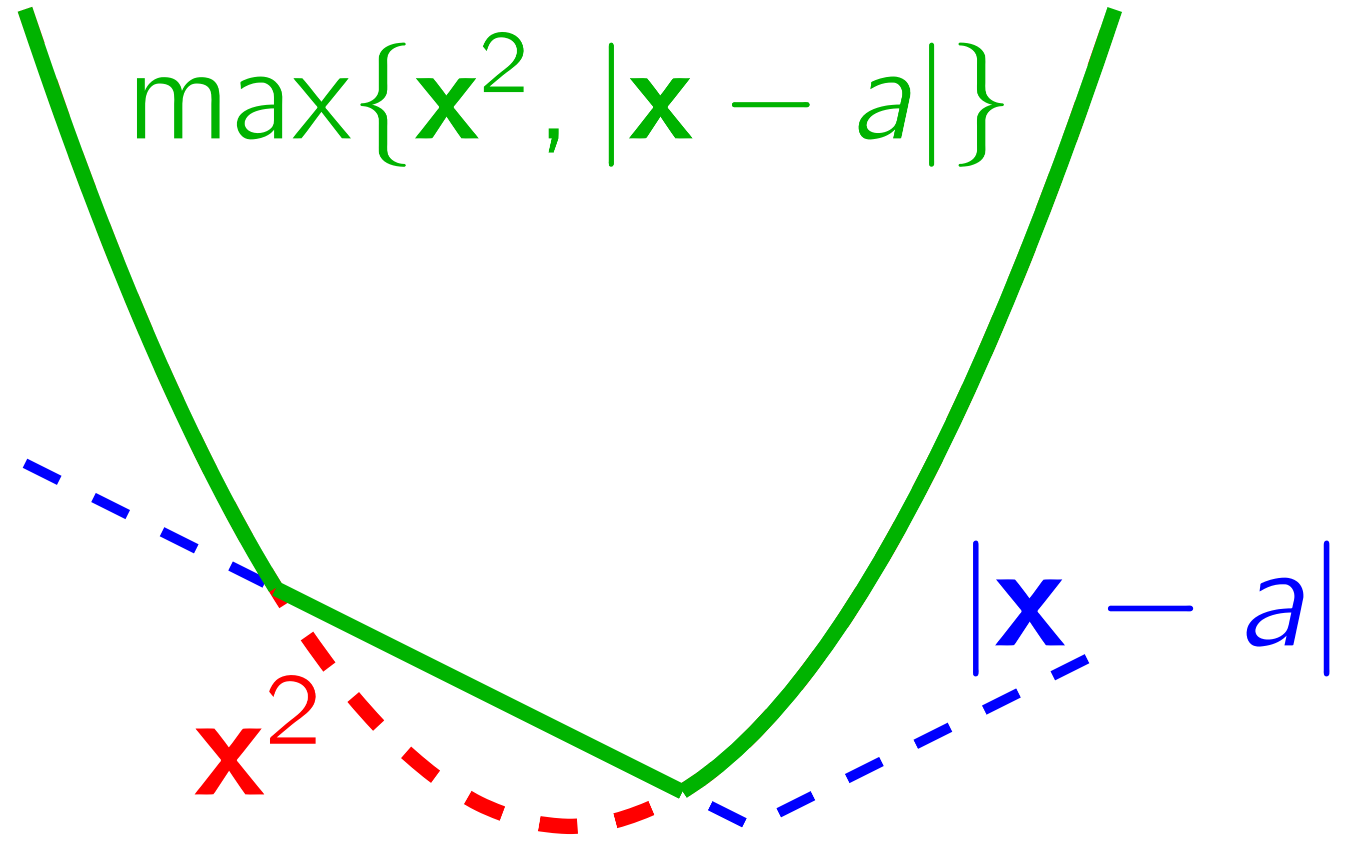

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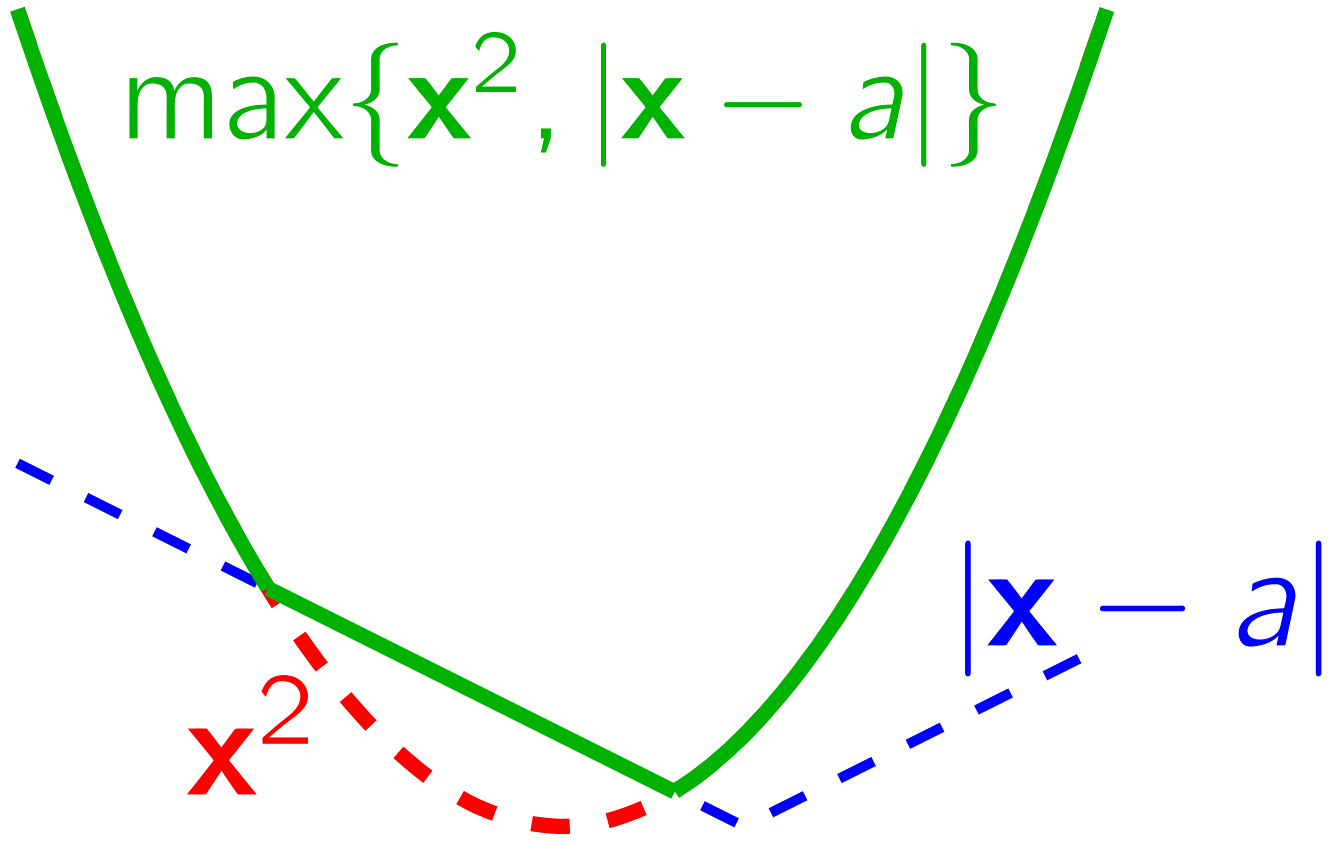

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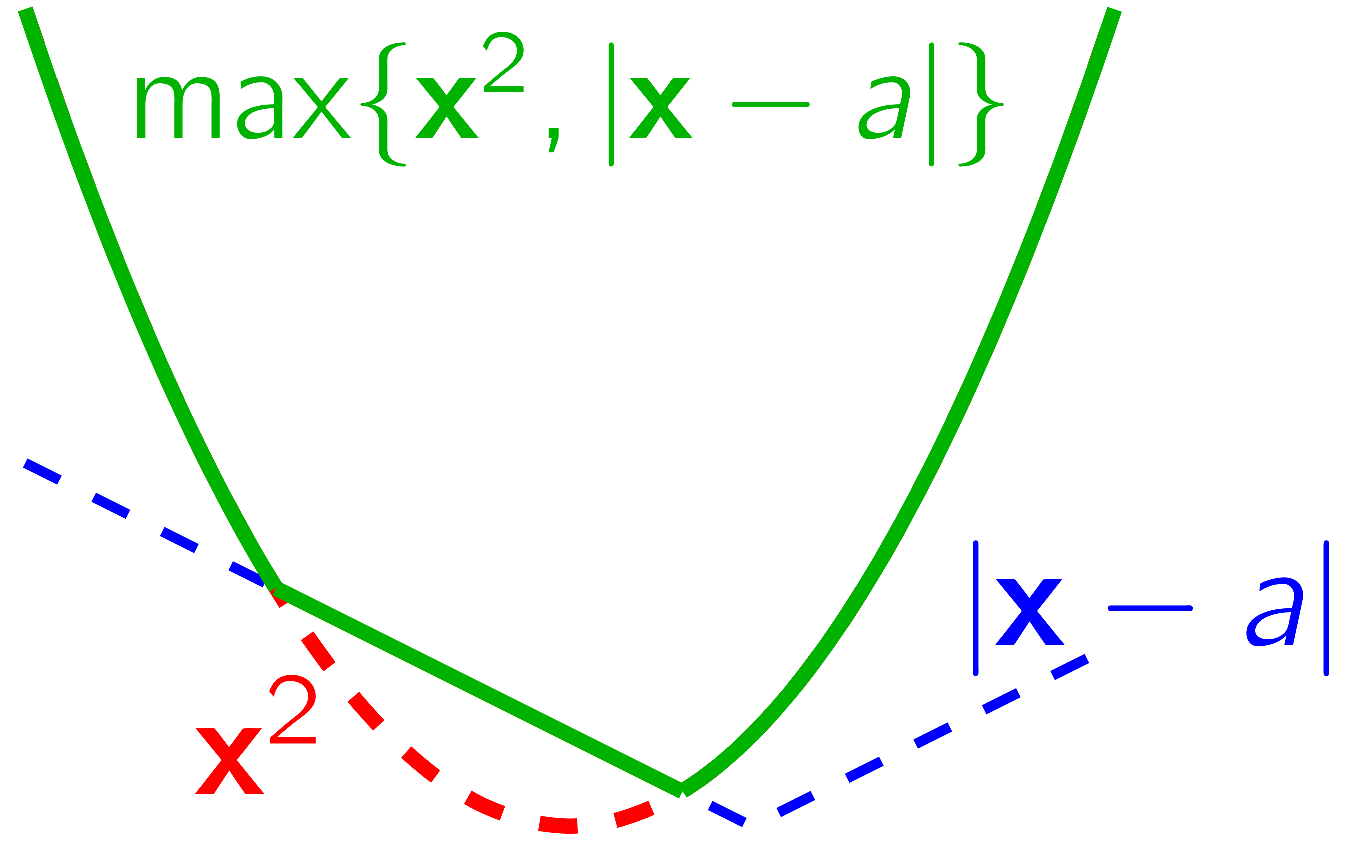

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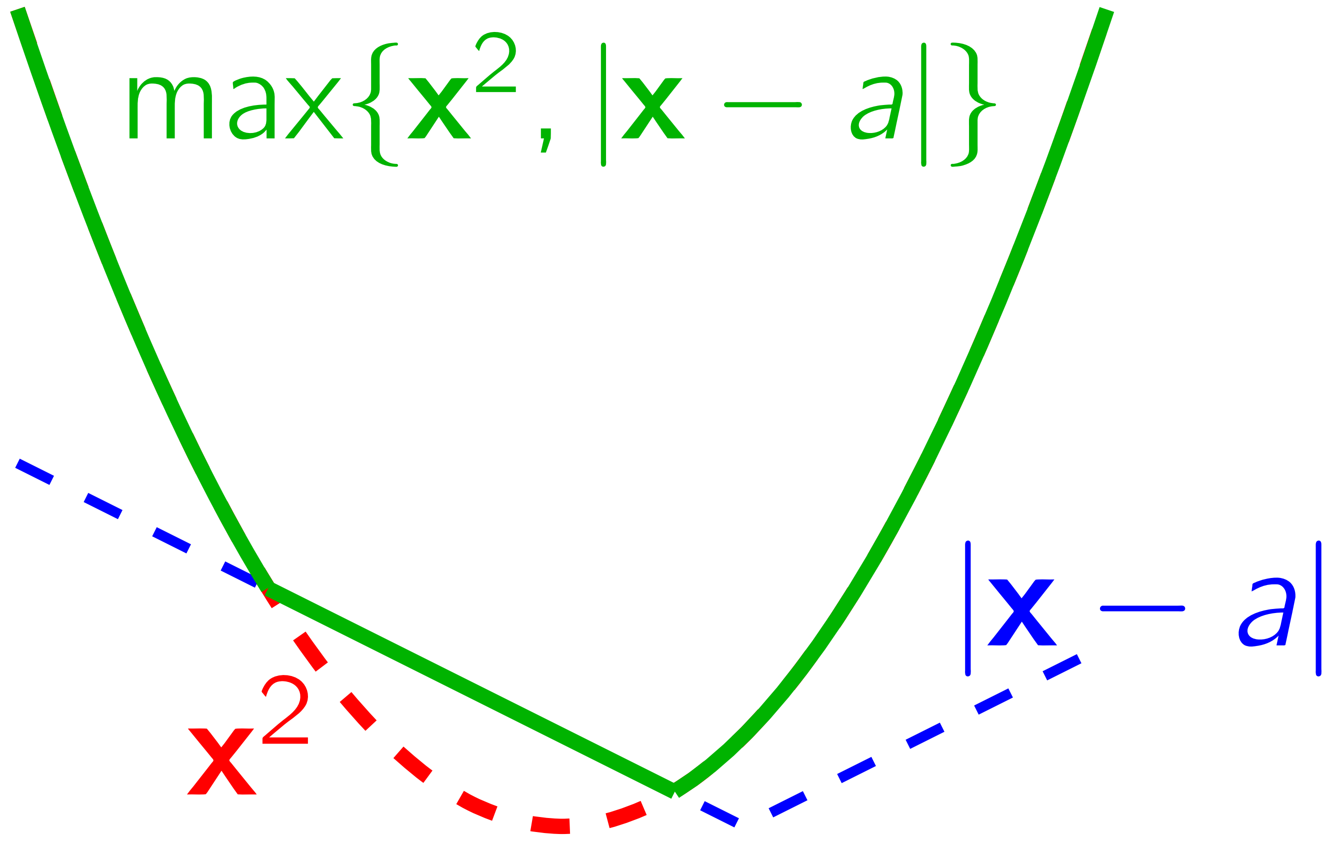

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Using convexity of maximum again: $\ell^{\mathrm{MM}}(\mathbf{z}) = \max\left\{0, \gamma + \max_{j \neq y} z_j - z_y\right\}$

Implies that $\ell^{\mathrm{MM}}(\mathbf{z})$ is convex in W

Multivariate Logistic Regression

As before $\mathbf{z} = W\mathbf{x}$

Define probability of class c to be $\mathbf{P}\left[j \mid \mathbf{z}\right] = \dfrac{e^{z_j}}{Z}$ where $Z = \sum_{j=1}^{k} e^{z_j}$

Loss: -log-probability of correct class $\ell^{LR}(\mathbf{z}) = -\log\left(P\left[y \mid \mathbf{x}\right]\right)$

$$\hat{y} = \arg\max_{j=1}^{k} z_j \neq y \qquad = \underbrace{\log\left(\sum_j \exp(z_j)\right)}_{\text{SoftMax}} - z_y$$

$$\text{SoftMax}(\mathbf{z}) \equiv \log\left(\sum_i e^{z_i}\right) \geq \max_i z_i$$

SoftMax

$$\ell^{\mathrm{LR}}(\mathrm{z}) = -\log\left(P\left[\mathrm{y}\,|\,\mathbf{x}\right]\right) \;=\; \underbrace{\log\left(\sum_j \exp(z_j)\right)}_{\text{SoftMax}} - \mathrm{z}_{\mathrm{y}}$$

Recall $\hat{\mathrm{y}} = \arg\max_{\mathrm{j}=1}^{\mathrm{k}} \mathrm{z}_{\mathrm{j}} \;\Rightarrow\; \mathrm{SoftMax}(\mathbf{z}) = \log\left(\sum_{\mathrm{j}} \mathrm{e}^{\mathrm{z}_{\mathrm{j}}}\right) \geq \log\left(\mathrm{e}^{\mathrm{z}_{\hat{\mathrm{y}}}}\right) = \mathrm{z}_{\hat{\mathrm{y}}}$

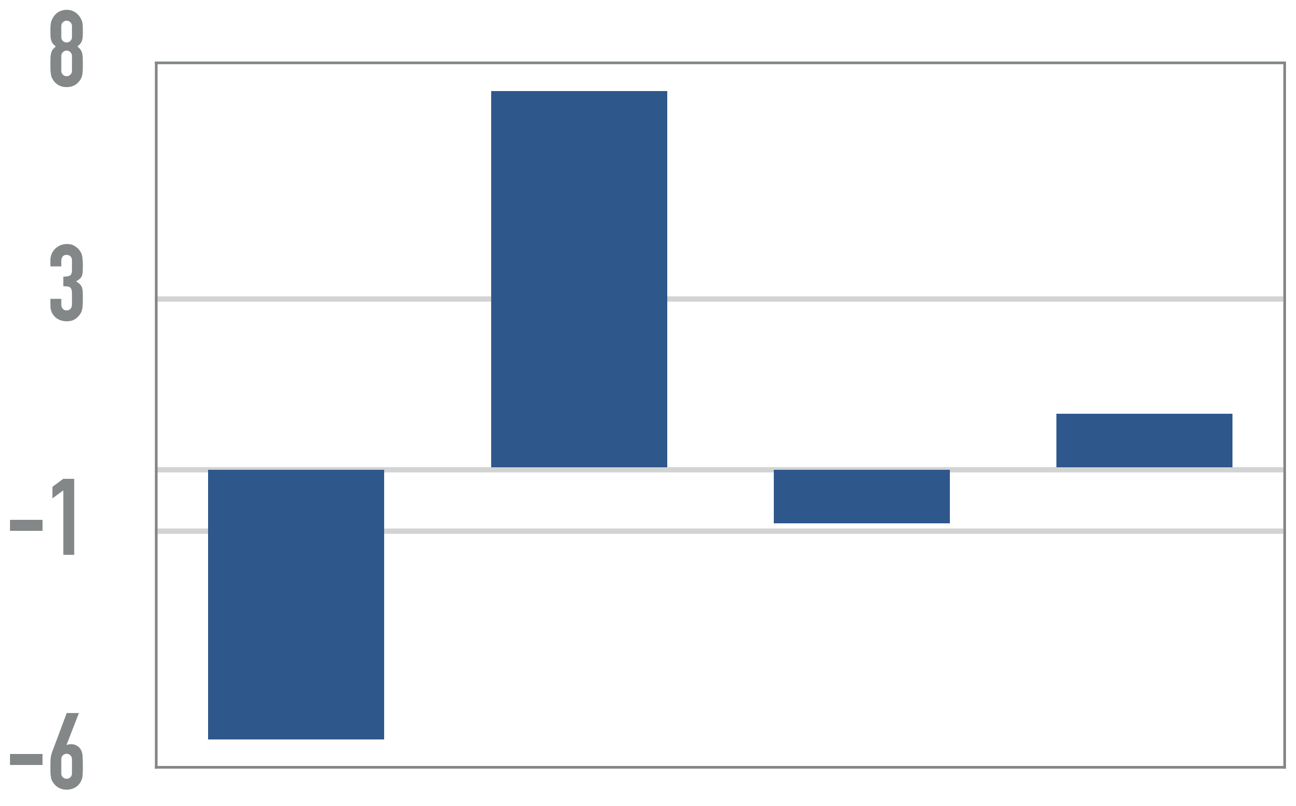
Case I: $\forall \mathrm{j} \neq \hat{\mathrm{y}} : \mathrm{z}_{\hat{\mathrm{y}}} \gg \mathrm{z}_{\mathrm{j}} \;\Rightarrow\; \mathrm{SoftMax}(\mathbf{z}) \approx \mathrm{z}_{\hat{\mathrm{y}}}$

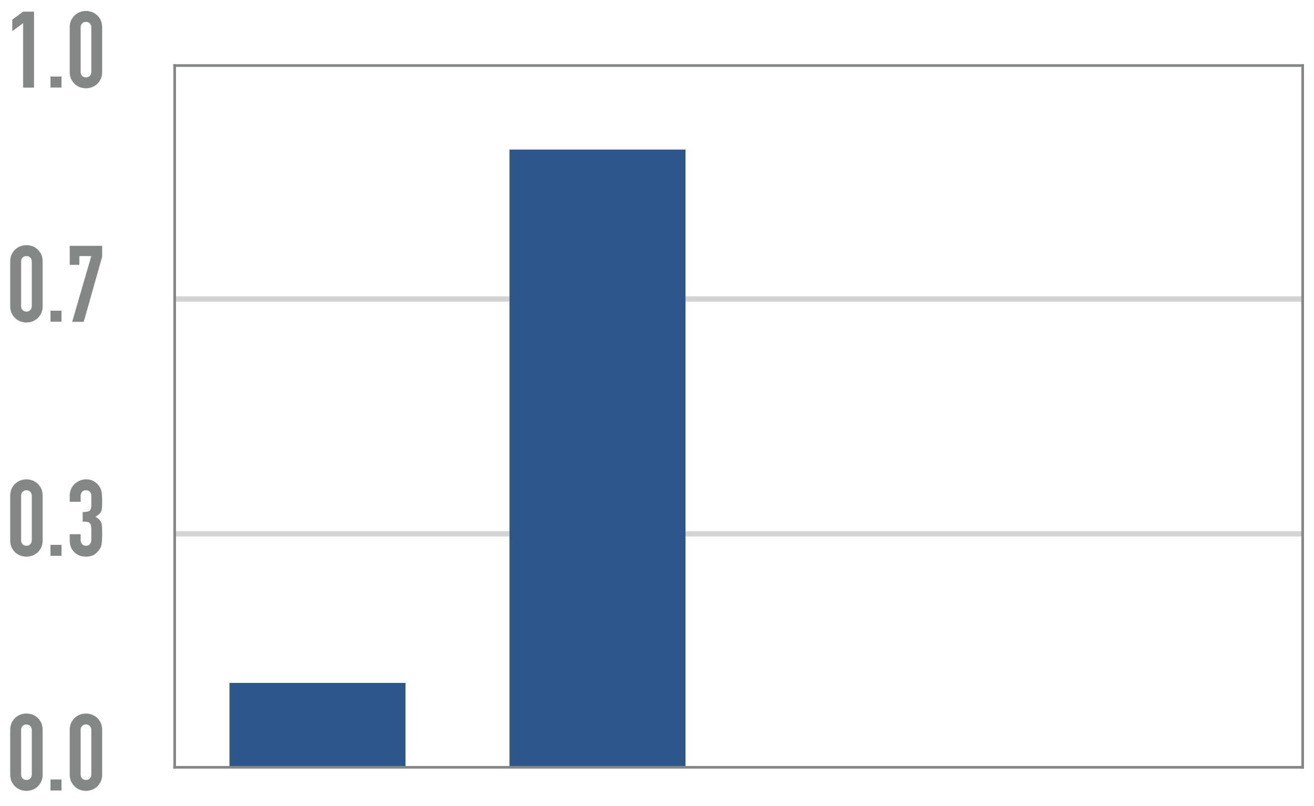
Case II: $\forall \mathrm{j} : \mathrm{z}_{\hat{\mathrm{y}}} \approx \mathrm{z}_{\mathrm{j}} \;\Rightarrow\; \mathrm{SoftMax}(\mathbf{z}) \approx \log\left(\sum_{\mathrm{j}} \mathrm{e}^{\mathrm{z}_{\hat{\mathrm{y}}}}\right) = \log(\mathrm{k})\,\mathrm{z}_{\hat{\mathrm{y}}}$

z	5	7	-1	1

p	0.1	0.9	0	0

$$\text{SoftMax}(\mathbf{z}) \approx 7.13$$



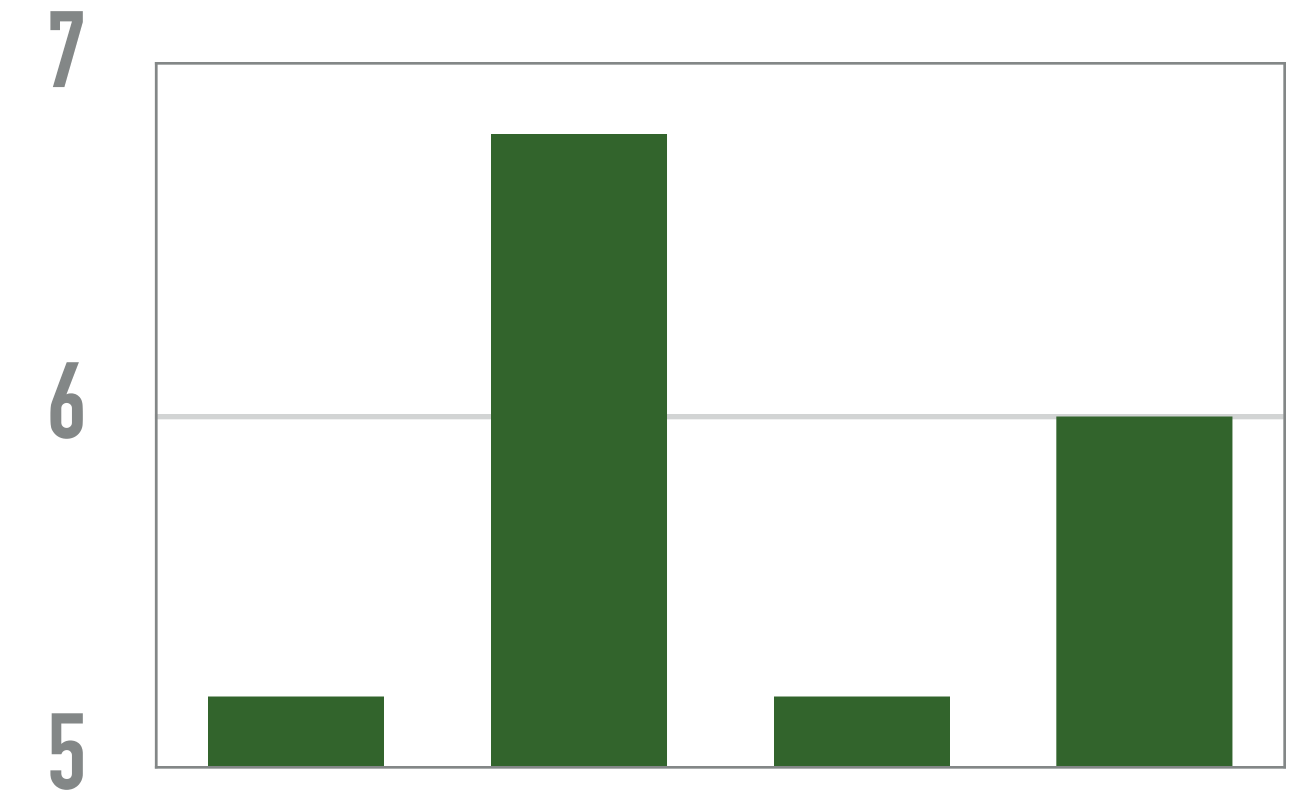


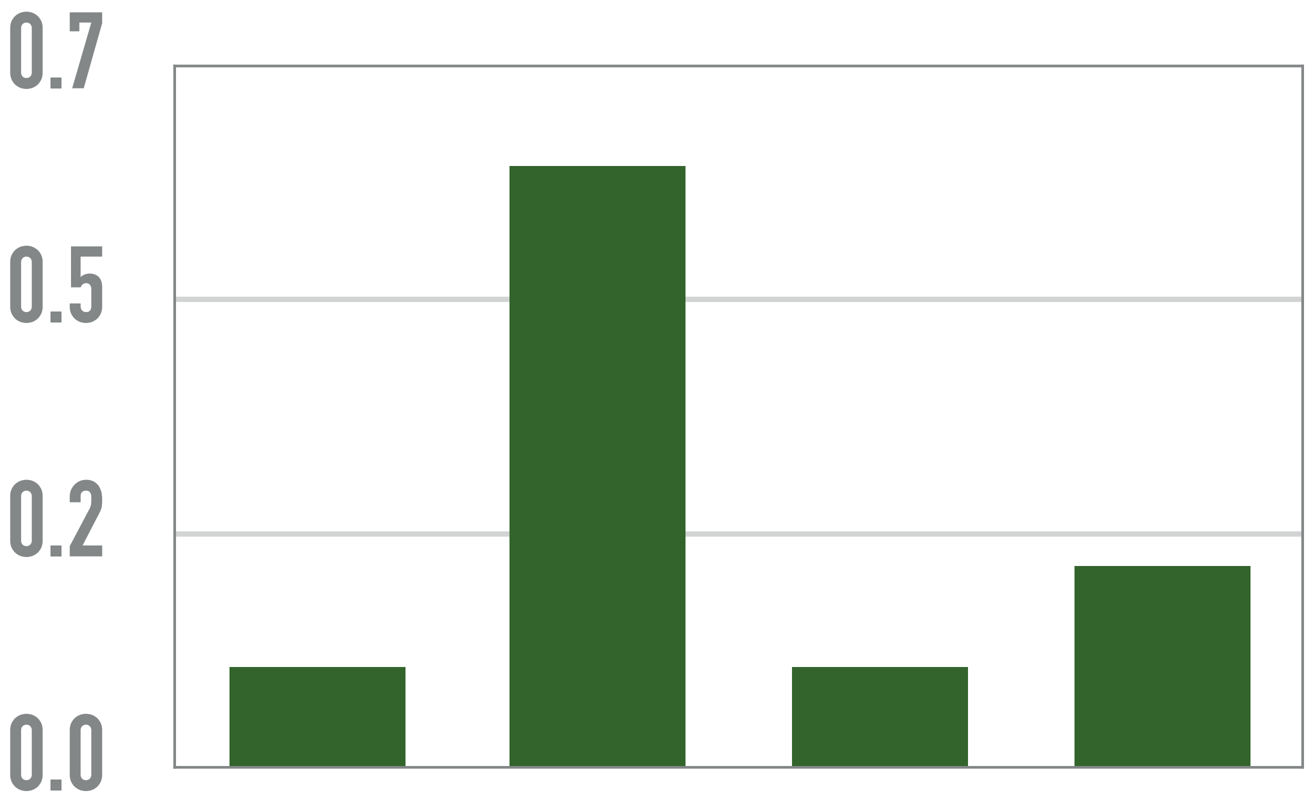
$$\ell^{\text{LR}}(\text{z}) = \text{SoftMax}(\mathbf{z}) - \text{z}_\text{y}$$
$$\approx 7.13 - 7 = 0.13$$

z	5	7	5	6

p	0.1	0.6	0.1	0.2

$$\text{SoftMax}(\mathbf{z}) \approx 7.5$$





$$\ell^{\text{LR}}(\text{z}) = \text{SoftMax}(\mathbf{z}) - \text{z}_\text{y}$$
$$\approx 7.5 - 7 = 0.5$$

Numerically Stable Evaluation

Exponentials of large values could cause overflow

Use the following properties:

➡ $$\log\Big(\sum_{\mathrm{j}} \exp(\mathrm{z_j})\Big) = \log\Big(\sum_{\mathrm{j}} \exp(\mathrm{z_j} - \mathrm{z_{\hat{y}}})\Big) + \mathrm{z_{\hat{y}}}$$

➡ $$\mathrm{P}[\mathrm{i}\,|\,\mathbf{x}] = \frac{\exp(\mathrm{z_i})}{\sum_{\mathrm{j}} \exp(\mathrm{z_j})} = \frac{\exp(\mathrm{z_i} - \mathrm{z_{\hat{y}}})}{\sum_{\mathrm{j}} \exp(\mathrm{z_j} - \mathrm{z_{\hat{y}}})} = \frac{\exp(\tilde{z}_i)}{\sum_j \exp(\tilde{z}_j)}$$

Transform $\mathbf{z} \mapsto \mathbf{z} - \mathrm{z_{\hat{y}}} = \tilde{\mathbf{z}}$

Define: $\ell^{\mathrm{LR}}(\tilde{\mathbf{z}}) = \mathrm{SoftMax}(\tilde{\mathbf{z}}) - \mathrm{z_y} + \mathrm{z_{\hat{y}}}$

Numerically Stable Evaluation

Exponentials of large values could cause overflow

Use the following properties:

- $$\log\Big(\sum_j \exp(z_j)\Big) = \log\Big(\sum_j \exp(z_j - z_{\hat{y}})\Big) + z_{\hat{y}}$$
- $$P[i\,|\,\mathbf{x}] = \frac{\exp(z_i)}{\sum_j \exp(z_j)} = \frac{\exp(z_i - z_{\hat{y}})}{\sum_j \exp(z_j - z_{\hat{y}})} = \frac{\exp(\tilde{z}_i)}{\sum_j \exp(\tilde{z}_j)}$$

Transform $\mathbf{z} \mapsto \mathbf{z} - z_{\hat{y}} = \tilde{\mathbf{z}}$

Define: $\ell^{\mathrm{LR}}(\tilde{\mathbf{z}}) = \mathrm{SoftMax}(\tilde{\mathbf{z}}) - z_y + z_{\hat{y}}$

MC Logistic Regression & Error

Multiclass prediction error:

$$\ell^{\mathsf{MC}}(\mathsf{y}, \mathbf{z}) = 1 \quad \Leftrightarrow \quad \hat{\mathsf{y}} = \arg\max_{\mathsf{j}=1}^{\mathsf{k}} \mathsf{z}_{\mathsf{j}} \neq \mathsf{y}$$

If $\hat{\mathsf{y}} \neq \mathsf{y}$ then $\ell^{\mathsf{LR}}(\mathsf{z}) = \log\left(\sum_j \exp(\mathsf{z}_j)\right) - \mathsf{z}_\mathsf{y}$

$$\geq \log\Big(\underbrace{\exp(\mathsf{z}_\mathsf{y}) + \exp(\mathsf{z}_{\hat{\mathsf{y}}})}_{\geq 2\exp(\mathsf{z}_\mathsf{y})}\Big) - \mathsf{z}_\mathsf{y} \geq \log(2)$$

Therefor $\ell^{\mathsf{MC}}(\mathsf{y}, \mathbf{z}) = 1 \quad \Rightarrow \quad \ell^{\mathsf{LR}}(\mathsf{y}, \mathbf{z}) \geq 2$

Multiclass LR & Max-Margin

If $\ell^{\mathrm{MM}}(\mathrm{z}) \geq \beta > 0 \quad \Rightarrow \quad \exists \mathrm{j} : \gamma + \mathrm{z_j} - \mathrm{z_y} \geq \beta$

Then $\ell^{\mathrm{LR}}(\mathrm{z}) = \log\left(\sum_j \exp(\mathrm{z}_j)\right) - \mathrm{z_y} \;\geq \log\left(\exp(\mathrm{z_y}) + \exp(\mathrm{z_j})\right) - \mathrm{z_y}$

Hence $\ell^{\mathrm{LR}}(\mathrm{z}) \geq \log\left((\exp(\mathrm{z_y}) + \mathrm{e}^{\beta-\gamma} \exp(\mathrm{z_y})\right) - \mathrm{z_y}$

$$\geq \log(1 + \mathrm{e}^{\beta-\gamma}) \geq \beta - \gamma$$

In summary: $\ell^{\mathrm{MM}}(\mathrm{y}, \mathbf{z}) = \beta \quad \Rightarrow \quad \ell^{\mathrm{LR}}(\mathrm{y}, \mathbf{z}) \geq \beta - \gamma$

SGD for Multiclass

Instead of $\mathbf{w}_t$ maintain a matrix W^t

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$$\begin{bmatrix} \| - \mathbf{w}_1 - \| \leq r \\ \| - \mathbf{w}_2 - \| \leq r \\ \vdots \\ \| - \mathbf{w}_k - \| \leq r \end{bmatrix}$$

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$$\begin{bmatrix} \| - \mathbf{w}_1 - \| \leq r \\ \| - \mathbf{w}_2 - \| \leq r \\ \vdots \\ \| - \mathbf{w}_k - \| \leq r \end{bmatrix} \qquad \begin{aligned} \mathbf{w}_j^{t+1/2} &\leftarrow \mathbf{w}_j^t - \eta_t \mathbf{g}_j^t \\ \mathbf{w}_j^{t+1} &\leftarrow \min\left\{1, r/\|\mathbf{w}_j^{t+1/2}\|\right\} \mathbf{w}_j^{t+1/2} \end{aligned}$$

Multiclass Logistic Regression

For each example ($\mathbf{x}$,y) in mini-batch calculate $\mathbf{z} = W\mathbf{x}$

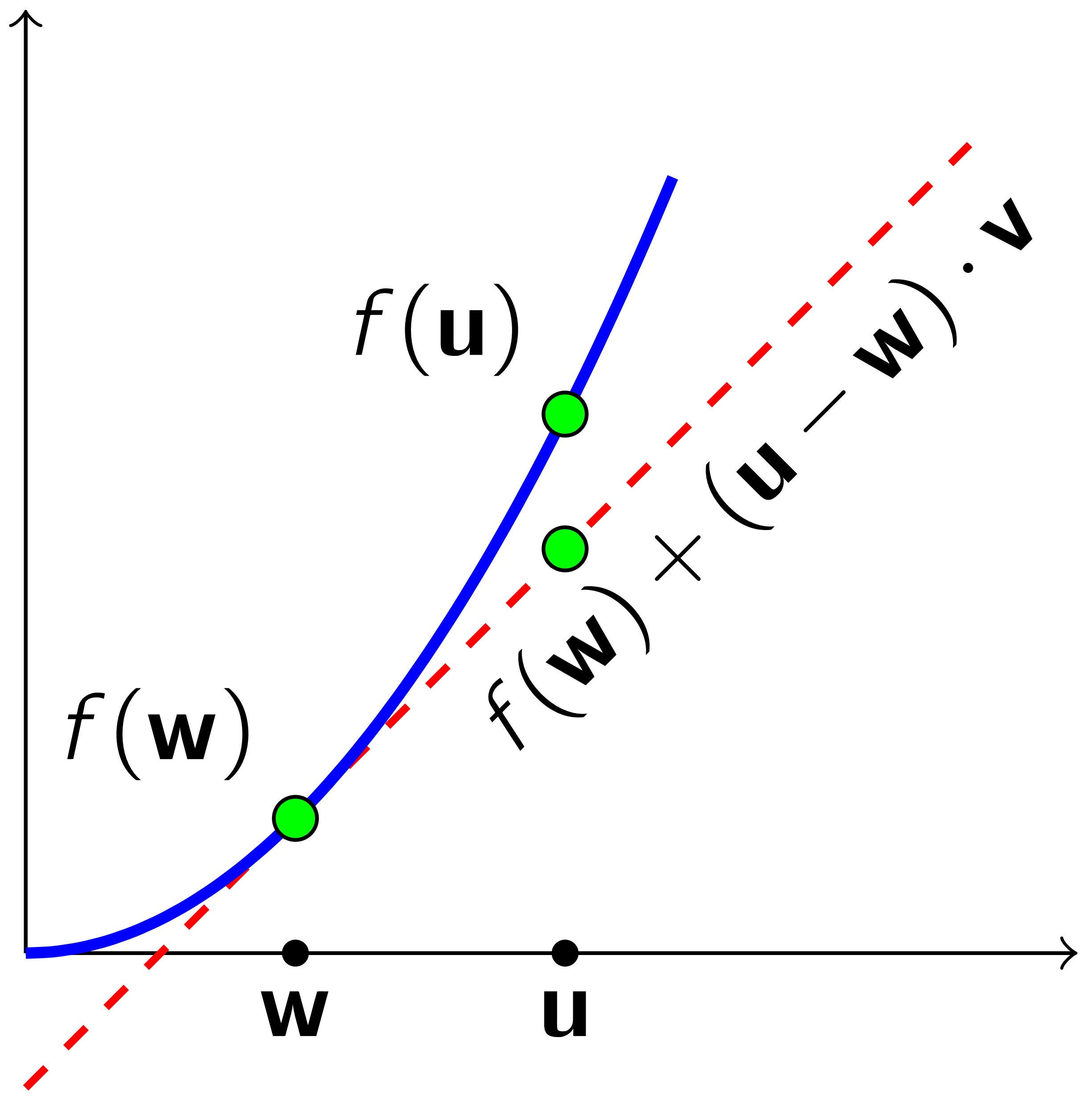
Define: $$v[j] = \frac{\exp(z_j)}{\sum_{i=1}^{k} \exp(z_i)} - \mathbf{1}[j=y]$$

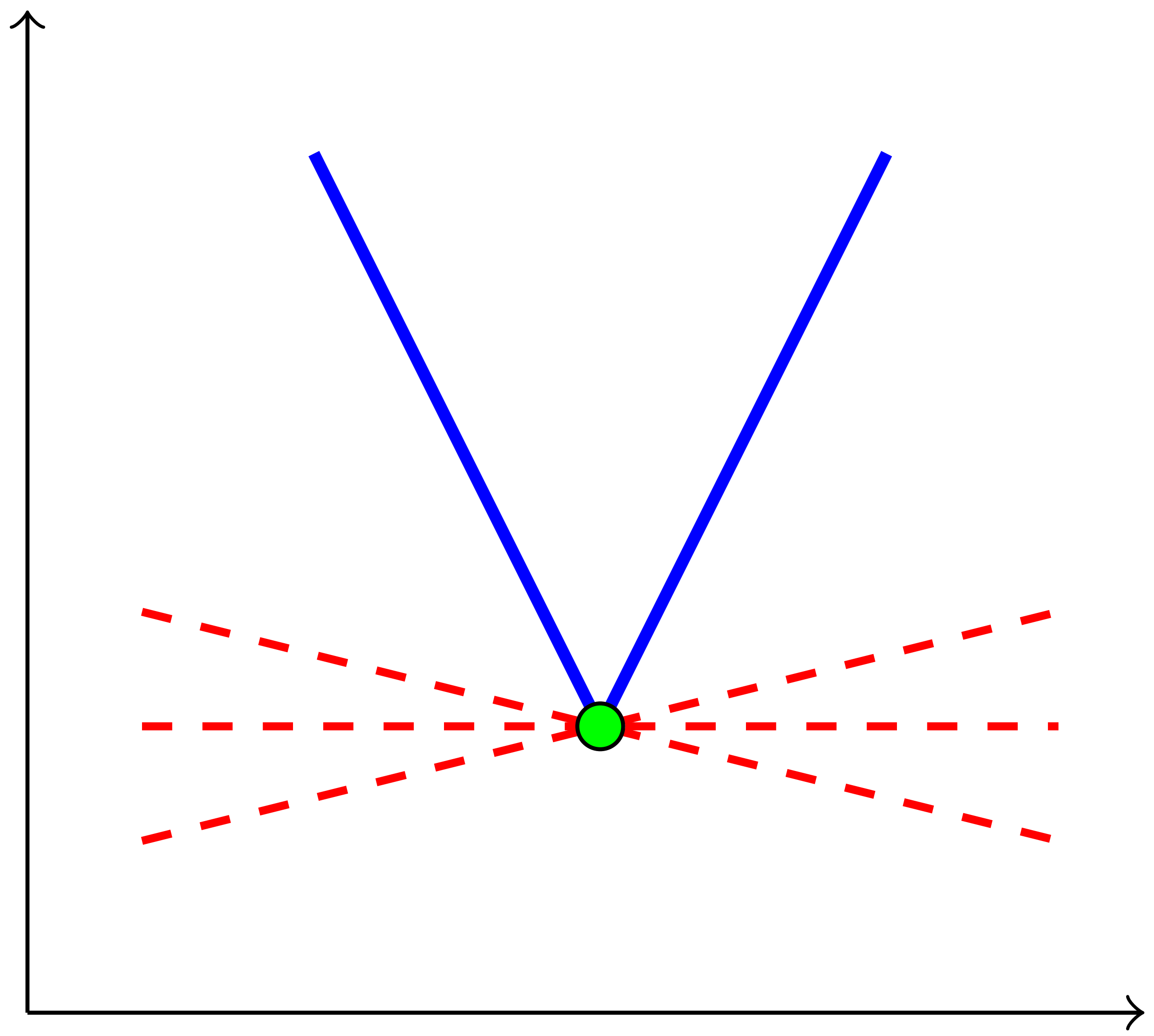
Gradient: $$\mathbf{v}\,\mathbf{x}^T = \begin{bmatrix} v[1]\,\mathbf{x} \\ v[2]\,\mathbf{x} \\ \vdots \\ v[k]\,\mathbf{x} \end{bmatrix}$$ and for mini-batch: $$G = \frac{1}{|S|} \sum_{i \in S} \mathbf{v_i}\,\mathbf{x_i}^T$$

Sub-gradients*

$\mathbf{w}$ is a sub-gradient of f at $\mathbf{w}$ if $\forall \mathbf{u},\quad \mathbf{f(u) \geq f(w) + v \cdot (u - w)}$

Differential set ∂f($\mathbf{w}$) is the set of sub-gradients of f at $\mathbf{w}$





Sub-gradient for Max Margin*

Set of labels with margin error $\Gamma = \{j \neq y \mid \gamma + z_j - z_y \geq 0\}$

Sub-gradients for MM loss are vectors **p** of the form:

$$p[y] = -1 \; ; \text{ for } j \notin \Gamma : p[j] = 0 \; ; \sum_{j \in \Gamma} p[j] = 1 \;\; (p[j] \geq 0)$$

Example: y = 2 **z** = [-2 3 2.5 1 7 4 1.9] $\gamma = 1$

$\Gamma = \{3, 5, 6\}$ **p** = [0 -1 1 0 0 0 0] or **p** = [0 -1 0.1 0 0.4 0.5 0] or …

Families of Updates

$y = 3 \quad \gamma = 2$

z	-1	2.5	3	4	1	2.5

For all forms of updates: $p[y] = 1$

Max only: $p[\hat{y}] = -1$

p	0	0	-1	1	0	0

Uniform: $\forall j \in \Gamma : p[j] = \dfrac{1}{|\Gamma|}$

p	0	1/3	-1	1/3	0	1/3

Margin-based: $\forall j \in \Gamma : p[j] = \dfrac{z_j - z_y}{Z}$ where $Z = \sum_{j \in \Gamma} z_j - z_y$

p	0	1.5	-1	3	0	1.5

/Z=6

p	0	1/4	-1	1/2	0	1/4

Mini-Batch Max-Margin Subgradient*

For each $i \in S$:

1. Calculate predicted values: $\mathbf{z}_i = W\,\mathbf{x}_i$

2. Calculate margin-error sets: $\Gamma = \{j \neq y_i \mid \gamma + z_i[j] - z_i[y] \geq 0\}$

3. Form update vectors: $\mathbf{p}_i$

4.Gradient: $G = \dfrac{1}{|S|} \sum_{i \in S} \mathbf{p}_i\,\mathbf{x}_i^T$

Max-Margin vs. Soft-Max*

Both updates of the form: $W^{t+1} \leftarrow W^t - \eta_t \, \mathbf{p} \, \mathbf{x}^\top$

Both satisfy $\sum_j p[j] = 0 \;\; ; \;\; \sum_{j \neq y} p[j] \leq 1$

If $\Gamma \neq \emptyset$ then for MM $p[y] = -1$ and for LR $p[y] > -1$

LR is a dense update $|\{j : p[j] > 0\}| = k - 1$

MM is a sparse update $|\{j : p[j] > 0\}| \leq |\Gamma|$

Cost-Sensitive Multiclass*

Classes often have semantic meaning and similarities

Image classification: Ape $\approx$ Baboon but Ape $\not\approx$ Subaru

Cost of confusing class y with class y': C(y,y')>0   [and C(y,y)=0]

Replace a fixed margin of γ with label-dependent margin C(y,y')

Cost Sensitive Multiclass*

Proxy for bounding $C(y, \hat{y})$

$$
\begin{aligned}
C(y, \hat{y}) &\le C(y, \hat{y}) + z_{\hat{y}} - z_y \\
&\le \underbrace{\max_r C(y, r) + z_r - z_y}_{\equiv \ell(y, \mathbf{z})}
\end{aligned}
$$

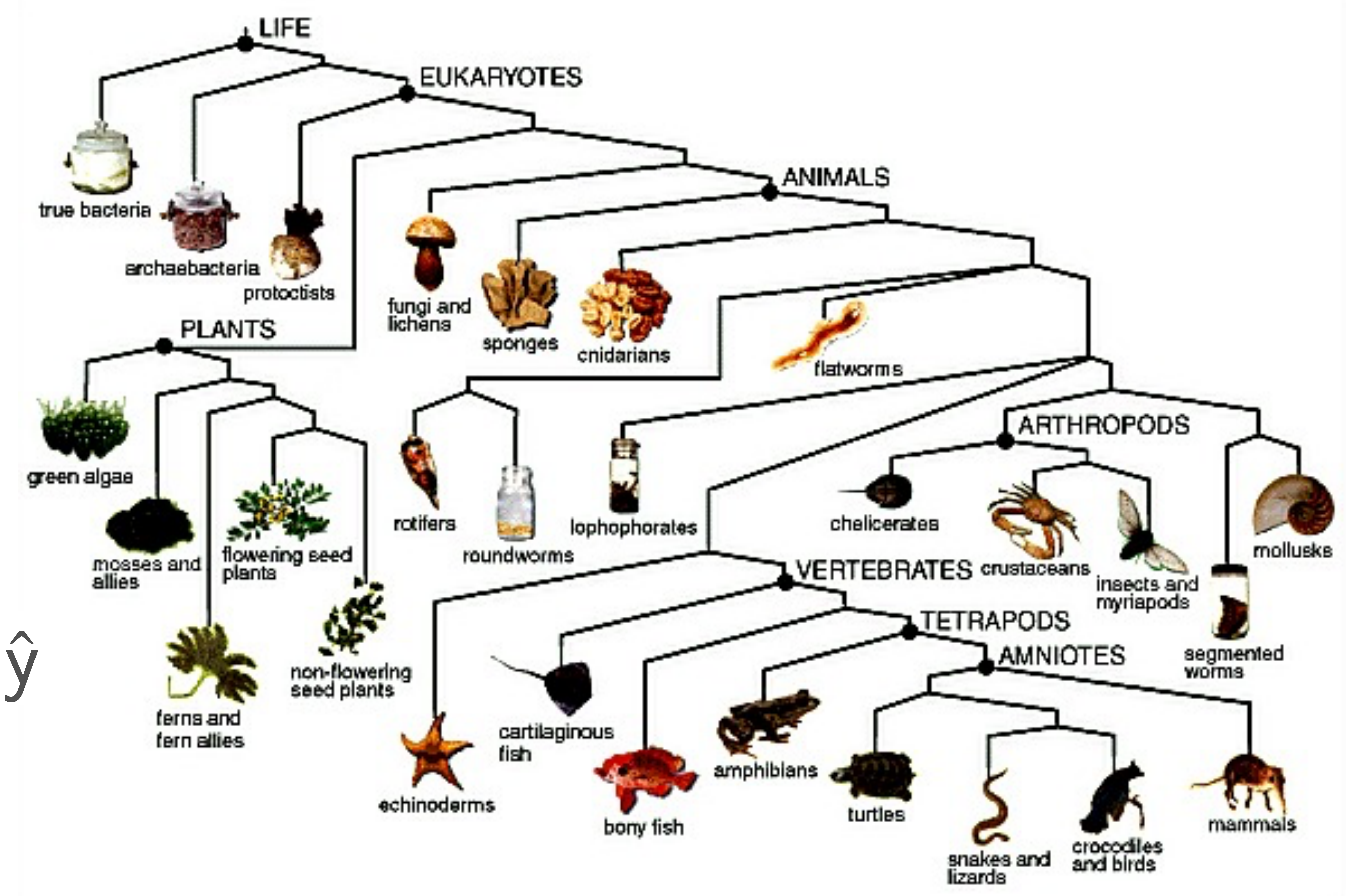
Usage: Hierarchical Classification*

Classes organized in a hierarchy

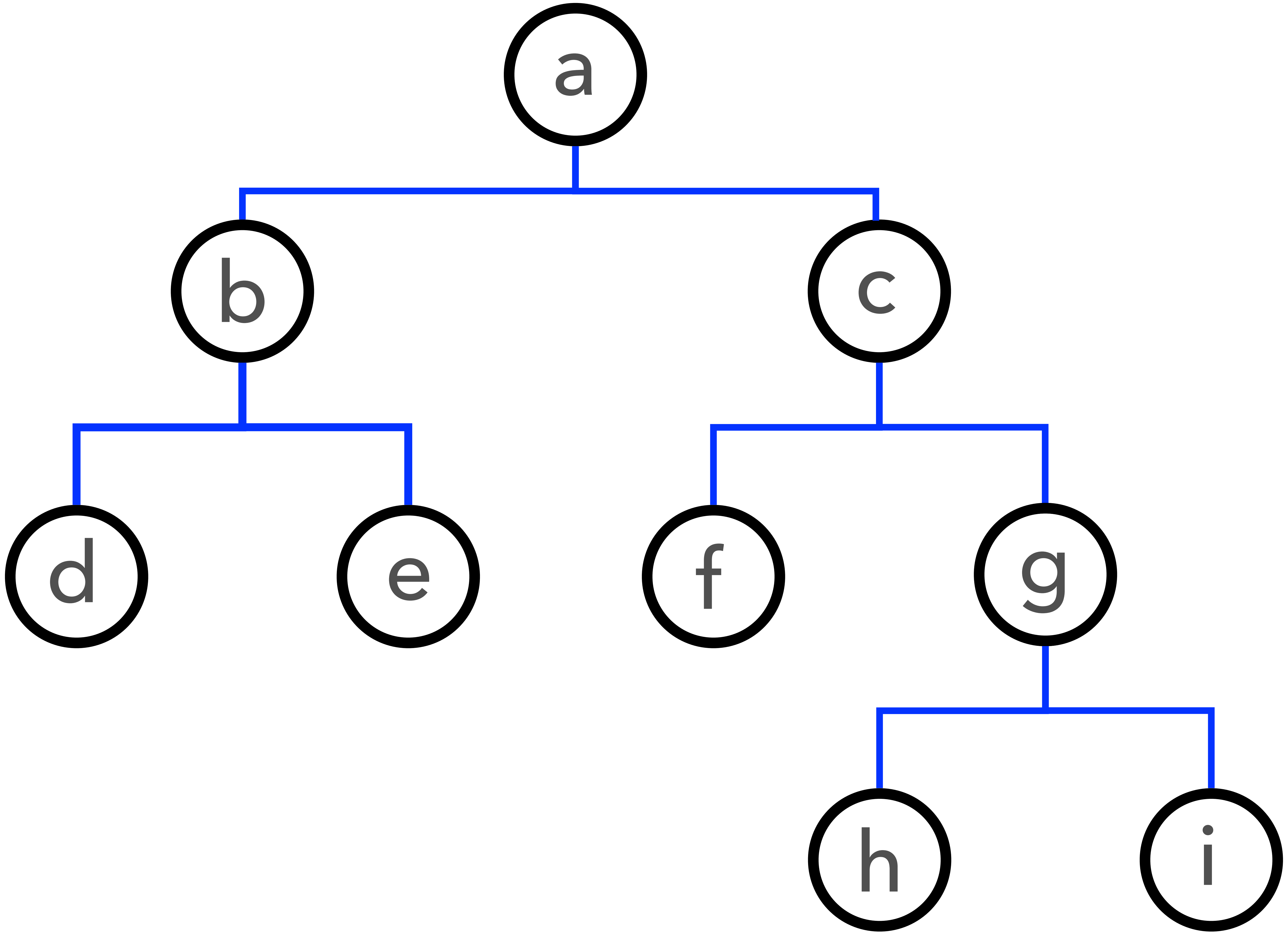
Cost of $C(y, \hat{y})$:

Length of (unique) path from y to $\hat{y}$

C(turtles, snakes) = 1
C(bacteria, mammals) = 14 ...

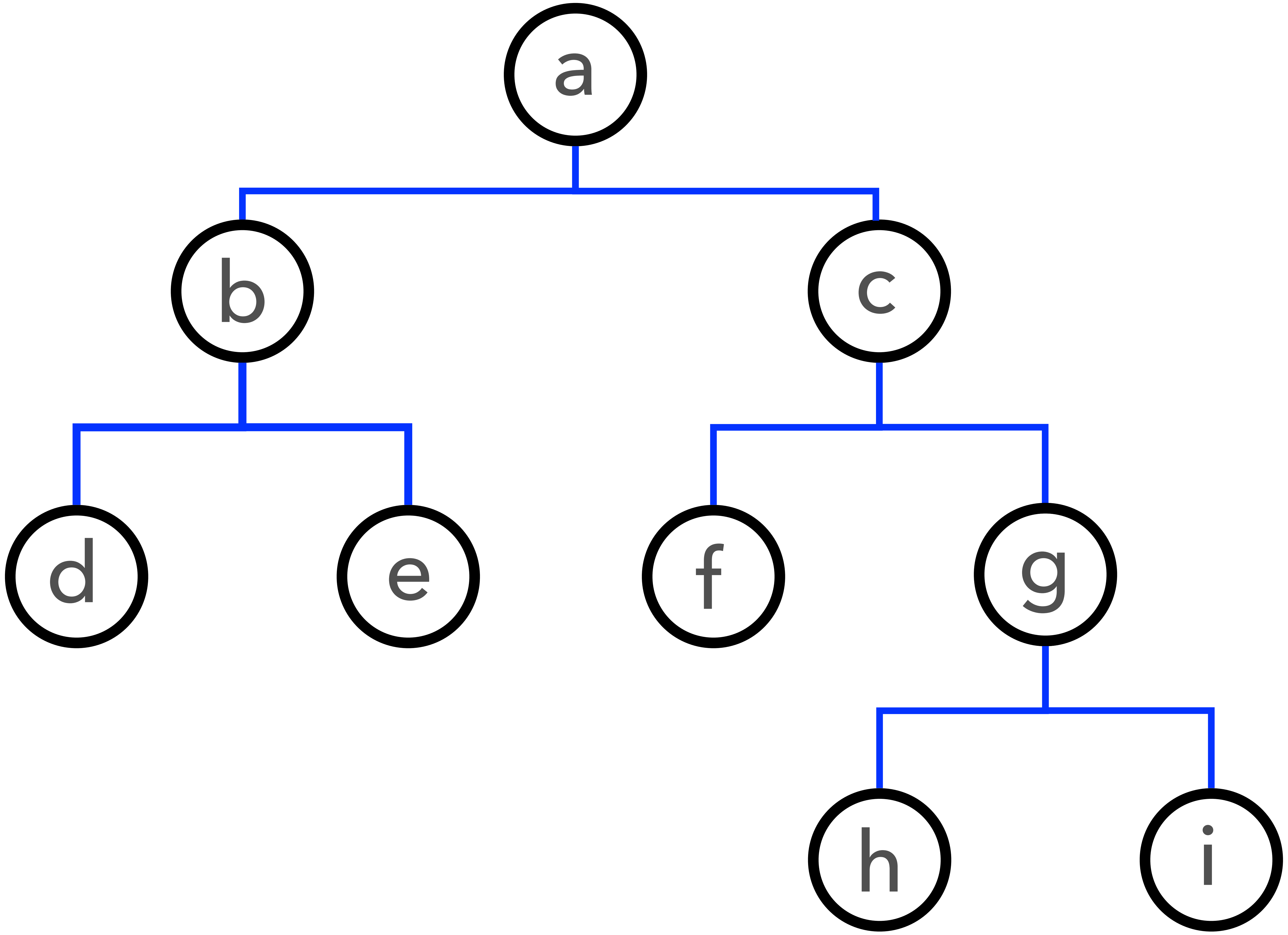


Hierarchical Cost*



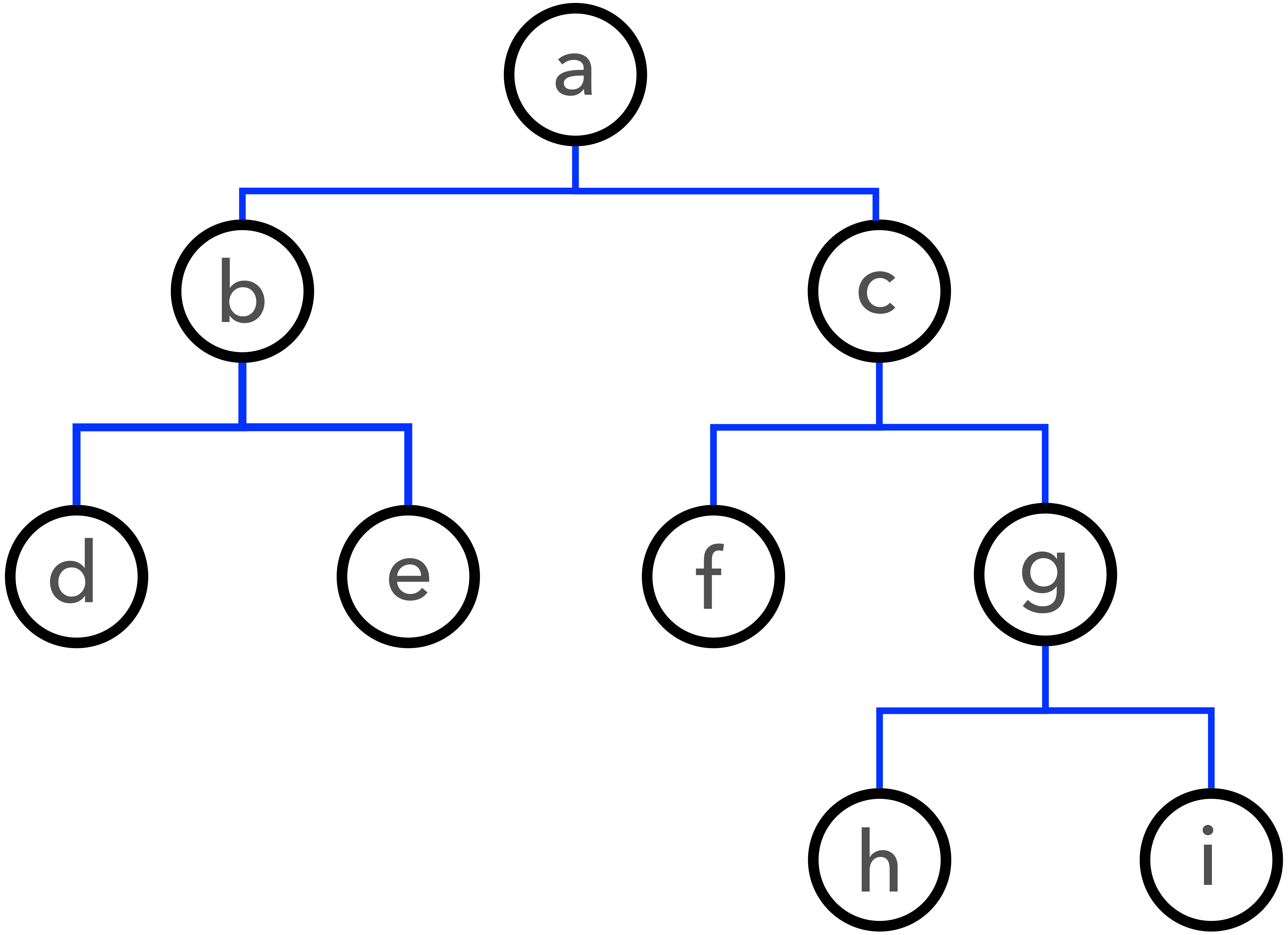
Hierarchical Cost*

$C(a,e) = ?$



Hierarchical Cost*

C(a,e) = 2



Hierarchical Cost*

C(a,e) = 2

C(b,h) = 4