

# Structured Prediction with Projection Oracles

Mathieu Blondel

NTT, Kyoto, Japan

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# Outline

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1. Background

2. Proposed framework

3. Experiments

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# Structured prediction

## Goal

Learn a mapping from **input** space to **output** space

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Typically assume  $f = \text{dec} \circ g$

$$x \in \mathcal{X} \xrightarrow[\text{model}]{g} \theta \in \Theta = \mathbb{R}^d \xrightarrow[\text{decoding}]{\text{dec}} \hat{y} \in \mathcal{Y}$$

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Non-convex, discontinuous!

# Surrogate losses

Surrogate loss risk

$$\mathcal{S}(g) \triangleq \mathbb{E}_{(X,Y) \sim p} S(g(X), Y) \quad S: \Theta \times \mathcal{Y} \rightarrow \mathbb{R}_+$$

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## Fisher consistency

$$\mathcal{S}(g_n) \rightarrow \inf_{g \in \mathcal{G}} \mathcal{S}(g) \longrightarrow \mathcal{L}(dec \circ g_n) \rightarrow \inf_{g \in \mathcal{G}} \mathcal{L}(dec \circ g)$$

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Extensively studied in the **multiclass** setting [Zhang 2004, Bartlett et al. 2006]

Only recently studied in the **structured** setting

[Ciliberto et al 2016,  
Osokin et al. 2017,  
Nowak-Vila et al. 2019]

# Structured perceptron loss

[Collins, 2002]

Loss

$$S(\theta, y) \triangleq \max_{y' \in \mathcal{Y}} \langle \theta, \varphi(y') \rangle - \langle \theta, \varphi(y) \rangle$$

$$\varphi: \mathcal{Y} \rightarrow \mathbb{R}^d$$

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[Tsochantaridis et al., 2005]

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# Conditional Random Field (CRF) loss

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$$p(y; \theta) \propto \exp\langle \varphi(y), \theta \rangle$$

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✗ Marginal inference is intractable for some tasks

# Squared loss

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None!

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- ✓ Smooth
- ✓ Consistent (when using calibrated decoding)
- ✗ Ignores structural information at training time

# Summary

Loss	Training oracle	Decoding	Smooth	Consistent
Perceptron	MAP	MAP	No	No
SVM	Loss-augmented MAP	MAP	No	No
CRF	Marginal	MAP Calibrated decoding	Yes	No Yes
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<b>Proposed</b>	<b>Projection</b>	<b>Calibrated decoding</b>	<b>Yes</b>	<b>Yes</b>

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# Proposed inference pipeline

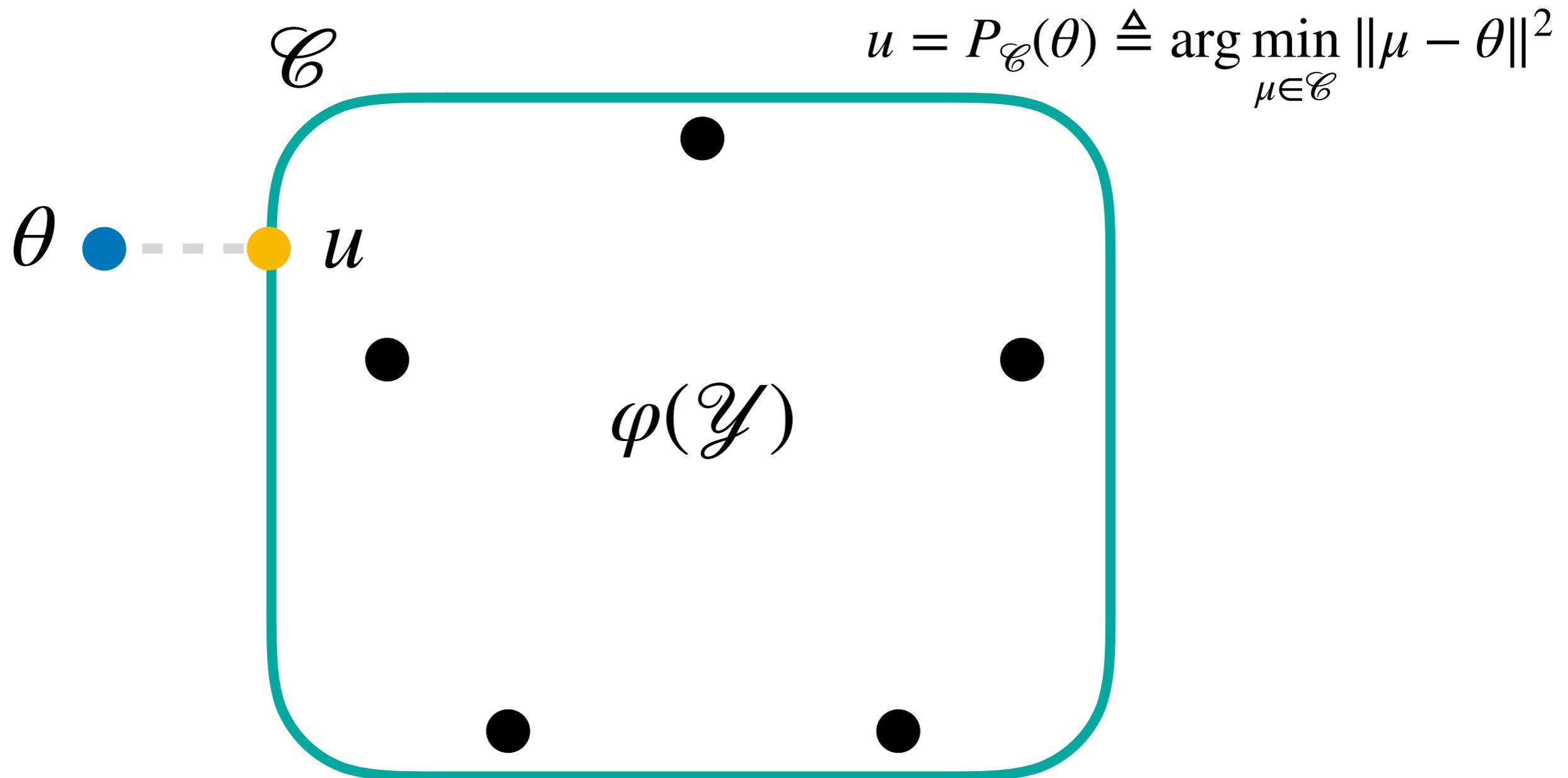
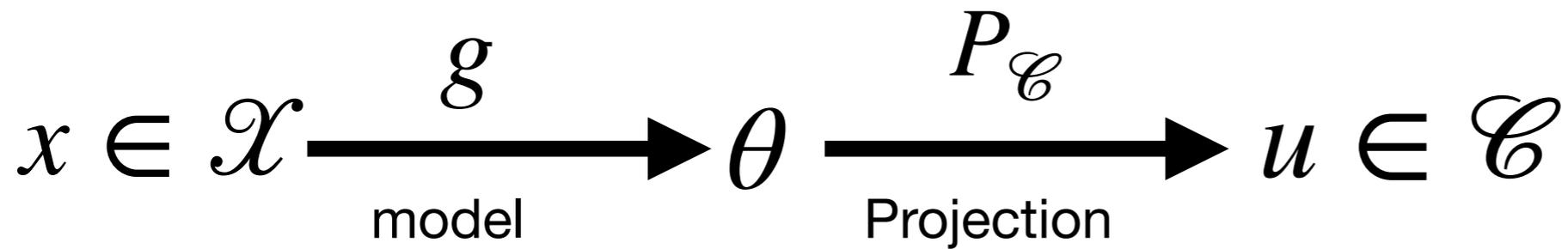
$$x \in \mathcal{X} \xrightarrow[\text{model}]{g} \theta$$

$\theta$  ●

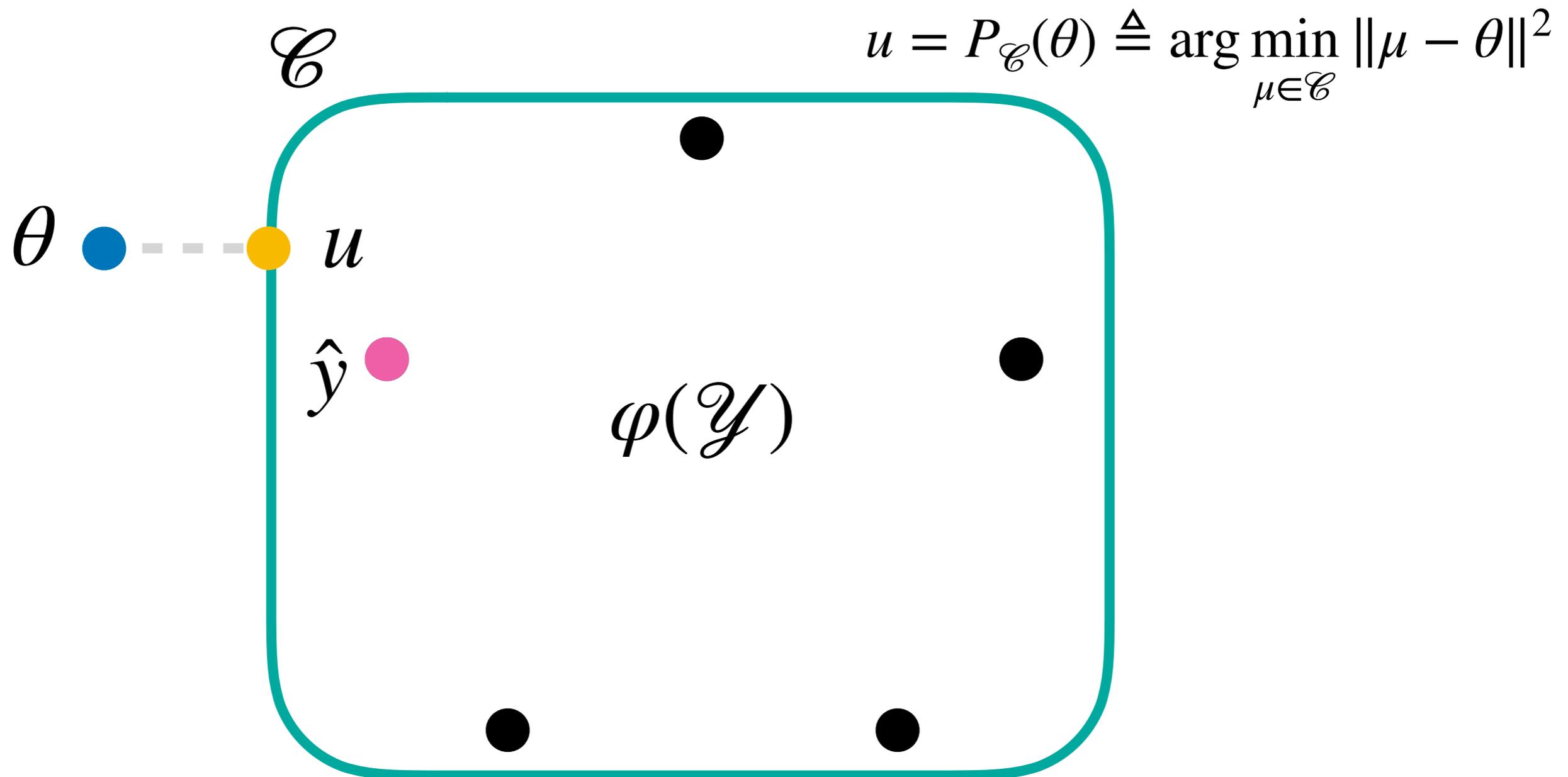
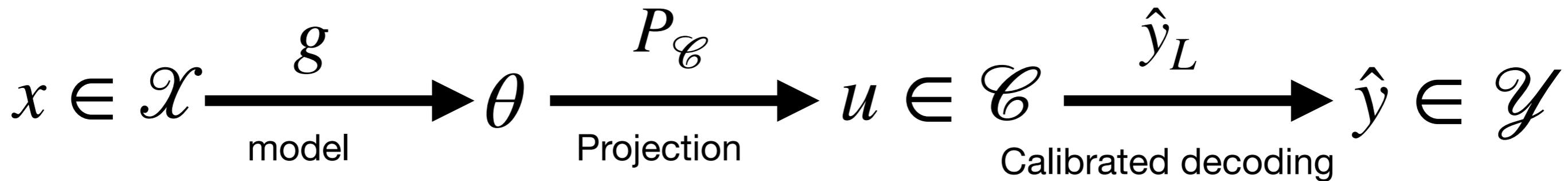
●  
 $\varphi(\mathcal{Y})$   
●



# Proposed inference pipeline

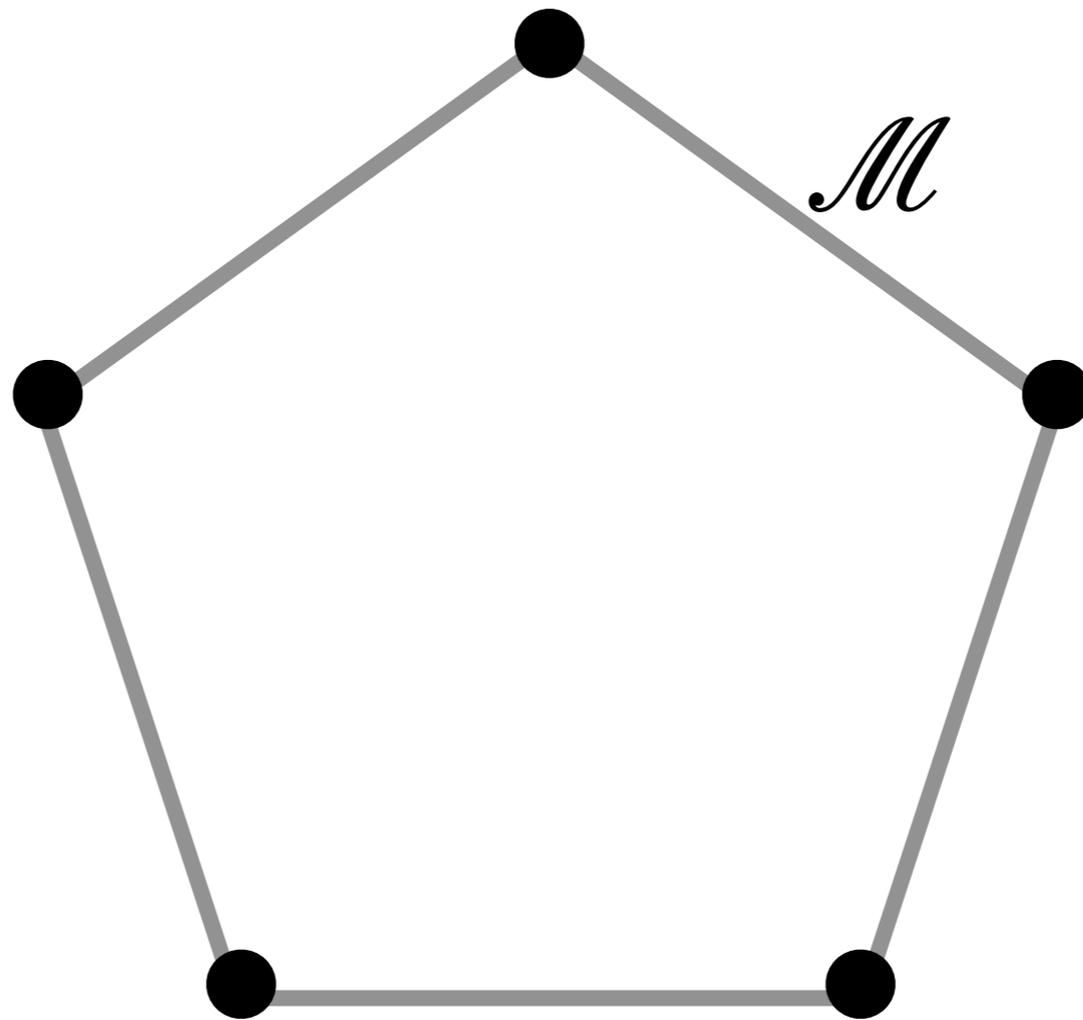


# Proposed inference pipeline



# Choice of the convex set

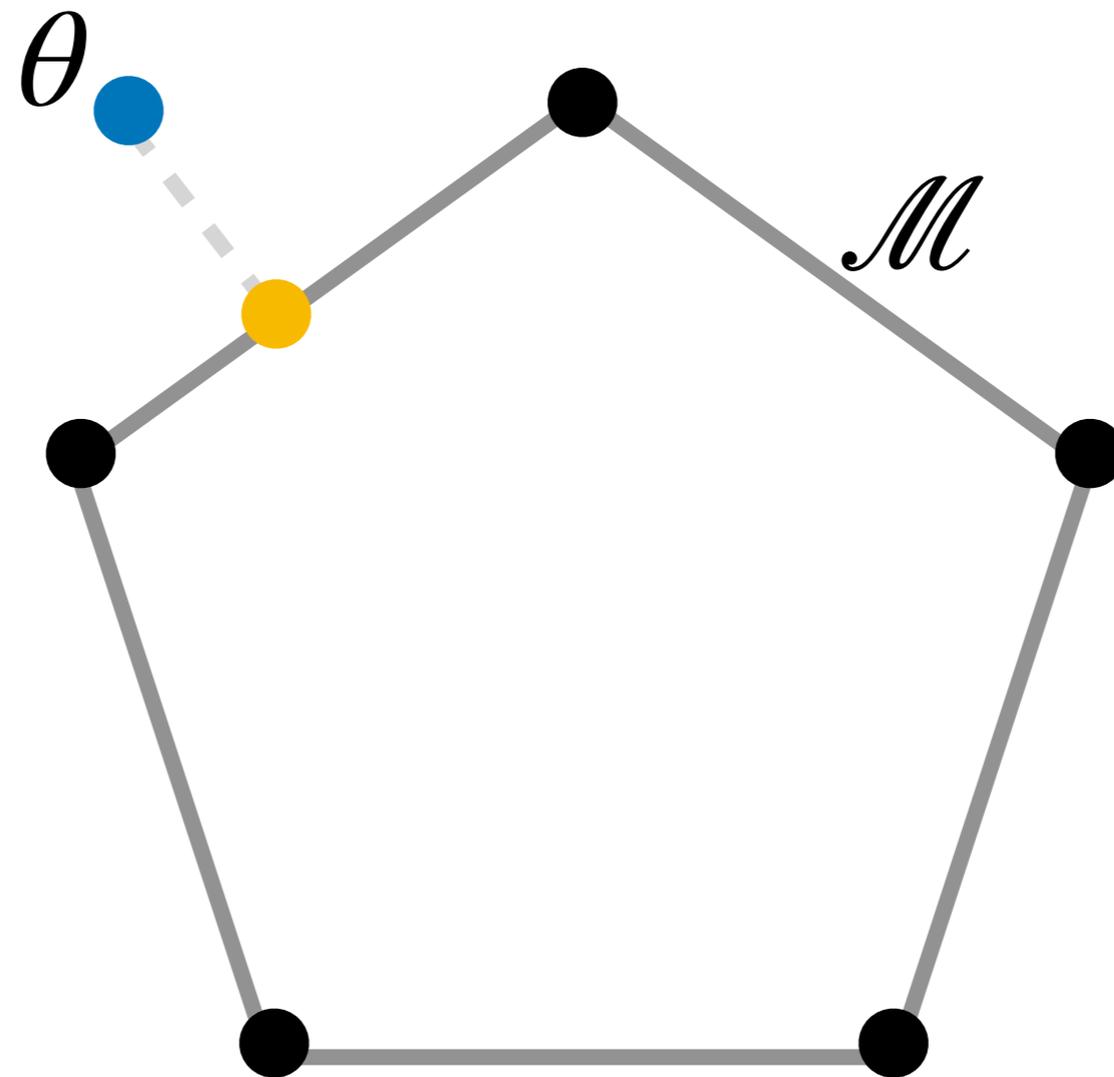
Smallest convex set = **convex hull** (a.k.a. marginal polytope)



$$\mathcal{M} \triangleq \text{conv}(\varphi(\mathcal{Y}))$$

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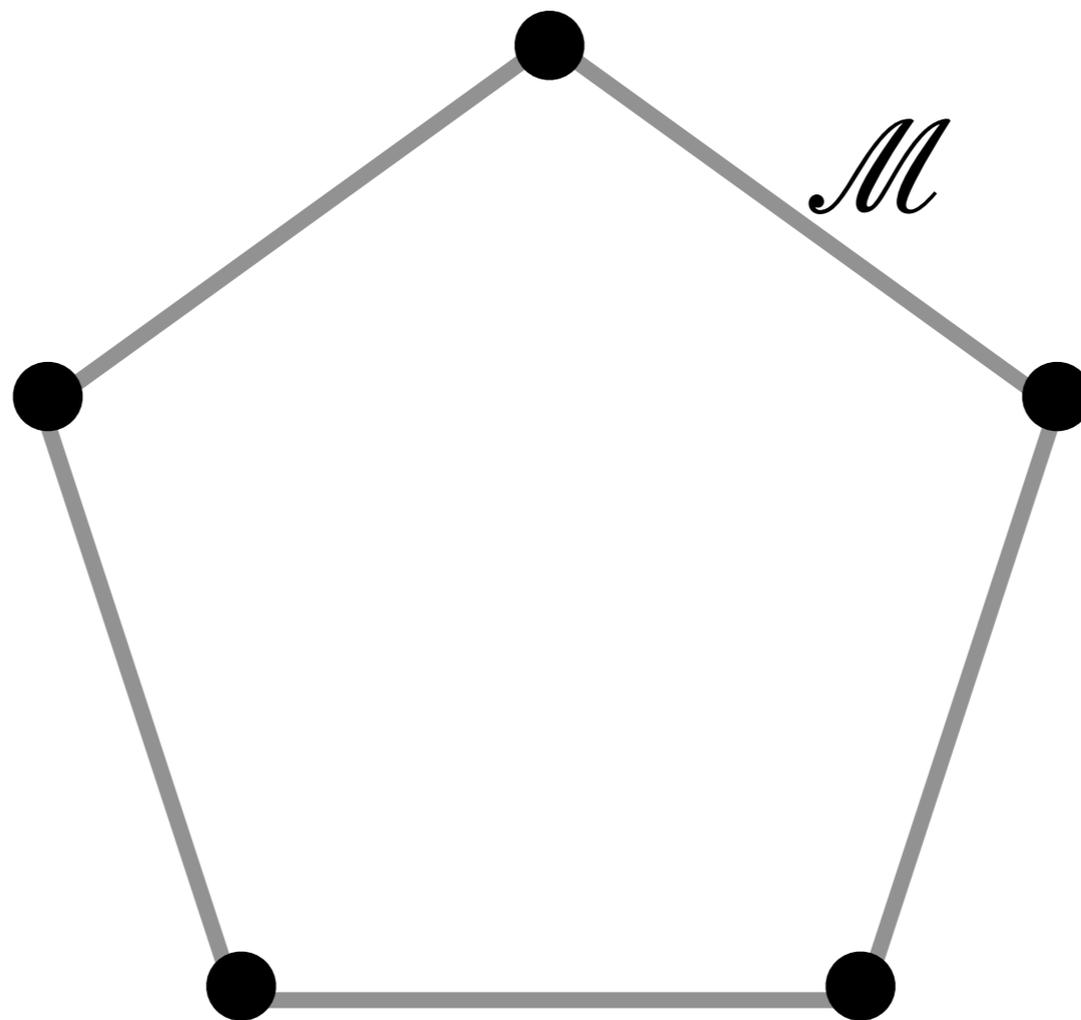
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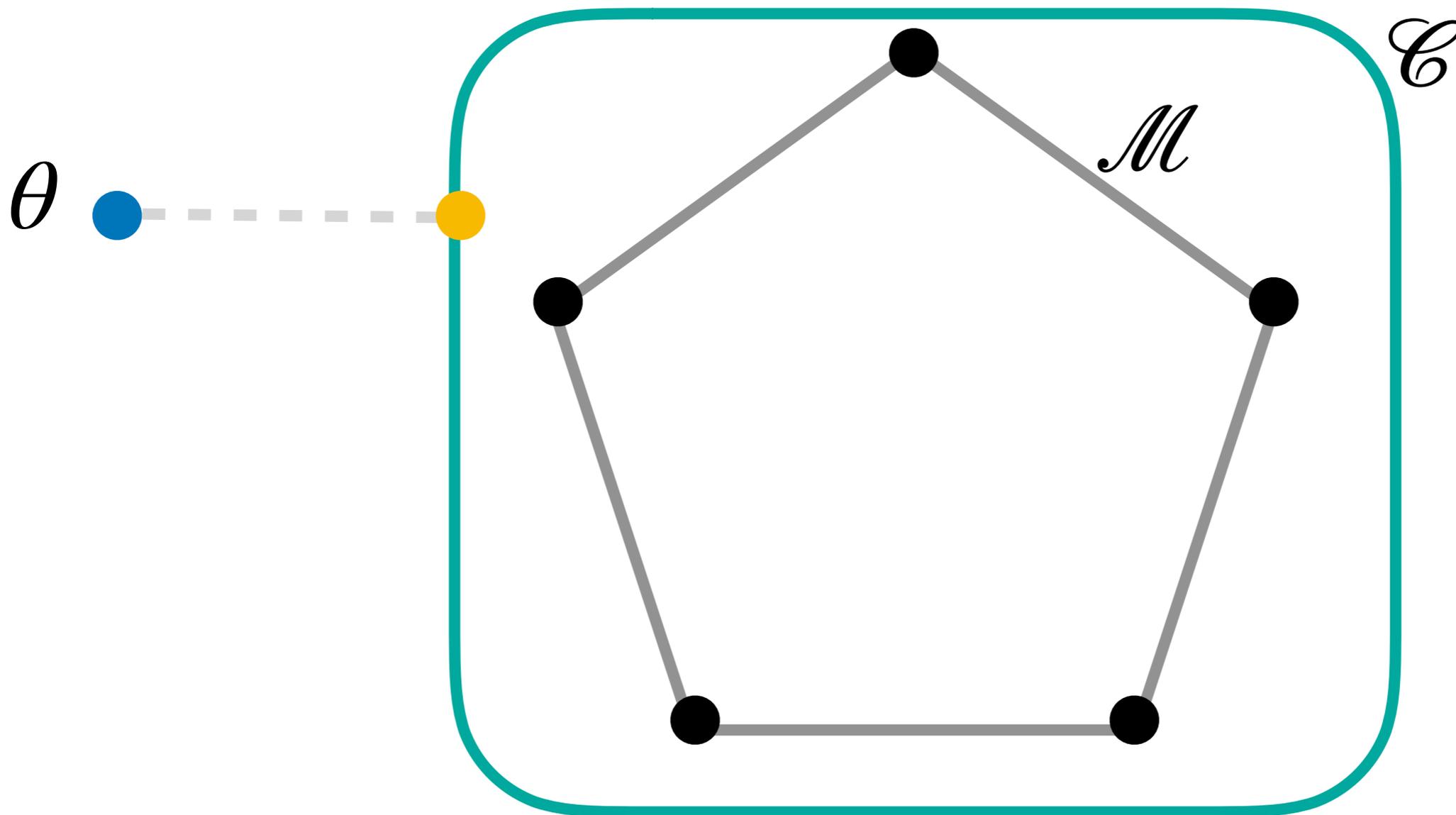


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Can use any **superset** with cheaper to compute projection



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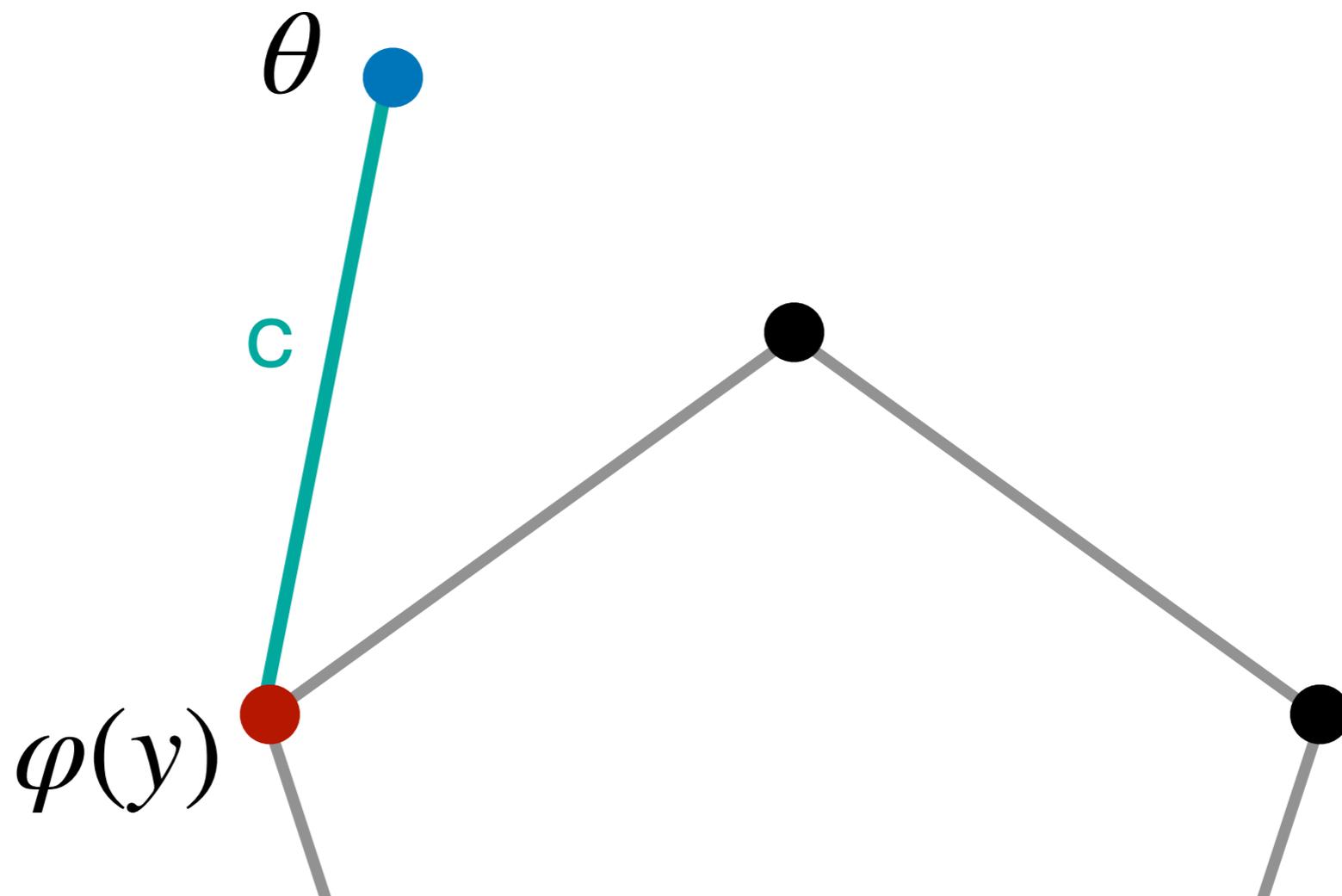
# Associated loss function

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**Squared loss**

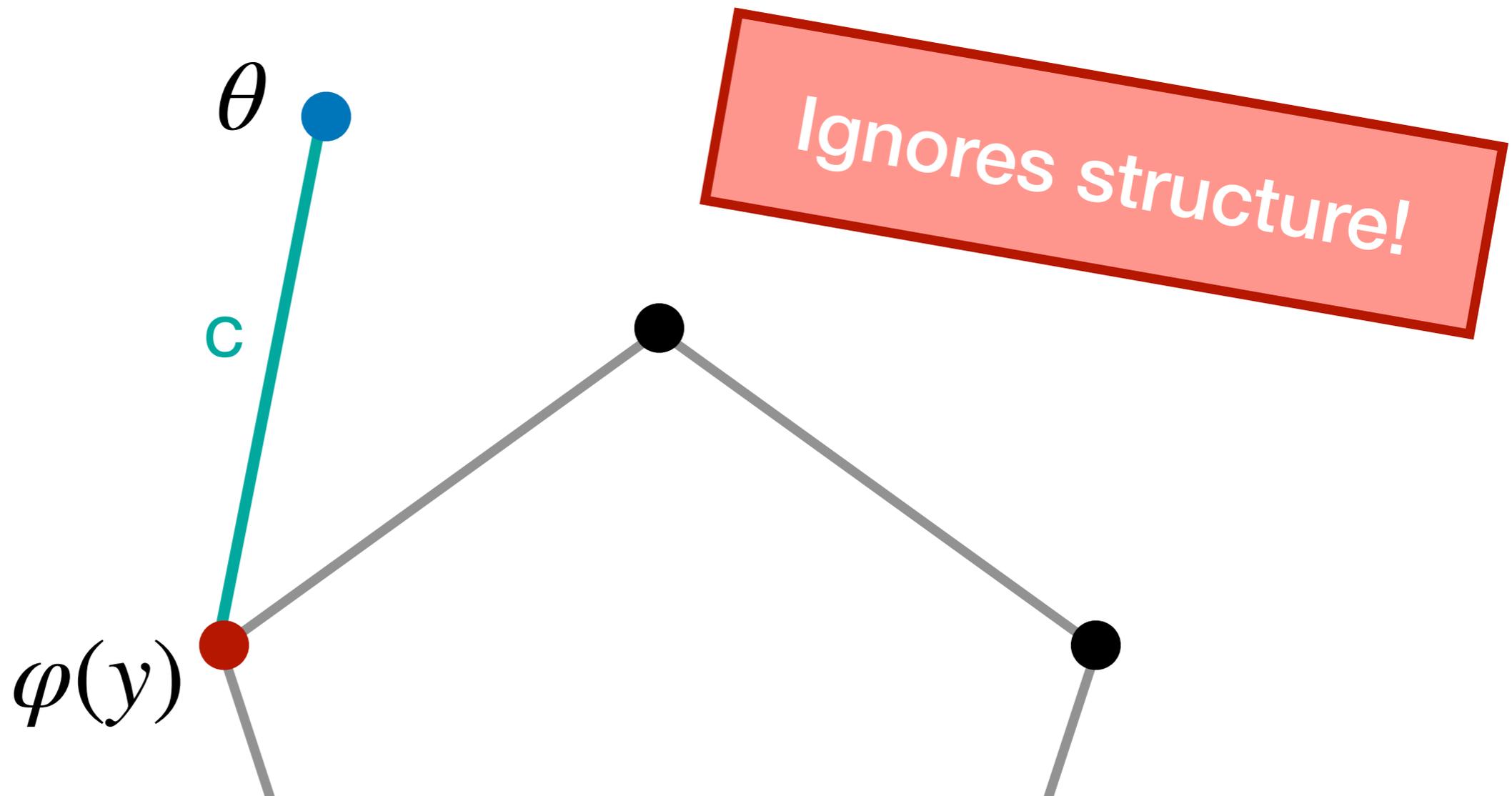
$$SQ(\theta, y) \triangleq \frac{1}{2} \|\varphi(y) - \theta\|^2 = c$$



# Associated loss function

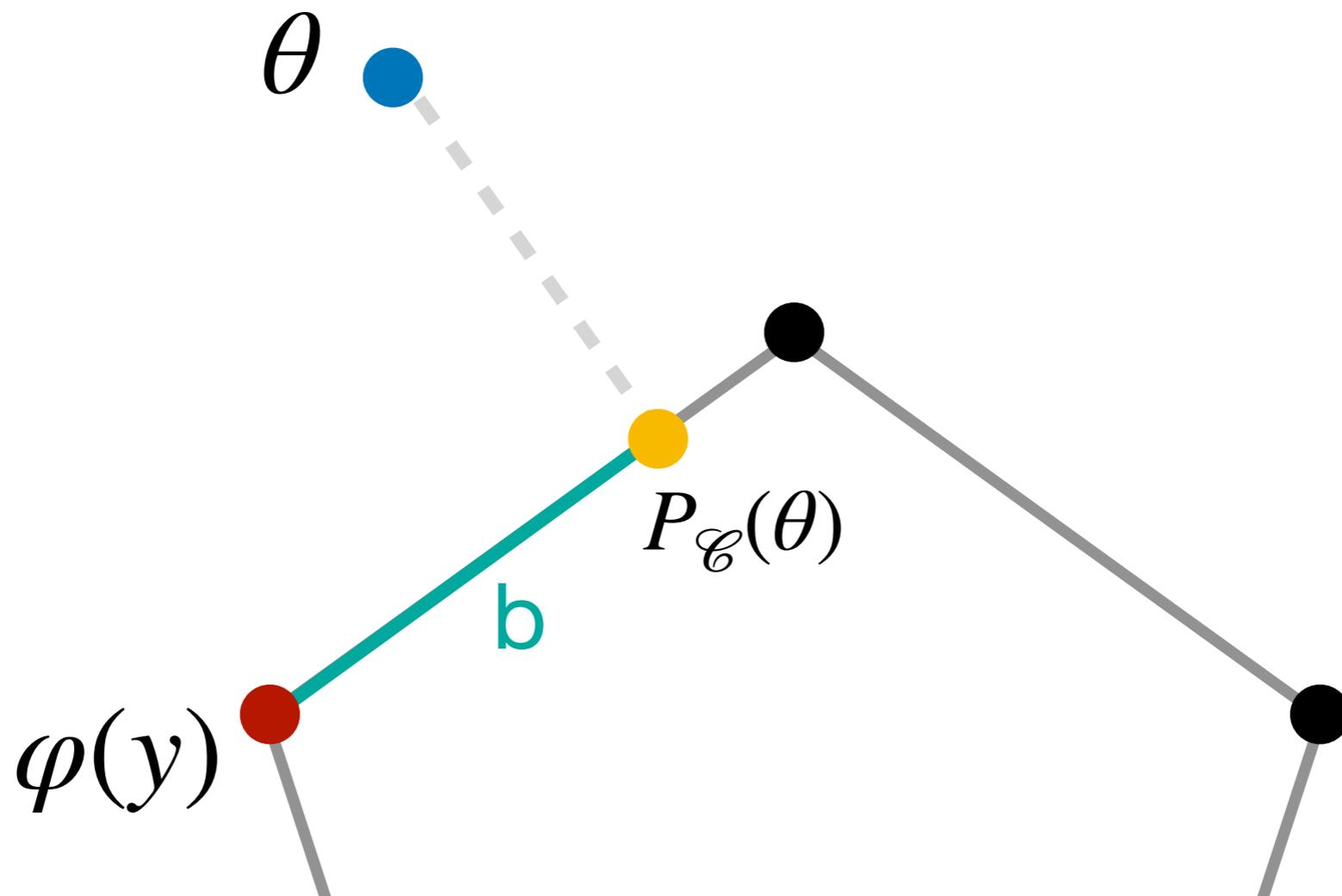
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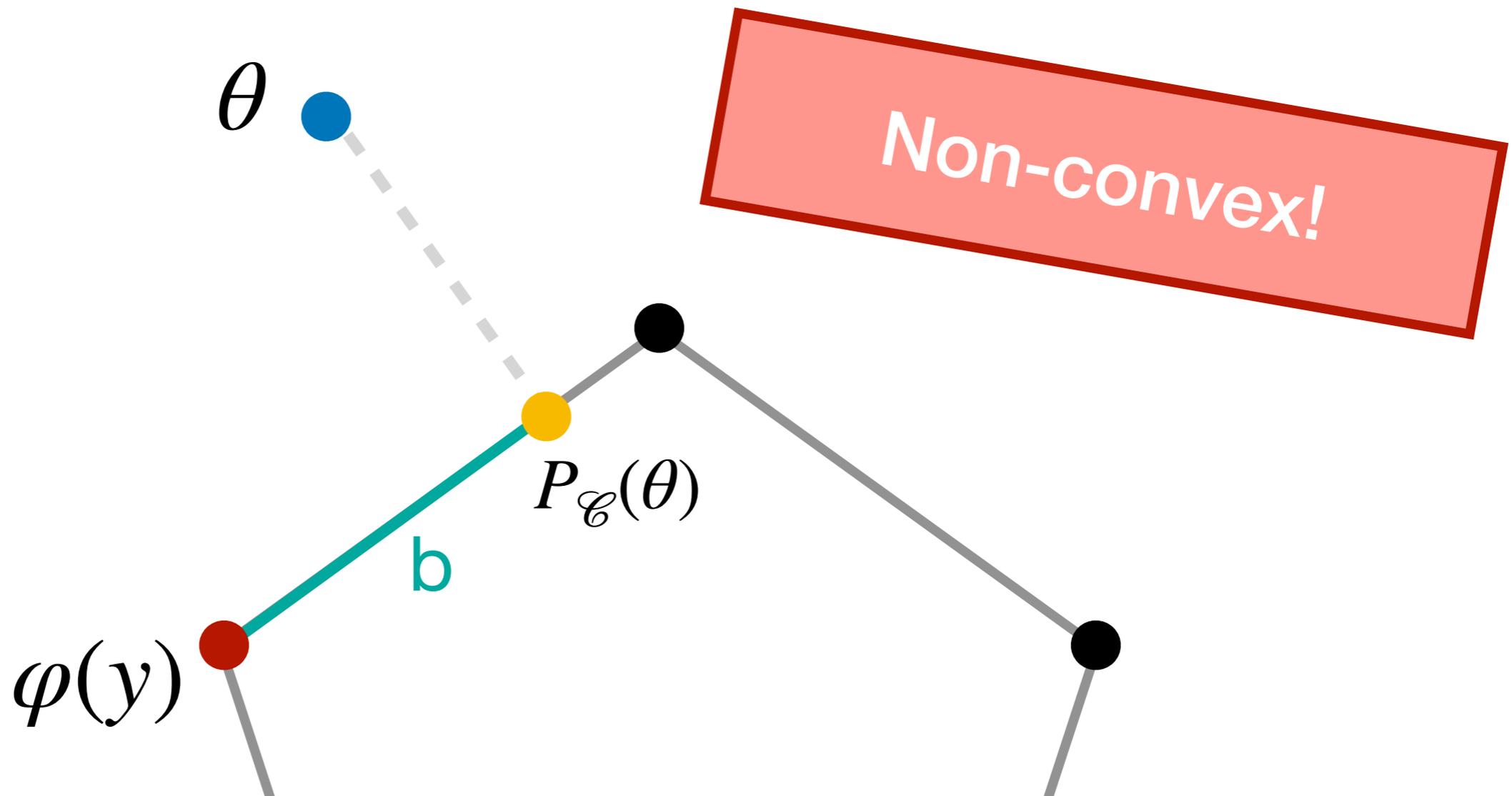
# Associated loss function

$$NC_{\mathcal{C}}(\theta, y) \triangleq \frac{1}{2} \|\varphi(y) - P_{\mathcal{C}}(\theta)\|^2 = b$$



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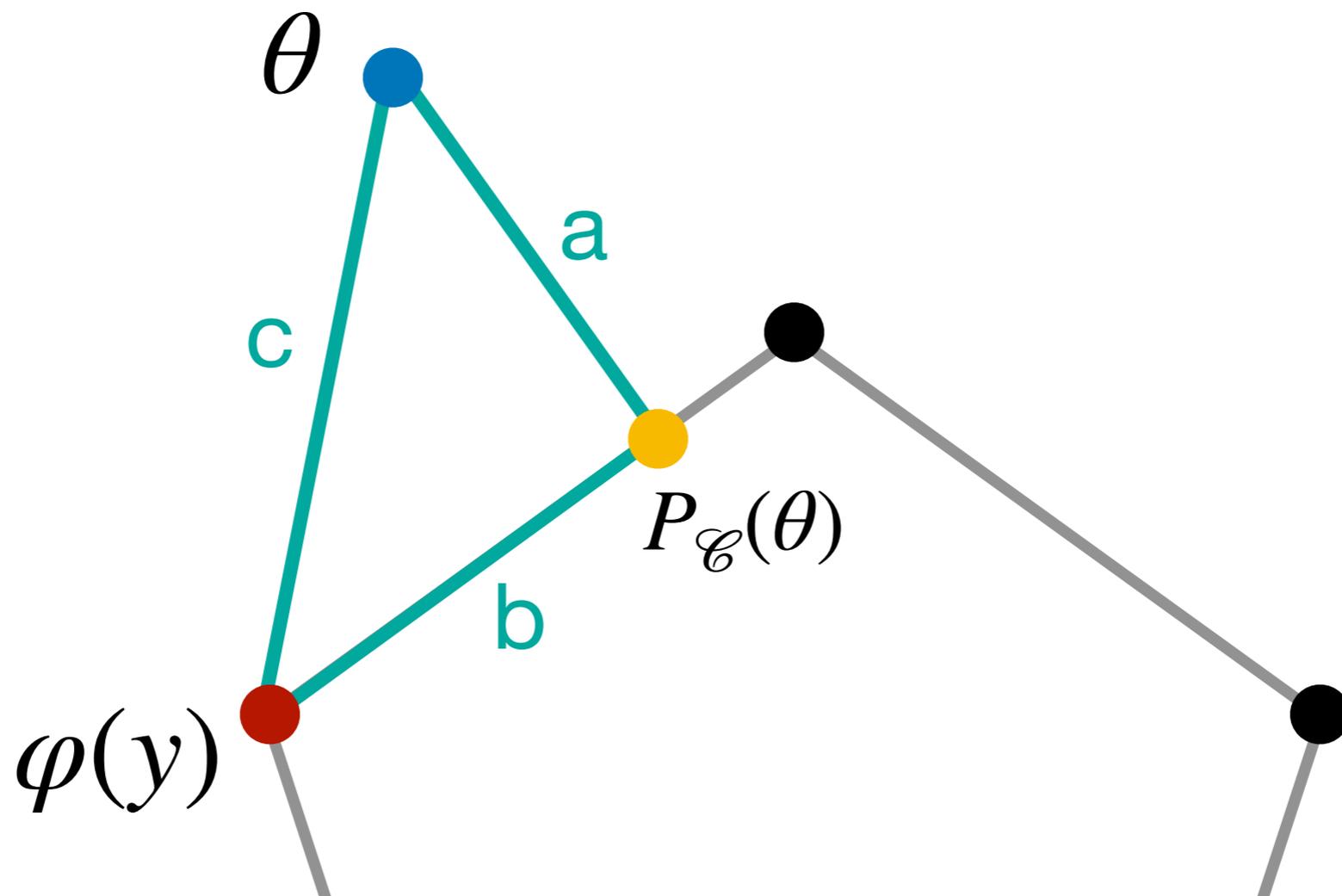
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# Associated loss function

Proposed loss

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# Associated loss function

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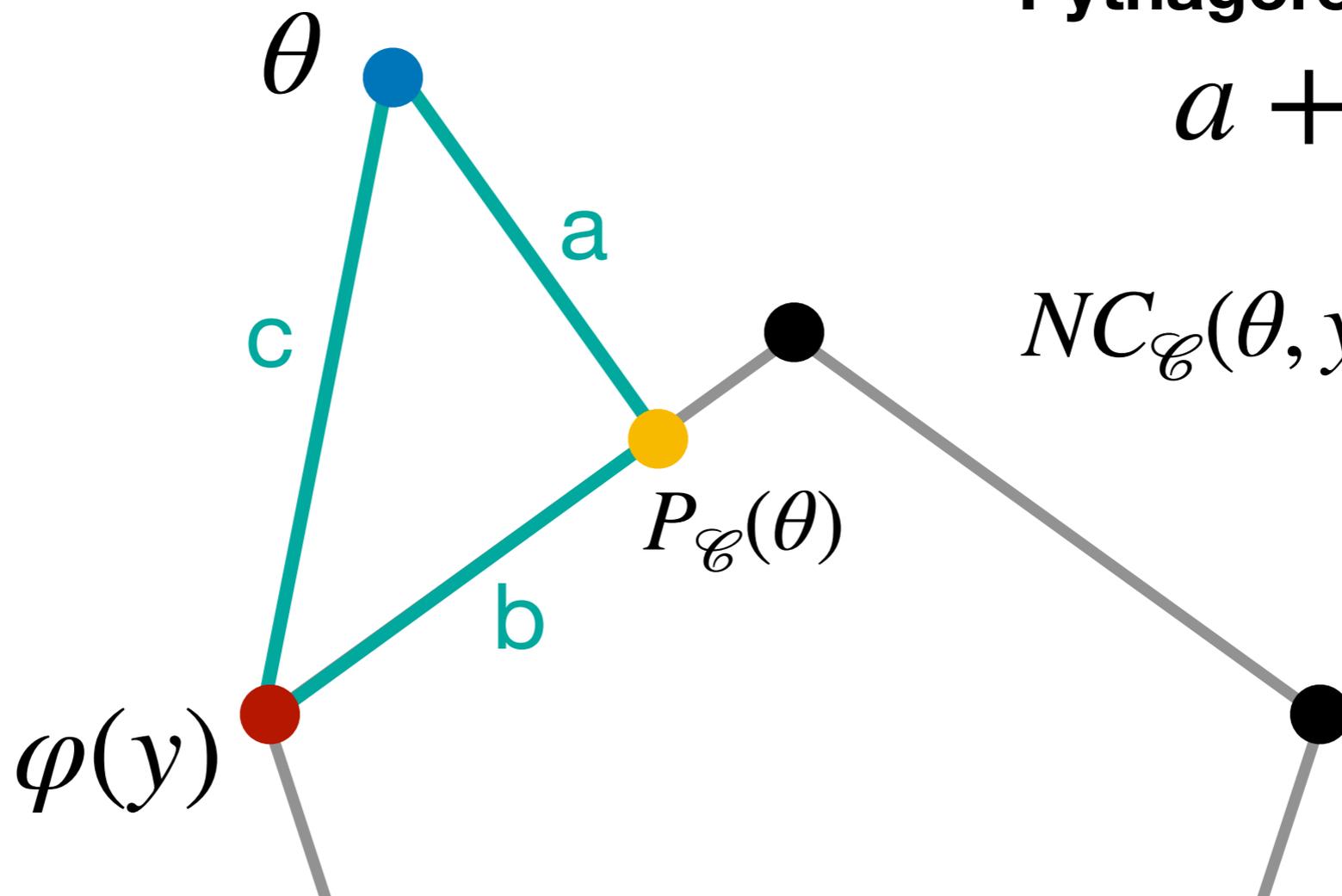
$$S_{\mathcal{C}}(\theta, y) \triangleq SQ(\theta, y) - \frac{1}{2} \|\theta - P_{\mathcal{C}}(\theta)\|^2 = c - a$$

Generalized  
Pythagorean theorem

$$a + b \leq c$$



$$NC_{\mathcal{C}}(\theta, y) \leq S_{\mathcal{C}}(\theta, y)$$



# Properties

1.  $S_{\mathcal{C}}(\theta, y)$  is convex w.r.t.  $\theta$
2.  $S_{\mathcal{C}}(\theta, y)$  is smooth w.r.t.  $\theta$  (gradient is Lipschitz cont.)
3.  $S_{\mathcal{C}}(\theta, y) \geq 0$
4.  $S_{\mathcal{C}}(\theta, y) = 0 \Leftrightarrow P_{\mathcal{C}}(\theta) = \varphi(y)$

# Upper bounds

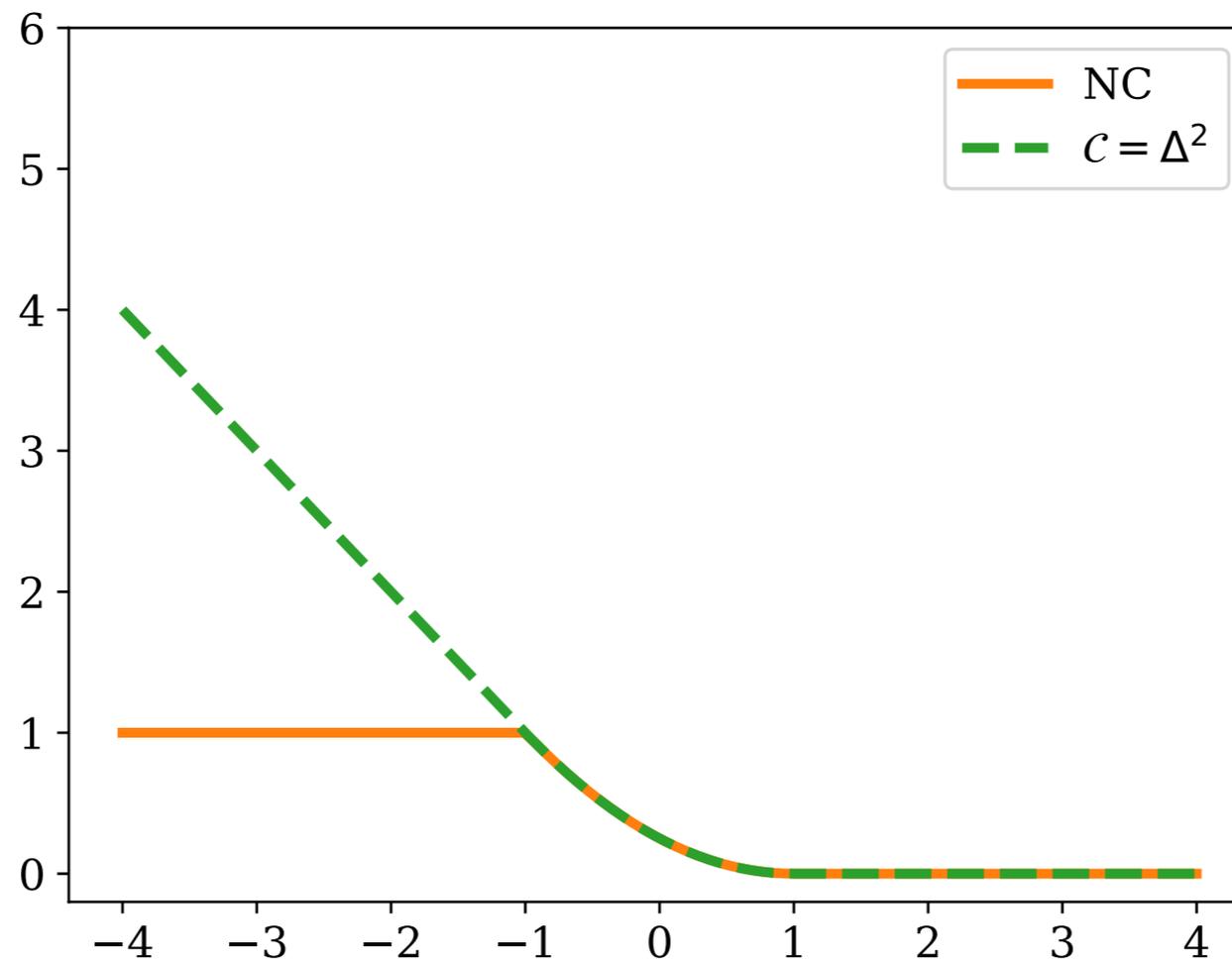
Convex upper bound

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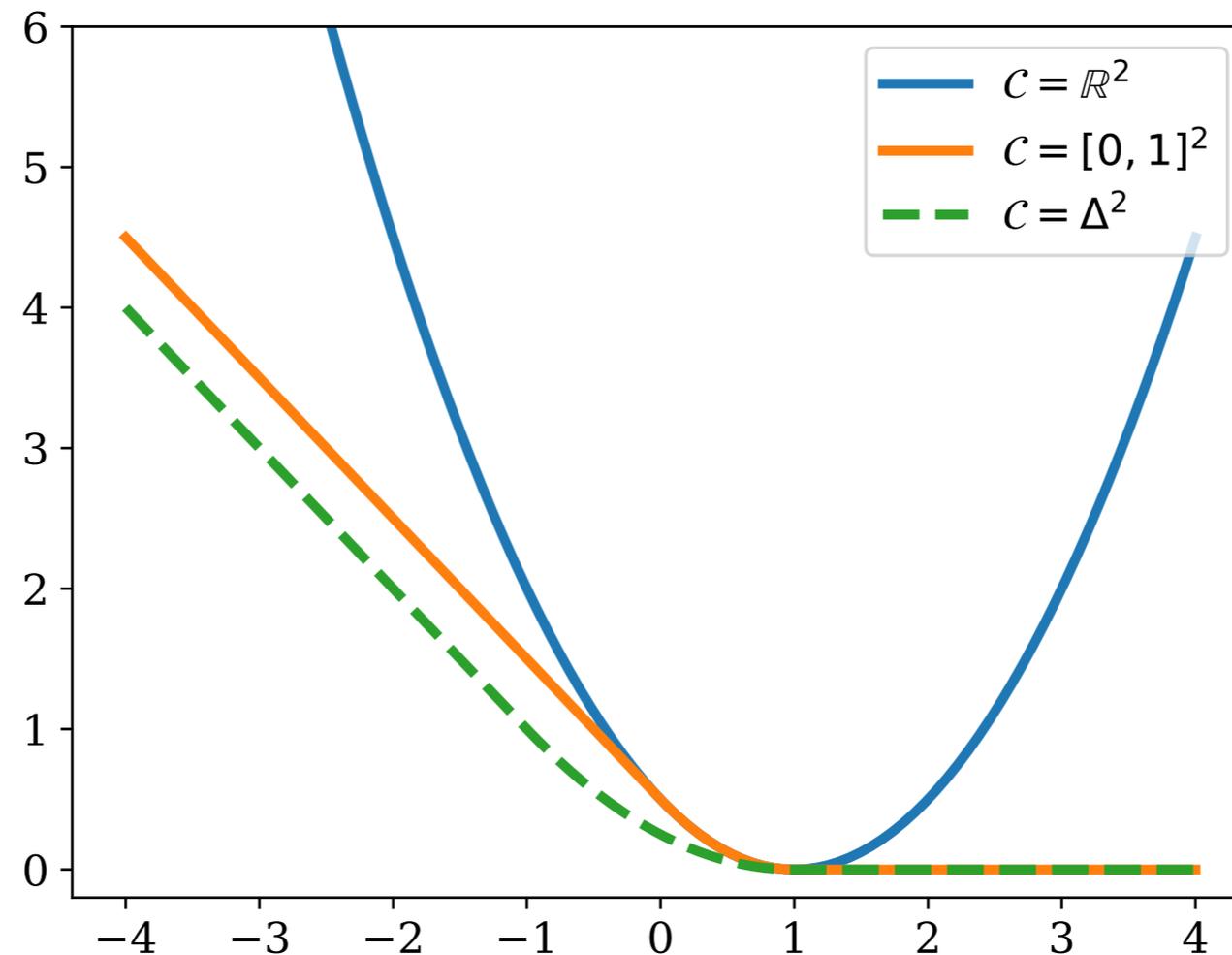
Superset upper bound

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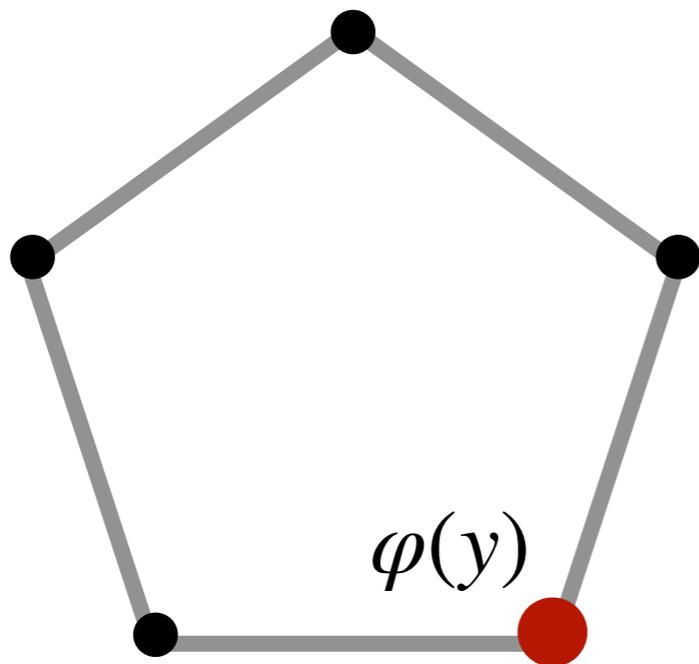
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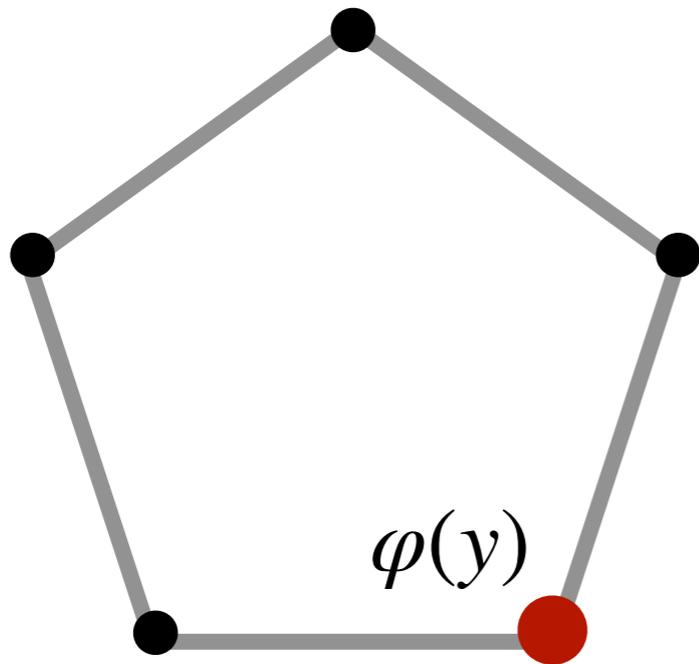
primal space  
 $\text{dom}(\Omega) = \mathcal{C}$



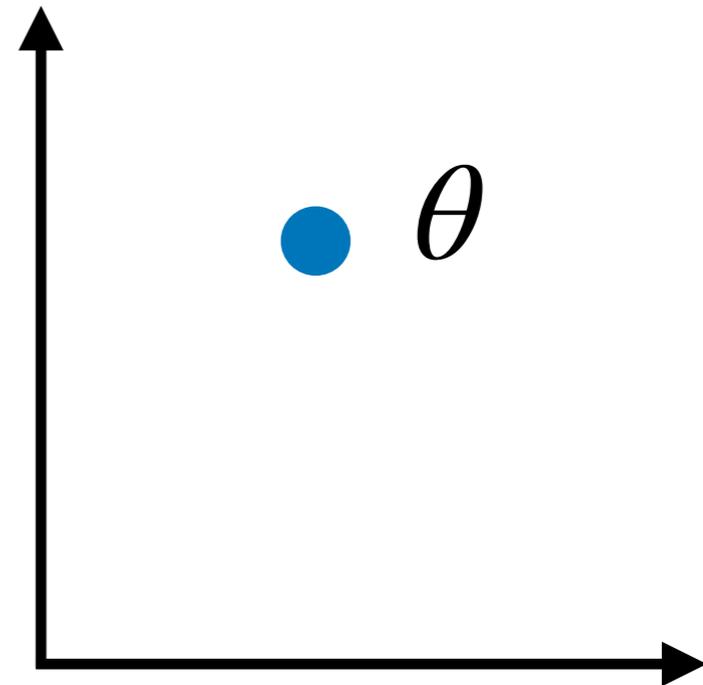
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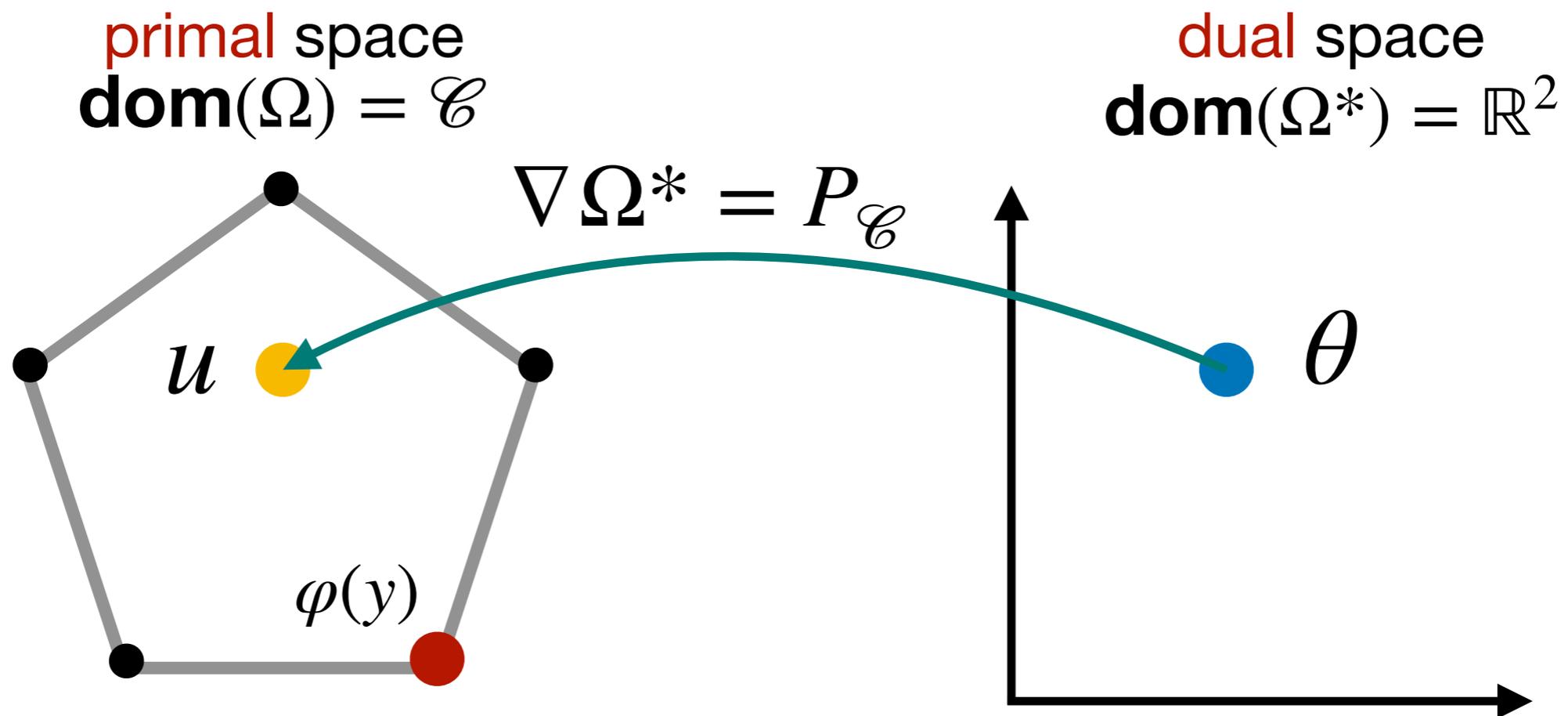


dual space  
 $\text{dom}(\Omega^*) = \mathbb{R}^2$



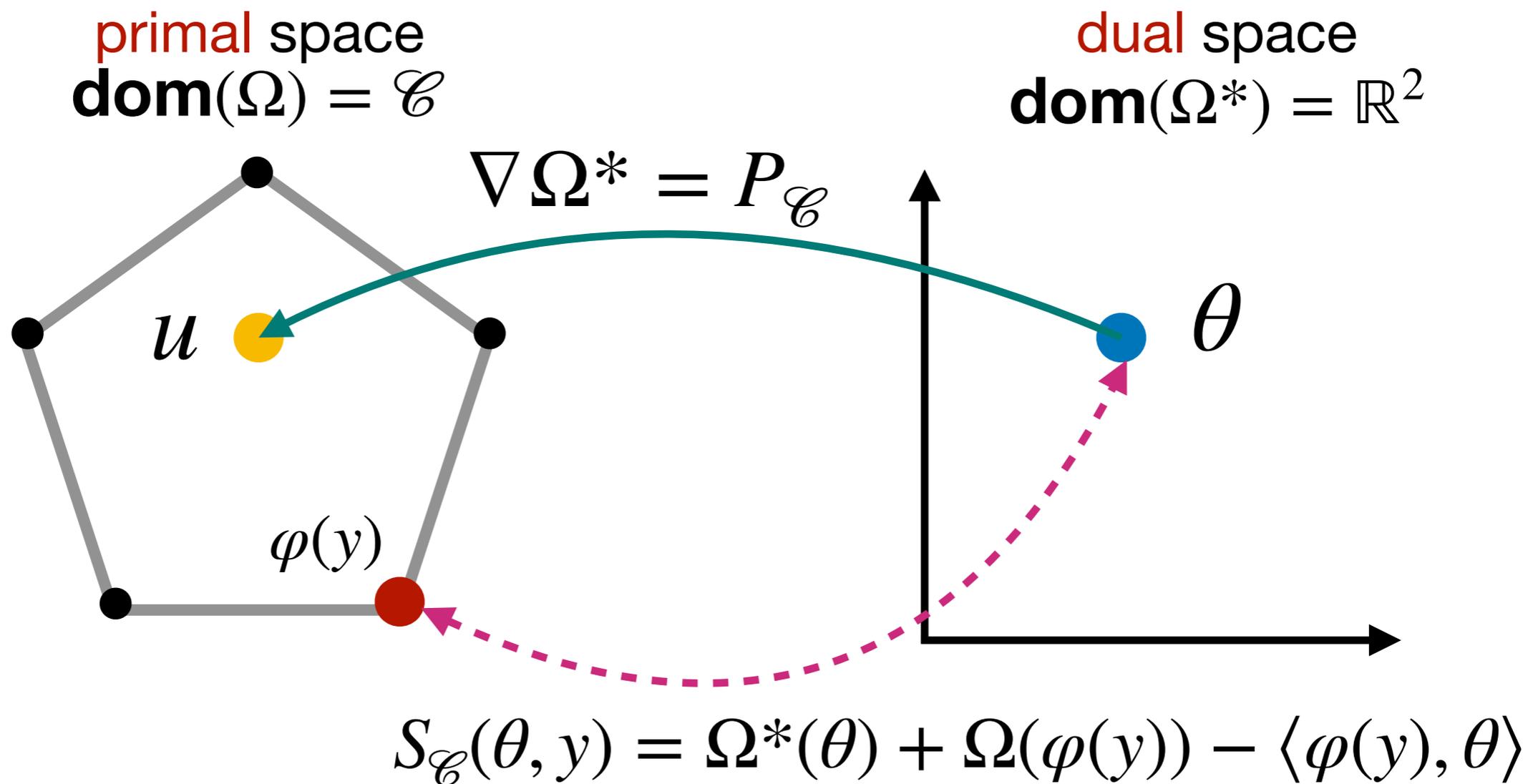
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## Proposition

Let  $\beta = \max_{u \in \mathcal{C}} \|u\|_1$ . Then,

$S_{\mathcal{C}}(\theta, y)$  is  $\beta$ -smooth with respect to  $\|\cdot\|_{\infty}$ .

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Smaller set  $\rightarrow$  smoother loss!

# Calibrated decoding

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Affine decomposition of the target loss

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Decomposition important both for **computational tractability**  
and **theoretical analysis**

# Consistency

## Excess risks

$$\delta\mathcal{L}(f) \triangleq \mathcal{L}(f) - \inf_{f': \mathcal{X} \rightarrow \mathcal{Y}} \mathcal{L}(f')$$

$$\delta\mathcal{S}_{\mathcal{C}}(g) \triangleq \mathcal{S}_{\mathcal{C}}(g) - \inf_{g': \mathcal{X} \rightarrow \Theta} \mathcal{S}_{\mathcal{C}}(g')$$

# Consistency

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## Calibration between excess risks

$$\forall g: \mathcal{X} \rightarrow \Theta : \frac{\delta\mathcal{L}(dec \circ g)^2}{8\beta\sigma^2} \leq \delta\mathcal{S}_{\mathcal{C}}(g)$$

$$dec \triangleq \hat{y}_L \circ P_{\mathcal{C}}$$

$$\beta \triangleq \text{Lipschitz constant of } P_{\mathcal{C}} \\ \text{w.r.t. } \|\cdot\|$$

$$\sigma \triangleq \sup_{y \in \mathcal{Y}} \|V^{\top} \varphi(y)\|$$

# Probability simplex

Output set

$$\mathcal{Y} = [k] \triangleq \{1, \dots, k\}$$

# Probability simplex

## Output set

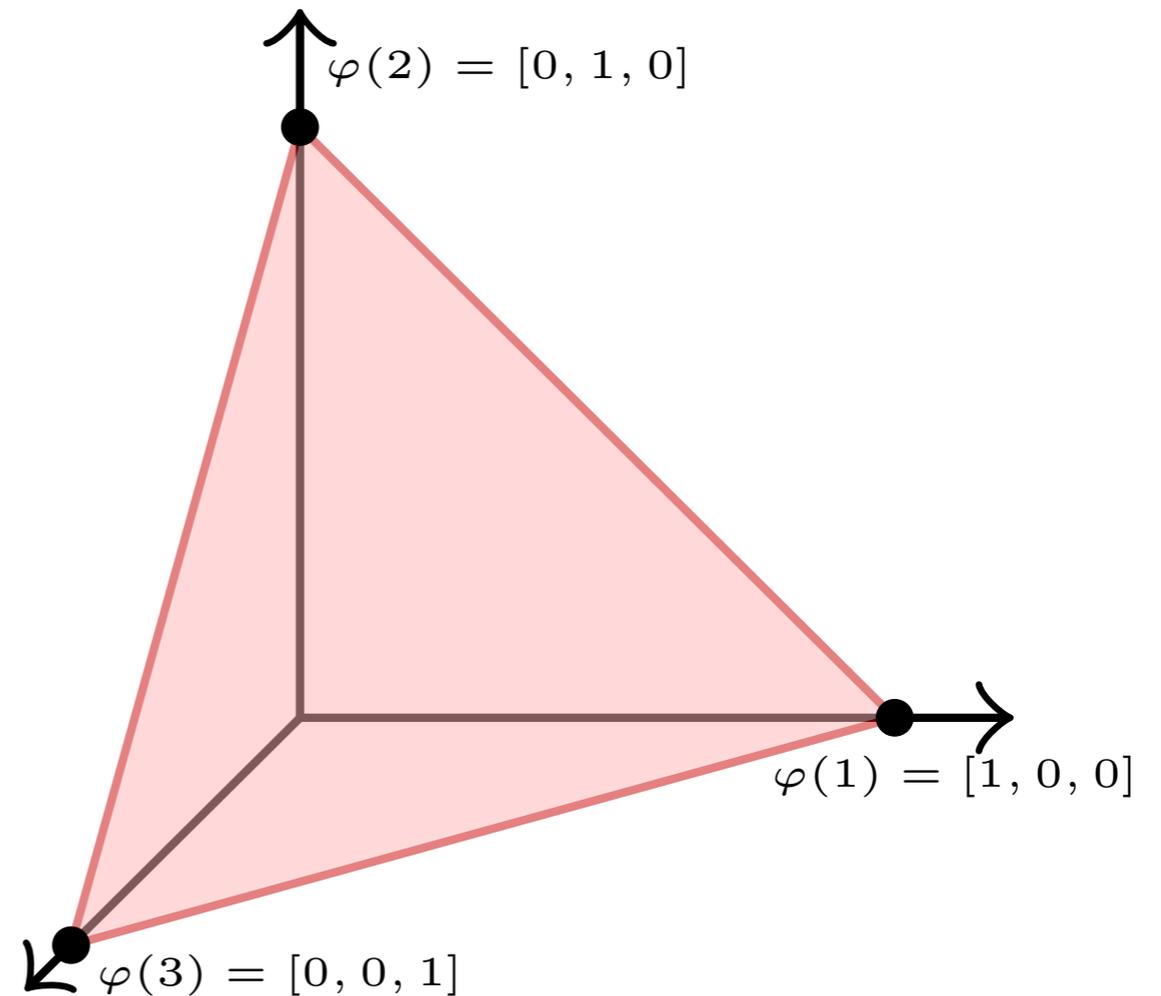
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## Encoding

$$\varphi(y) = e_y$$

## Marginal polytope

$$\mathcal{M} = \text{conv}(\varphi(\mathcal{Y})) = \Delta^k$$



# Probability simplex

## Output set

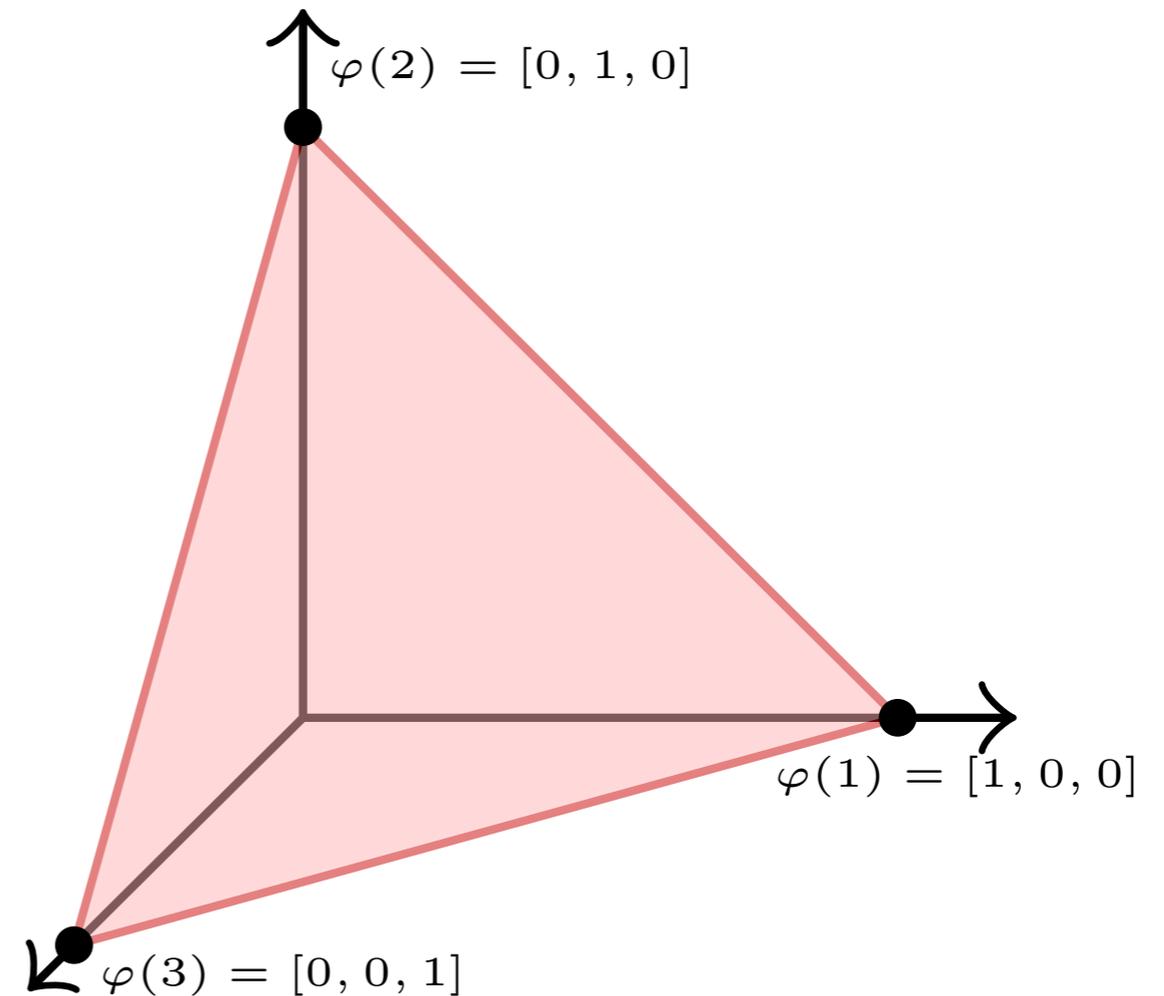
$$\mathcal{Y} = [k] \triangleq \{1, \dots, k\}$$

## Encoding

$$\varphi(y) = e_y$$

## Marginal polytope

$$\mathcal{M} = \text{conv}(\varphi(\mathcal{Y})) = \triangle^k$$



## Oracles

MAP:  $O(k)$

Euclidean: sparsemax,  $O(k)$  or  $O(k \log k)$

KL: softmax,  $O(k)$

# Unit cube

Output set

$$\mathcal{Y} = 2^{[k]}$$

# Unit cube

Output set

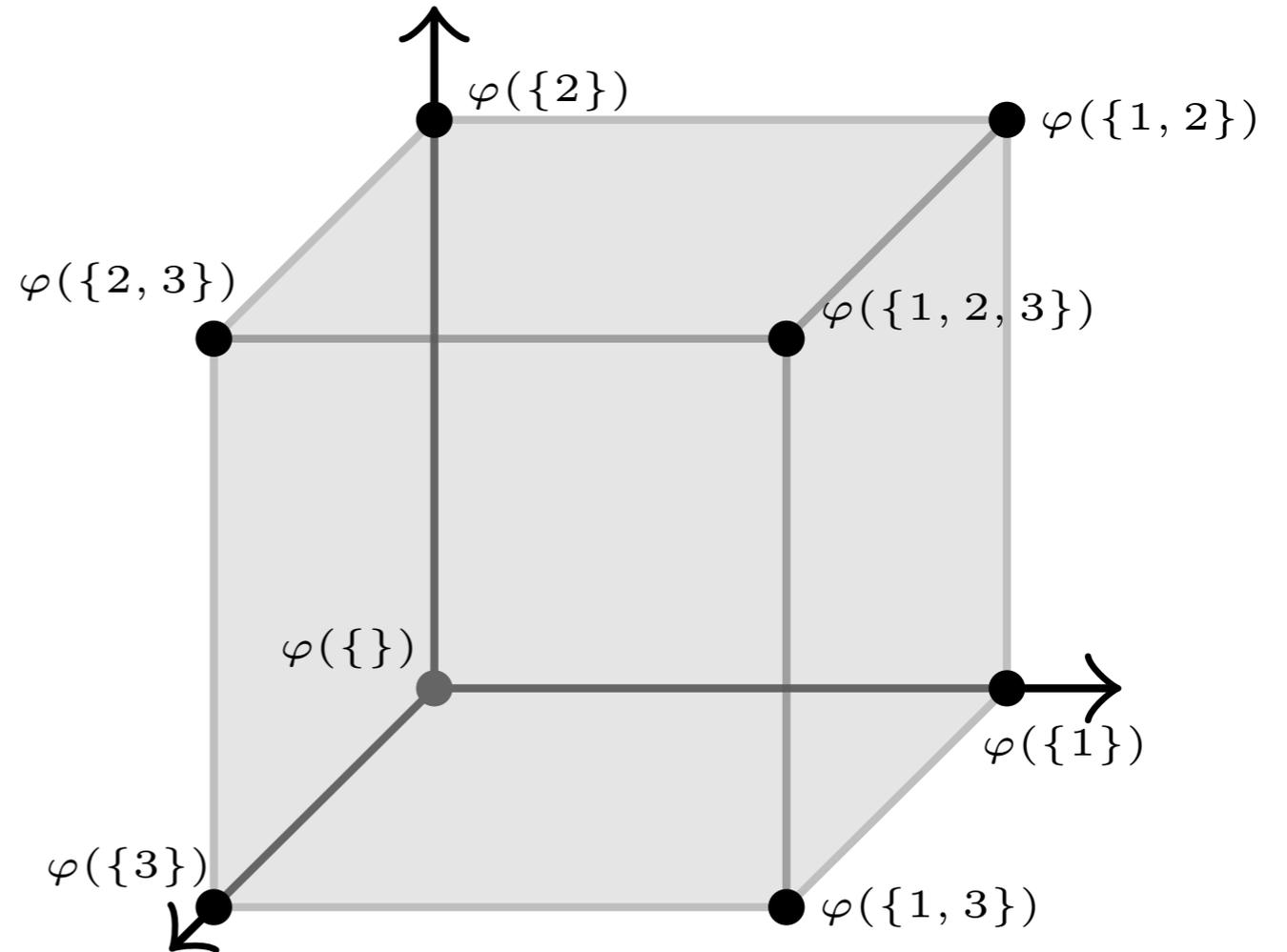
$$\mathcal{Y} = 2^{[k]}$$

Encoding

$$\varphi(y) = \sum_{i=1}^{|y|} e_{y_i}$$

Marginal polytope

$$\mathcal{M} = [0, 1]^k$$



# Unit cube

## Output set

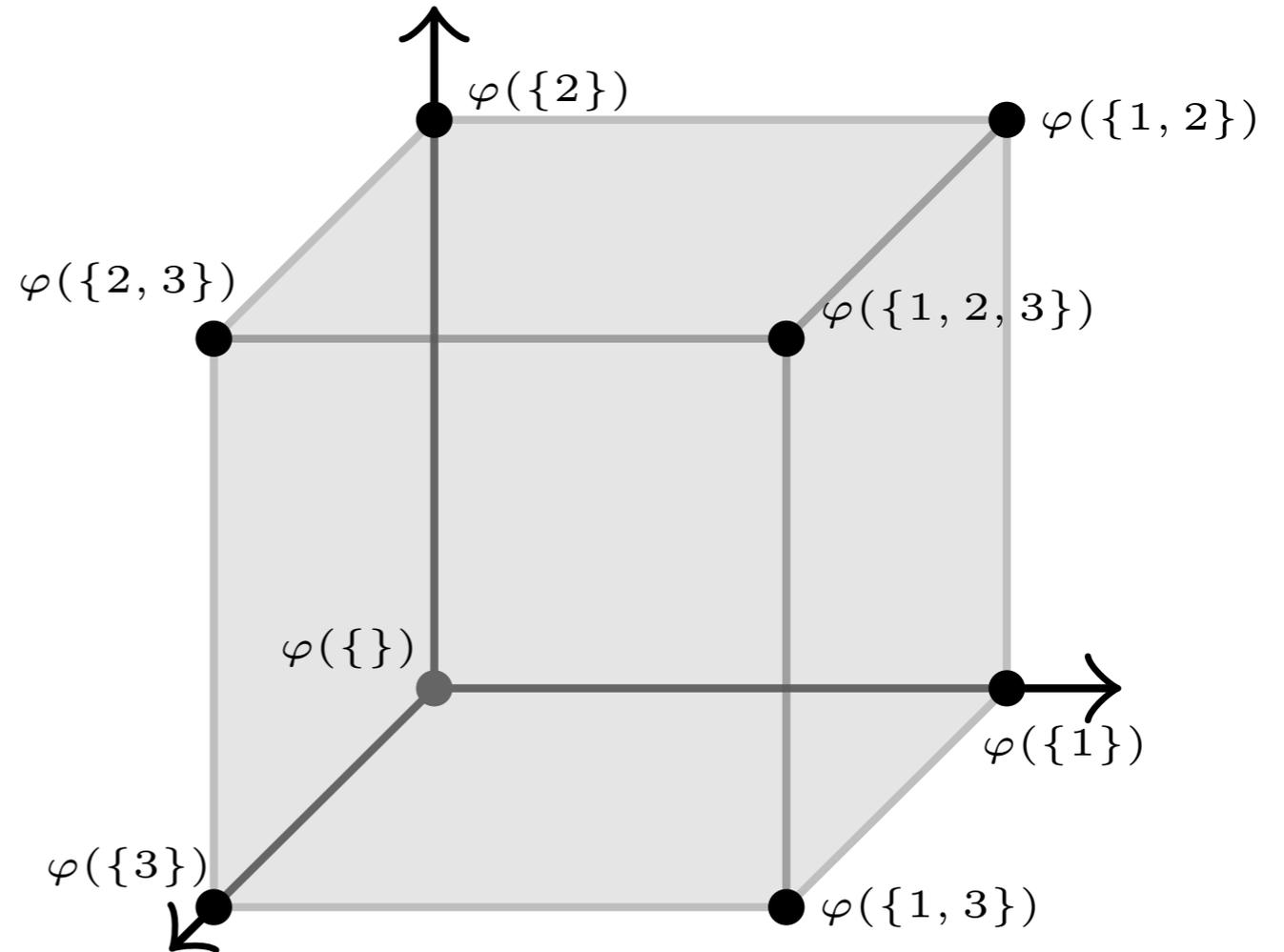
$$\mathcal{Y} = 2^{[k]}$$

## Encoding

$$\varphi(y) = \sum_{i=1}^{|y|} e_{y_i}$$

## Marginal polytope

$$\mathcal{M} = [0,1]^k$$



## Oracles

MAP:  $O(k)$

Euclidean: clipping to  $[0,1]$ ,  $O(k)$

KL:  $O(k)$

# Budget polytope

Output set

$$\mathcal{Y} = \{y \in 2^{[k]} : l \leq |y| \leq u\}$$

# Budget polytope

## Output set

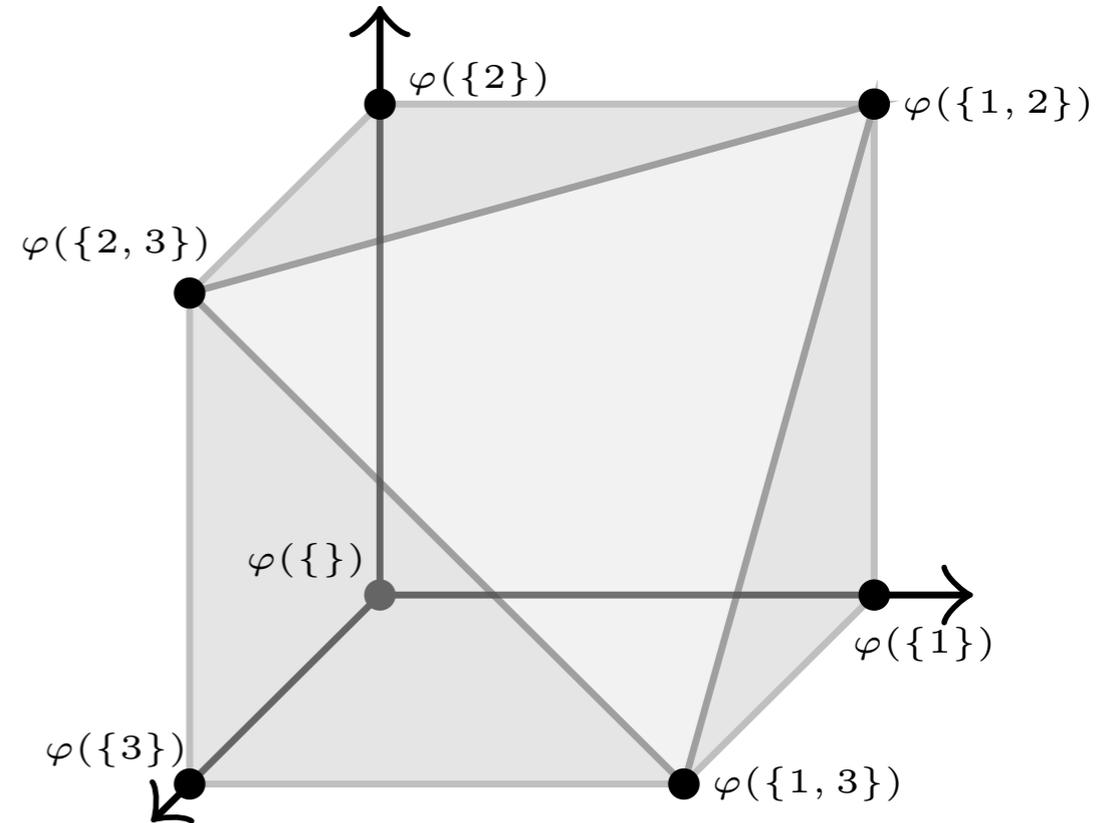
$$\mathcal{Y} = \{y \in 2^{[k]} : l \leq |y| \leq u\}$$

## Encoding

$$\varphi(y) = \sum_{i=1}^{|y|} e_{y_i}$$

## Marginal polytope

$$\mathcal{M} = \{y \in [0,1]^k : l \leq y^\top \mathbf{1} \leq m\}$$



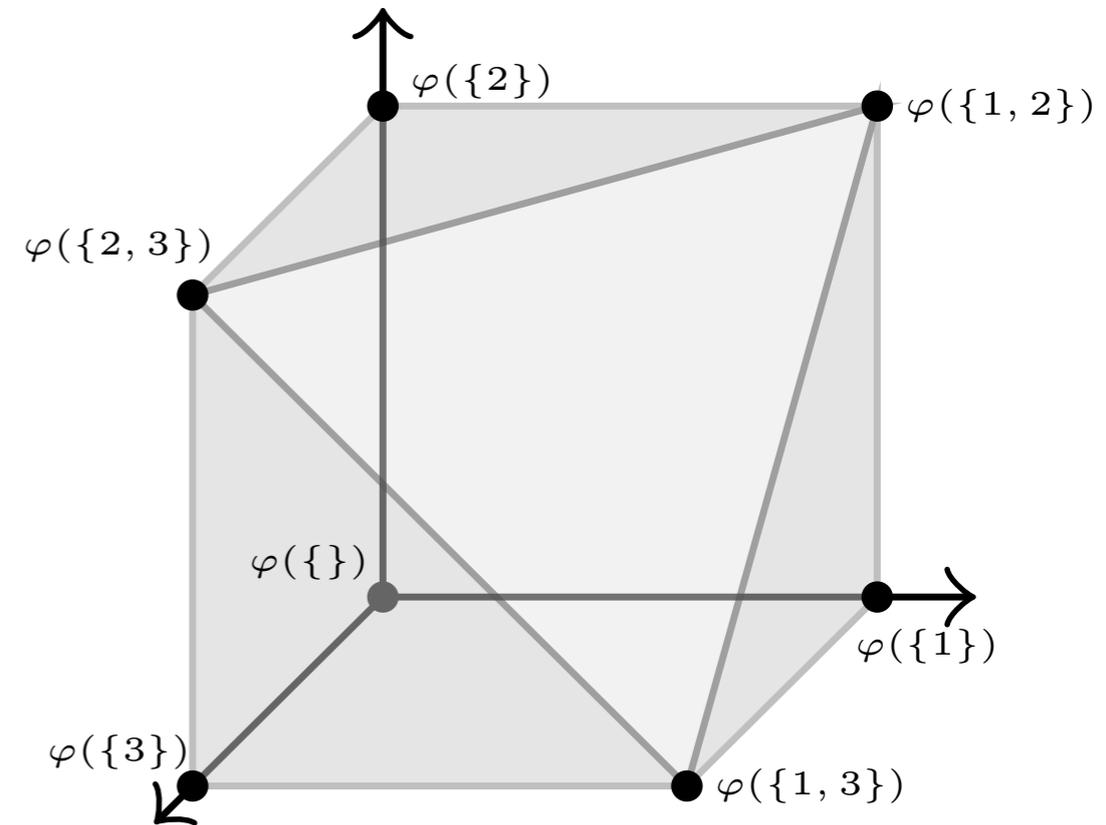
# Budget polytope

## Output set

$$\mathcal{Y} = \{y \in 2^{[k]} : l \leq |y| \leq u\}$$

## Encoding

$$\varphi(y) = \sum_{i=1}^{|y|} e_{y_i}$$



## Marginal polytope

$$\mathcal{M} = \{y \in [0,1]^k : l \leq y^\top \mathbf{1} \leq m\}$$

## Oracles

MAP:  $O(k \log k)$

Euclidean:  $O(k)$

KL:  $O(k \log k)$

# Order simplex

Output set

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

# Order simplex

## Output set

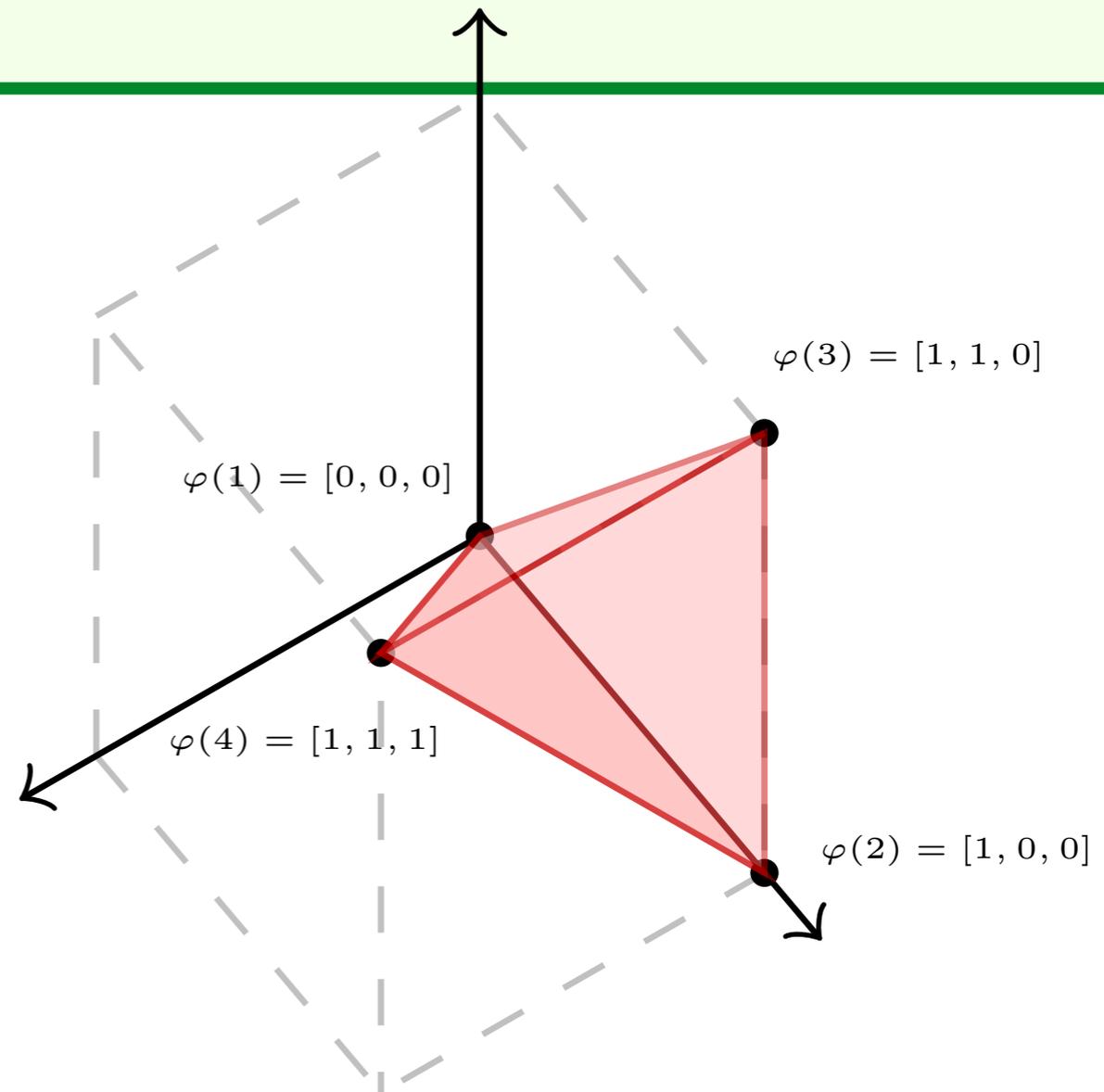
$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

## Encoding

$$\varphi(y) = \sum_{1 \leq i < y \leq k} e_i \in \mathbb{R}^{k-1}$$

## Marginal polytope

$$\mathcal{M} = \{\mu \in \mathbb{R}^{k-1} : 1 \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_{k-1} \geq 0\}$$



# Order simplex

## Output set

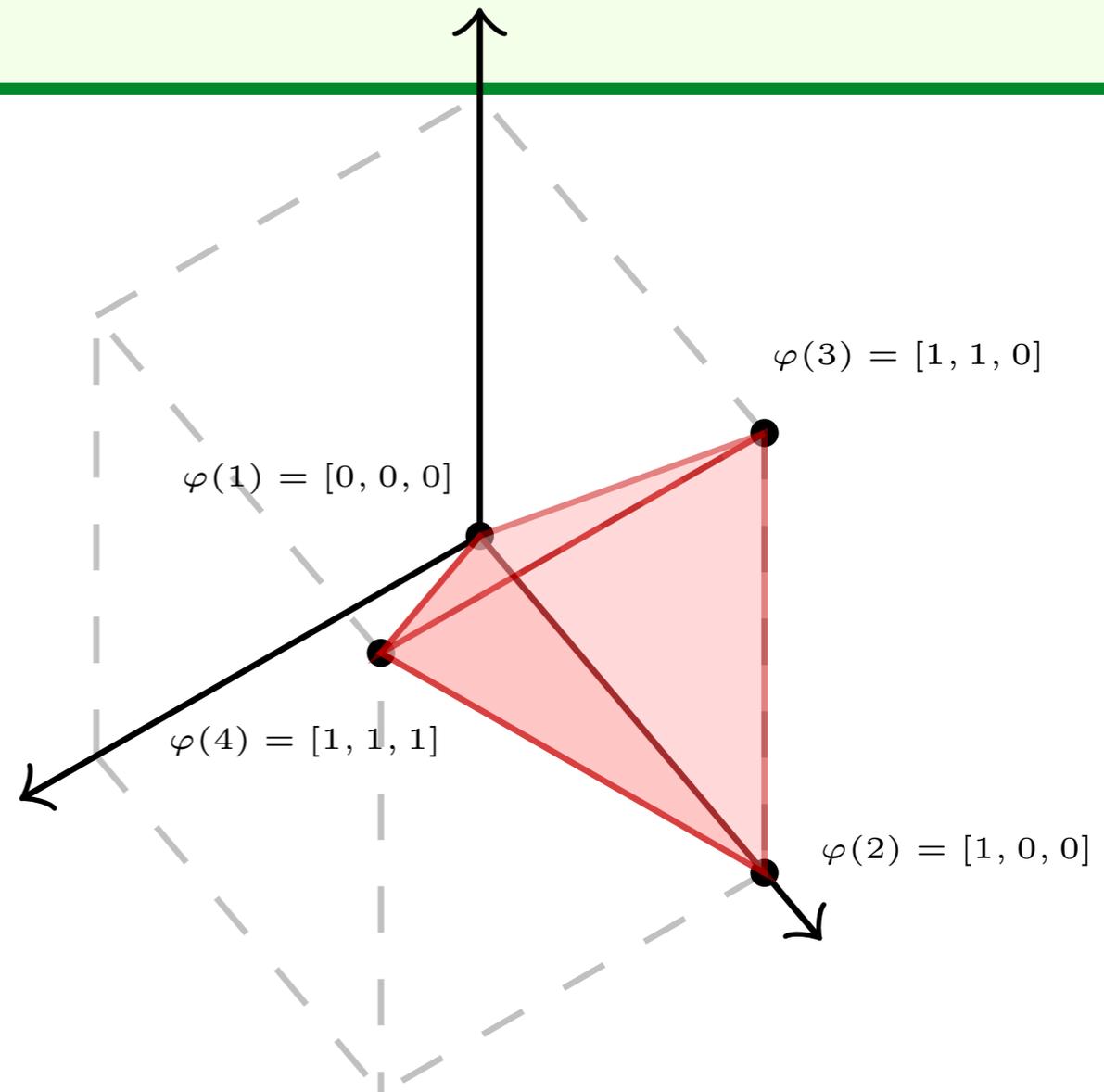
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$$\varphi(y) = \sum_{1 \leq i < y \leq k} e_i \in \mathbb{R}^{k-1}$$

## Marginal polytope

$$\mathcal{M} = \{\mu \in \mathbb{R}^{k-1} : 1 \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_{k-1} \geq 0\}$$



## Oracles

MAP:  $O(k)$

Eucl: isotonic reg,  $O(k)$

KL: isotonic optimization

# Birkhoff polytope

Output set

$$\mathcal{Y} = \text{Permutations}([m])$$

# Birkhoff polytope

## Output set

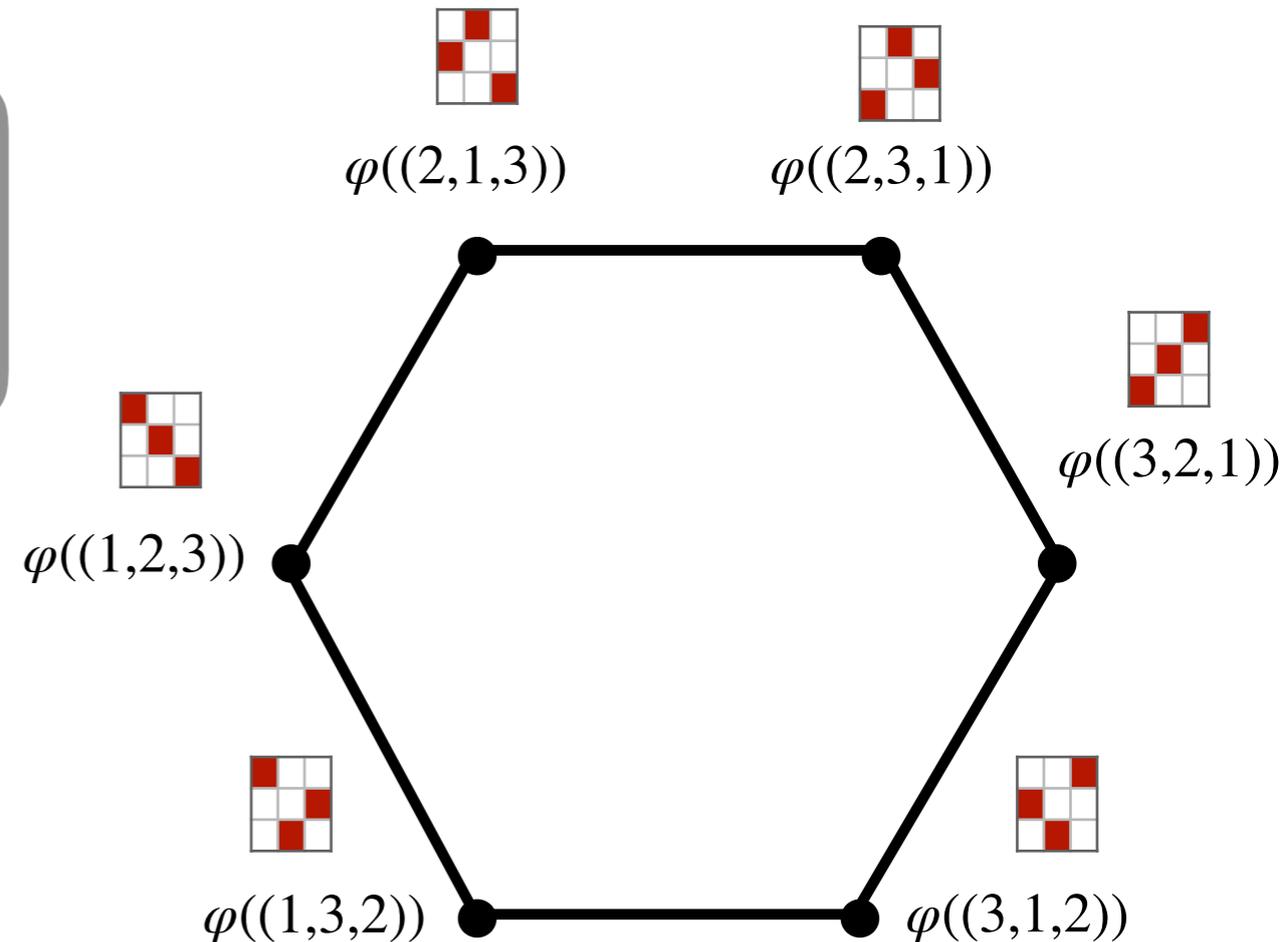
$$\mathcal{Y} = \text{Permutations}([m])$$

## Encoding

$$\varphi(y) = \text{permutation matrix associated with } y$$

## Marginal polytope

$$\mathcal{M} = \{P \in \mathbb{R}^{m \times m} : P^T \mathbf{1}_m = \mathbf{1}, P \mathbf{1}_m = \mathbf{1}, 0 \leq P \leq 1\}$$



# Birkhoff polytope

## Output set

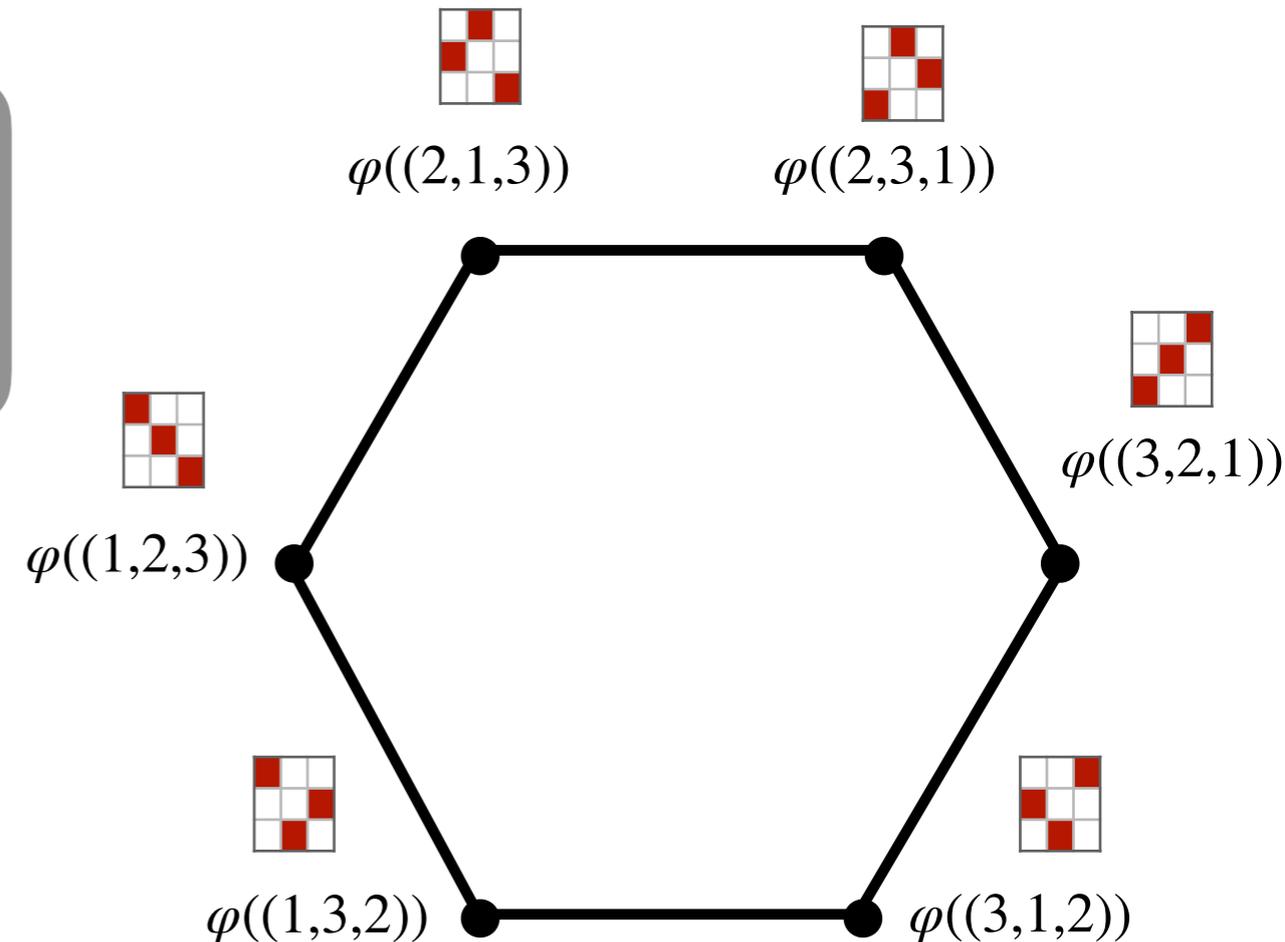
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## Oracles

- MAP: Hungarian,  $O(m^3)$
- Eucl: LBFGS dual,  $O(m^2/\epsilon)$
- KL: Sinkhorn,  $O(m^2/\epsilon)$
- Marginal: **intractable**

# Birkhoff polytope

## Output set

$$\mathcal{Y} = \text{Permutations}([m])$$

## Encoding

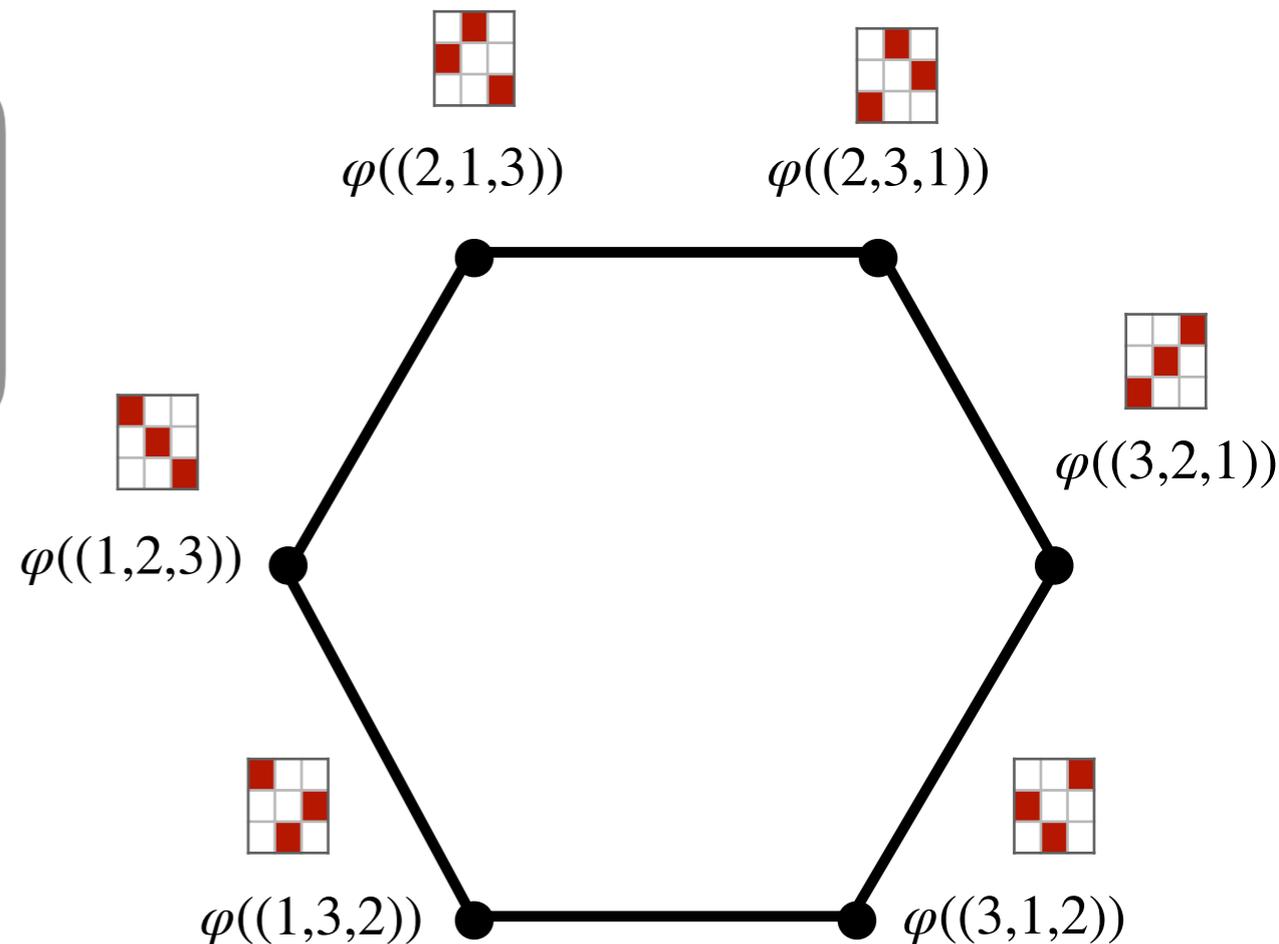
$$\varphi(y) = \text{permutation matrix associated with } y$$

## Marginal polytope

$$\mathcal{M} = \{P \in \mathbb{R}^{m \times m} : P^T \mathbf{1}_m = \mathbf{1}, P \mathbf{1}_m = \mathbf{1}, 0 \leq P \leq 1\}$$

$$\Delta^{m \times m} \triangleq \{P \in \mathbb{R}^{m \times m} : P^T \mathbf{1}_m = \mathbf{1}, 0 \leq P \leq 1\} \supset \mathcal{M}$$

Row-stochastic matrices



## Oracles

MAP: Hungarian,  $O(m^3)$

Eucl: LBFGS dual,  $O(m^2/\epsilon)$

KL: Sinkhorn,  $O(m^2/\epsilon)$

Marginal: **intractable**

# Permutahedron

Output set

$$\mathcal{Y} = \text{Permutations}([m])$$

# Permutahedron

## Output set

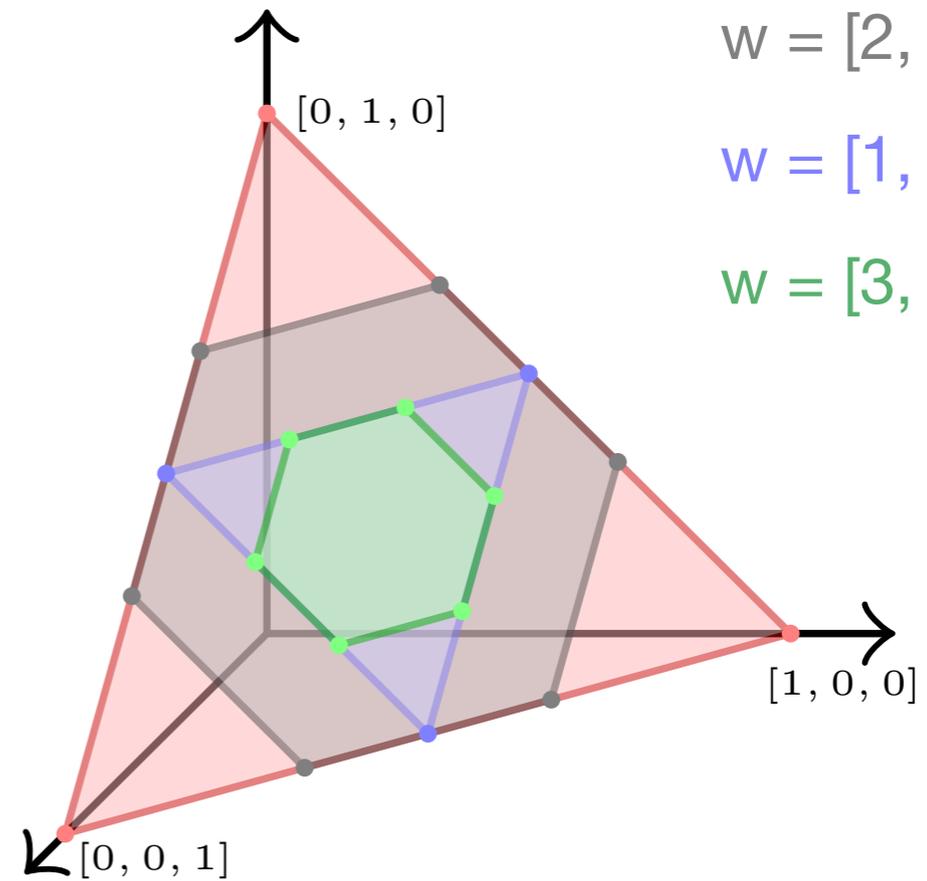
$$\mathcal{Y} = \text{Permutations}([m])$$

## Encoding

$$\varphi(y) = \text{permutation of a vector } w \text{ according to } y$$

## Marginal polytope

$$\mathcal{M} = \left\{ \mu \in \mathbb{R}^m : \sum_{i \in S} \mu_i \leq \sum_{i=1}^{|S|} w_i \forall S \subset [m], \sum_{i=1}^m \mu_i = \sum_{i=1}^m w_i \right\}$$



$$w = [1, 0, 0]$$

$$w = [2, 1, 0] / 3$$

$$w = [1, 1, 0] / 2$$

$$w = [3, 2, 1] / 6$$

# Permutahedron

## Output set

$$\mathcal{Y} = \text{Permutations}([m])$$

## Encoding

$$\varphi(y) = \text{permutation of a vector } w \text{ according to } y$$

## Marginal polytope

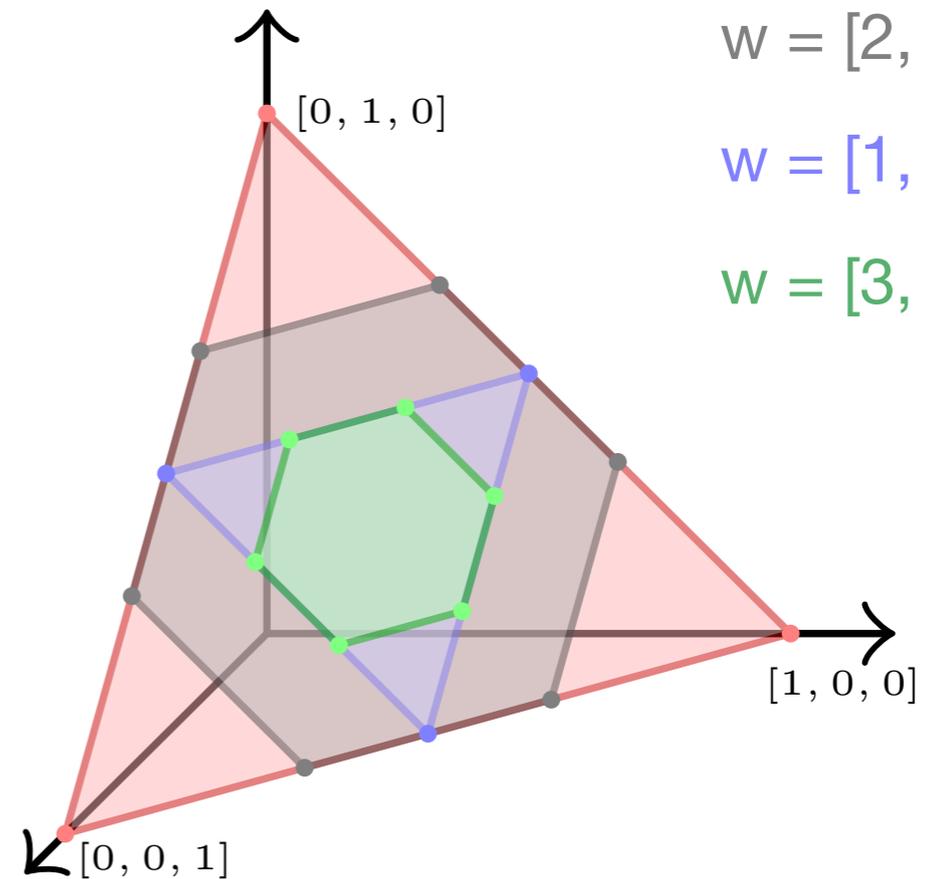
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## Oracles

MAP:  $O(m \log m)$

Eucl: isotonic reg,  $O(m \log m)$

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$$w = [1, 0, 0]$$

$$w = [2, 1, 0] / 3$$

$$w = [1, 1, 0] / 2$$

$$w = [3, 2, 1] / 6$$

# Outline

---

1. Background

2. Proposed framework

3. Experiments

# Experiments

---

$$\frac{1}{n} \sum_{i=1}^n S_{\mathcal{E}}(Wx_i, y_i) + \lambda \|W\|_F^2$$

- Label ranking
- Ordinal regression
- Multilabel classification

# Label ranking

---

Full-ranking supervision setting (no relevance scores)

e.g.  $2 \succ 1 \succ 3 \succ 4$

# Label ranking

Full-ranking supervision setting (no relevance scores)

e.g.  $2 \succ 1 \succ 3 \succ 4$

Projection	$\mathbb{R}^{m \times m}$
Decoding	$\mathcal{B}$
Authorship	5.70
Glass	7.11
Iris	19.26
Vehicle	9.04
Vowel	10.57
Wine	<b>1.23</b>

= squared loss

L = Hamming loss

Using **Euclidean** projections

# Label ranking

Full-ranking supervision setting (no relevance scores)

e.g.  $2 \succ 1 \succ 3 \succ 4$

Projection	$\mathbb{R}^{m \times m}$	$[0, 1]^{m \times m}$
Decoding	$\mathcal{B}$	$\mathcal{B}$
Authorship	5.70	5.18
Glass	7.11	5.68
Iris	19.26	4.44
Vehicle	9.04	7.57
Vowel	10.57	9.56
Wine	<b>1.23</b>	1.85

= squared loss

L = Hamming loss

Using **Euclidean** projections

# Label ranking

Full-ranking supervision setting (no relevance scores)

e.g.  $2 \succ 1 \succ 3 \succ 4$

Projection	$\mathbb{R}^{m \times m}$	$[0, 1]^{m \times m}$	$\Delta^{m \times m}$
Decoding	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{B}$
Authorship	5.70	5.18	5.70
Glass	7.11	5.68	5.04
Iris	19.26	4.44	<b>1.48</b>
Vehicle	9.04	7.57	6.99
Vowel	10.57	9.56	9.18
Wine	<b>1.23</b>	1.85	1.85

= squared loss

L = Hamming loss

Using **Euclidean** projections

# Label ranking

Full-ranking supervision setting (no relevance scores)

e.g.  $2 \succ 1 \succ 3 \succ 4$

Projection	$\mathbb{R}^{m \times m}$	$[0, 1]^{m \times m}$	$\Delta^{m \times m}$	$\mathcal{B}$
Decoding	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{B}$	$\mathcal{B}$
Authorship	5.70	5.18	5.70	<b>5.10</b>
Glass	7.11	5.68	5.04	<b>4.65</b>
Iris	19.26	4.44	<b>1.48</b>	2.96
Vehicle	9.04	7.57	6.99	<b>5.88</b>
Vowel	10.57	9.56	9.18	<b>8.76</b>
Wine	<b>1.23</b>	1.85	1.85	1.85

= squared loss

L = Hamming loss

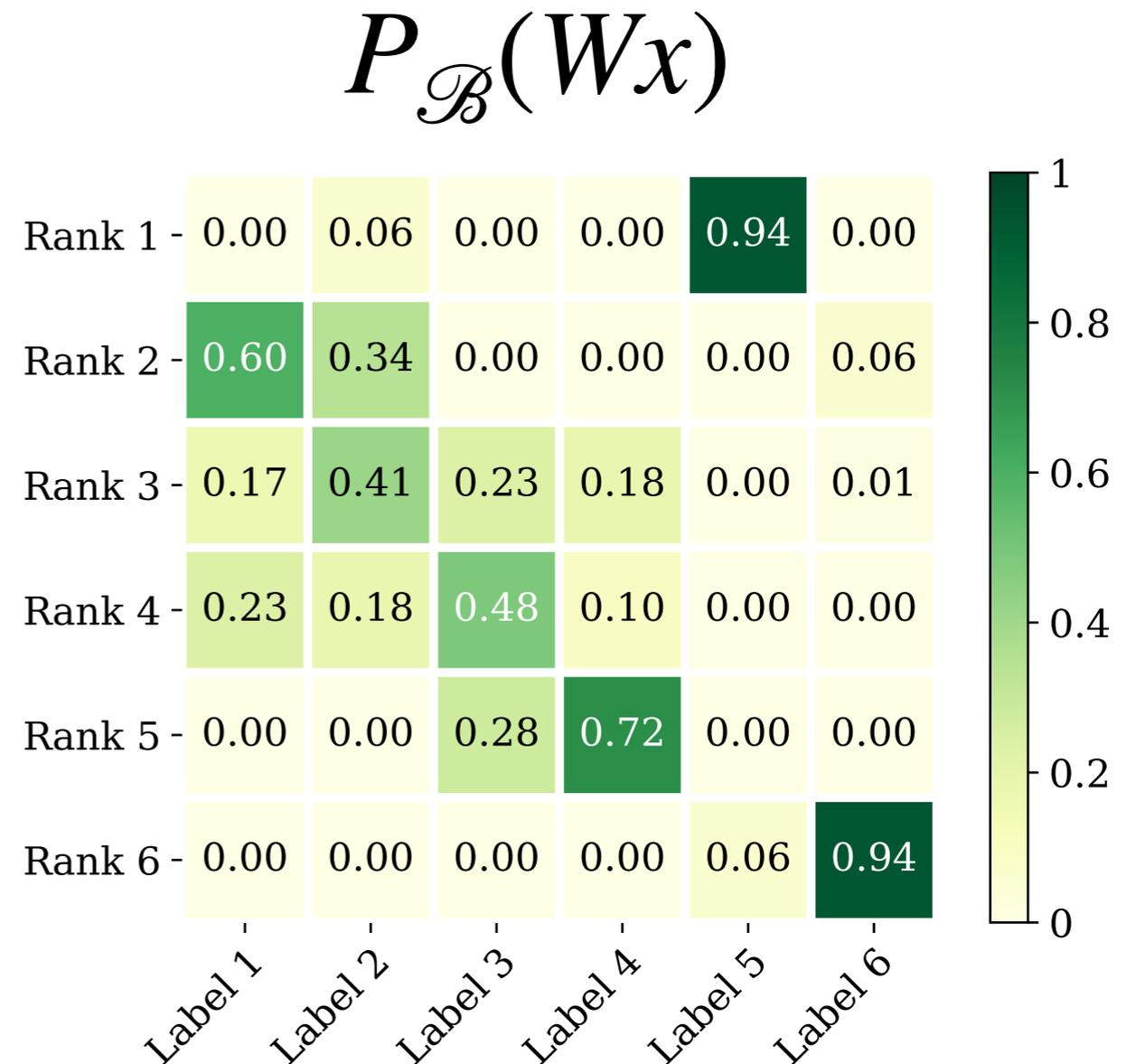
Using **Euclidean** projections

# Label ranking

	Euclidean	vs. KL
Projection	<i>B</i>	<i>B</i>
Decoding	<i>B</i>	<i>B</i>
Authorship	<b>5.10</b>	<b>5.10</b>
Glass	<b>4.65</b>	<b>4.65</b>
Iris	2.96	2.96
Vehicle	<b>5.88</b>	<b>6.25</b>
Vowel	<b>8.76</b>	<b>9.17</b>
Wine	1.85	<b>1.85</b>

# Label ranking

	Euclidean	vs. KL
Projection	$\mathcal{B}$	$\mathcal{B}$
Decoding	$\mathcal{B}$	$\mathcal{B}$
Authorship	<b>5.10</b>	<b>5.10</b>
Glass	<b>4.65</b>	<b>4.65</b>
Iris	2.96	2.96
Vehicle	<b>5.88</b>	<b>6.25</b>
Vowel	<b>8.76</b>	<b>9.17</b>
Wine	1.85	<b>1.85</b>



“soft permutation matrix”

# Label ranking

Birkhoff vs. permutahedron

		Linear	Poly 2	Poly 3
Projection	$\mathcal{B}$	$\mathcal{P}$	$\mathcal{P}$	$\mathcal{P}$
Decoding	$\mathcal{B}$	$\mathcal{P}$	$\mathcal{P}$	$\mathcal{P}$
Authorship	<b>5.10</b>	10.06	10.50	8.59
Glass	<b>4.65</b>	7.49	7.10	8.14
Iris	2.96	27.41	20.00	5.93
Vehicle	<b>5.88</b>	11.62	8.30	9.26
Vowel	<b>8.76</b>	14.35	11.74	10.21
Wine	1.85	8.02	3.08	6.79
	$W \in \mathbb{R}^{p \times m^2}$	$W \in \mathbb{R}^{p \times m}$	$W \in \mathbb{R}^{n \times m}$	$W \in \mathbb{R}^{n \times m}$

Using **Euclidean** projections

# Ordinal regression

---

$$y = [k] \quad 1 < \dots < k$$

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline
Average MAE	0.78
Average rank	4.75

Averaged over 16 datasets

L = MAE = Mean Absolute Error

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline	$\mathbb{R}$ Round
Average MAE	0.78	0.72
Average rank	4.75	2.9

Averaged over 16 datasets

L = MAE = Mean Absolute Error

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline	$\mathbb{R}$ Round
Average MAE	0.78	0.72
Average rank	4.75	2.9

Averaged over 16 datasets

L = MAE = Mean Absolute Error

OS = Order Simplex

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline	$\mathbb{R}$ Round	$\mathbb{R}^{k-1}$ <i>OS</i>
Average MAE	0.78	0.72	0.47
Average rank	4.75	2.9	2.1

Averaged over 16 datasets

L = MAE = Mean Absolute Error

OS = Order Simplex

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline	$\mathbb{R}$ Round	$\mathbb{R}^{k-1}$ <i>OS</i>	$[0, 1]^{k-1}$ <i>OS</i>
Average MAE	0.78	0.72	0.47	0.45
Average rank	4.75	2.9	2.1	1.6

Averaged over 16 datasets

L = MAE = Mean Absolute Error

OS = Order Simplex

# Ordinal regression

$$\mathcal{Y} = [k] \quad 1 < \dots < k$$

Projection Decoding	Baseline	$\mathbb{R}$ Round	$\mathbb{R}^{k-1}$ <i>OS</i>	$[0, 1]^{k-1}$ <i>OS</i>	<i>OS</i> <i>OS</i>
Average MAE	0.78	0.72	0.47	0.45	0.43
Average rank	4.75	2.9	2.1	1.6	<b>1.5</b>

Averaged over 16 datasets

L = MAE = Mean Absolute Error

OS = Order Simplex

# Multilabel classification

---

$$\text{lower bound} = 0 \quad \text{upper bound} = \lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$$

# Multilabel classification

lower bound = 0      upper bound =  $\lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$

---

Projection	$[0, 1]^k$
Decoding	$[0, 1]^k$

---

Birds	38.87
Emotions	56.60
Scene	61.06

---

$\mathcal{K}$ : budget polytope

F<sub>1</sub> score

# Multilabel classification

lower bound = 0      upper bound =  $\lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$

---

Projection	$[0, 1]^k$	$\mathbb{R}^k$
Decoding	$[0, 1]^k$	$\mathcal{K}$
Birds	38.87	37.75
Emotions	56.60	51.73
Scene	61.06	50.33

---

$\mathcal{K}$ : budget polytope

F<sub>1</sub> score

# Multilabel classification

lower bound = 0      upper bound =  $\lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$

---

Projection	$[0, 1]^k$	$\mathbb{R}^k$	$[0, 1]^k$
Decoding	$[0, 1]^k$	$\mathcal{K}$	$\mathcal{K}$
Birds	38.87	37.75	39.21
Emotions	56.60	51.73	53.98
Scene	61.06	50.33	58.95

---

$\mathcal{K}$ : budget polytope

F<sub>1</sub> score

# Multilabel classification

lower bound = 0      upper bound =  $\lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$

---

	$[0, 1]^k$	$\mathbb{R}^k$	$[0, 1]^k$	$\mathcal{K}$
Projection	$[0, 1]^k$	$\mathbb{R}^k$	$[0, 1]^k$	$\mathcal{K}$
Decoding	$[0, 1]^k$	$\mathcal{K}$	$\mathcal{K}$	$\mathcal{K}$
Birds	38.87	37.75	39.21	<b>39.43</b>
Emotions	56.60	51.73	53.98	<b>62.57</b>
Scene	61.06	50.33	58.95	<b>69.01</b>

---

$\mathcal{K}$ : budget polytope

F<sub>1</sub> score

# Multilabel classification

lower bound = 0      upper bound =  $\lceil \mathbb{E}[|Y|] + \sqrt{\mathbb{V}[|Y|]} \rceil$

Projection	$[0, 1]^k$	$\mathbb{R}^k$	$[0, 1]^k$	$\mathcal{K}$
Decoding	$[0, 1]^k$	$\mathcal{K}$	$\mathcal{K}$	$\mathcal{K}$
Birds	38.87	37.75	39.21	<b>39.43</b>
Cal500	34.62	<b>35.86</b>	34.63	34.61
Emotions	56.60	51.73	53.98	<b>62.57</b>
Mediamill	<b>56.22</b>	55.35	<b>56.22</b>	54.53
Scene	61.06	50.33	58.95	<b>69.01</b>
TMC	<b>60.45</b>	58.61	60.37	60.25
Yeast	<b>60.24</b>	60.20	60.23	60.06

$\mathcal{K}$ : budget polytope

F<sub>1</sub> score

# Conclusion

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- We proposed a generic framework for deriving a **loss** from the **projection** onto a convex set

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- If its projection is affordable, the **marginal polytope** is the best convex set

# Conclusion

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- We proposed a generic framework for deriving a **loss** from the **projection** onto a convex set
- If its projection is affordable, the **marginal polytope** is the best convex set
- If not, any convex **superset** with cheaper projection can be used (e.g., unit cube)