# Cost-Sensitive Label Embedding for Multi-Label Classification

Kuan-Hao Huang and Hsuan-Tien Lin

Department of Computer Science & Information Engineering National Taiwan University



ECML PKDD, September 20, 2017

0/14

#### Multi-Label Classification

- ▶ an extension of the multi-class classification
- allow instance with multiple associated classes

ECML PKDD 2017

#### Multi-Label Classification

- an extension of the multi-class classification
- ▶ allow instance with multiple associated classes

### Example: Image with Animals (dog, cat, rabbit, shark)

image				
class	{ dog, cat }	{ dog, cat, rabbit }	{ dog }	{ shark }
label	(1, 1, 0, 0)	(1, 1, 1, 0)	(1,0,0,0)	(0,0,0,1)

#### Notation

- ▶ feature vector (image):  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$
- ▶ label vector (classes):  $\mathbf{y} \in \mathcal{Y} \subseteq \{0,1\}^K$

#### Notation

- feature vector (image):  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$
- ▶ label vector (classes):  $\mathbf{y} \in \mathcal{Y} \subseteq \{0,1\}^K$

#### Multi-Label Classification

- $\blacktriangleright$  given training instances  $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$
- learn a **predictor** h from  $\mathcal{D}$
- for testing instance  $(\mathbf{x}, \mathbf{y})$ , prediction  $\tilde{\mathbf{y}} = h(\mathbf{x})$
- let the prediction  $\tilde{\mathbf{y}}$  be close to ground truth  $\mathbf{y}$

#### Notation

- feature vector (image):  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$
- ▶ label vector (classes):  $\mathbf{y} \in \mathcal{Y} \subseteq \{0,1\}^K$

#### Multi-Label Classification

- $\blacktriangleright$  given training instances  $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$
- learn a **predictor** h from  $\mathcal{D}$
- for testing instance  $(\mathbf{x}, \mathbf{y})$ , prediction  $\tilde{\mathbf{y}} = h(\mathbf{x})$
- let the prediction  $\tilde{\mathbf{y}}$  be close to ground truth  $\mathbf{y}$

#### **Evaluation of Closeness**

- ightharpoonup cost function  $c(\mathbf{y}, \tilde{\mathbf{y}})$ : the penalty of predicting  $\mathbf{y}$  as  $\tilde{\mathbf{y}}$
- ► Hamming loss, 0/1 loss, Rank loss, F1 score(loss), Accuracy score(loss)

# Cost-Sensitive Multi-Label Classification (CSMLC)

#### Notation

- feature vector (image):  $\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$
- ▶ label vector (classes):  $\mathbf{y} \in \mathcal{Y} \subseteq \{0,1\}^K$

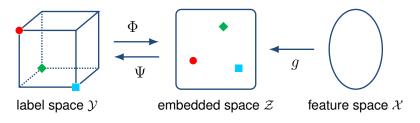
#### Cost-Sensitive Multi-Label Classification (CSMLC)

- ▶ given training instances  $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$  and cost function c
- learn a predictor h from both D and c
- for testing instance  $(\mathbf{x}, \mathbf{y})$ , prediction  $\tilde{\mathbf{y}} = h(\mathbf{x})$
- lackbox let the prediction  $\tilde{\mathbf{y}}$  be close to ground truth  $\mathbf{y}$

#### **Evaluation of Closeness**

- ightharpoonup cost function  $c(\mathbf{y}, \tilde{\mathbf{y}})$ : the penalty of predicting  $\mathbf{y}$  as  $\tilde{\mathbf{y}}$
- ► Hamming loss, 0/1 loss, Rank loss, F1 score(loss), Accuracy score(loss)

### Label Embedding

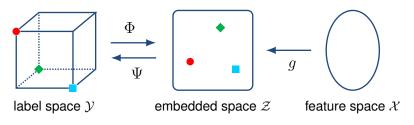


### Training Stage

- lacktriangle embedding function  $\Phi$ : label vector  $\mathbf{y} \to \mathbf{e}$ mbedded vector  $\mathbf{z}$
- $\blacktriangleright$  learn a regressor g from  $\{(\mathbf{x}^{(n)},\mathbf{z}^{(n)})\}_{n=1}^N$

ECML PKDD 2017

### Label Embedding



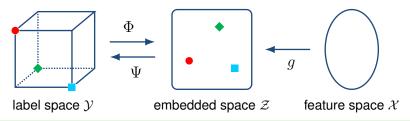
### Training Stage

- ightharpoonup embedding function  $\Phi$ : label vector  $\mathbf{y} \to \mathsf{embedded}$  vector  $\mathbf{z}$
- $\blacktriangleright \ \ \text{learn a regressor} \ g \ \text{from} \ \{(\mathbf{x}^{(n)},\mathbf{z}^{(n)})\}_{n=1}^{N}$

### **Predicting Stage**

- for testing instance x, predicted embedded vector  $\tilde{\mathbf{z}} = g(\mathbf{x})$
- ▶ decoding function  $\Psi$ : predicted embedded vector  $\tilde{\mathbf{z}}$  → predicted label vector  $\tilde{\mathbf{y}}$

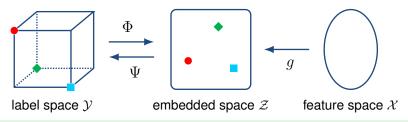
### Cost-Sensitive Label Embedding



### **Existing Works**

- ▶ label embedding: PLST, FaIE, RAkEL, ECC-based [Tai et al., 2012; Lin et al., 2014; Tsoumakas et al., 2011; Ferng et al., 2013]
- cost-sensitivity: CFT, PCC [Li et al., 2014; Dembczynski et al., 2010]
- cost-sensitivity + label embedding: no existing works

### Cost-Sensitive Label Embedding



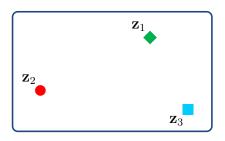
### **Existing Works**

- ▶ label embedding: PLST, FaIE, RAkEL, ECC-based [Tai et al., 2012; Lin et al., 2014; Tsoumakas et al., 2011; Ferng et al., 2013]
- cost-sensitivity: CFT, PCC [Li et al., 2014; Dembczynski et al., 2010]
- cost-sensitivity + label embedding: no existing works

#### Cost-Sensitive Label Embedding

▶ consider cost function c when designing embedding function  $\Phi$  and decoding function  $\Psi$  (cost-sensitive embedded vectors  $\mathbf{z}$ )

### Cost-Sensitive Embedding

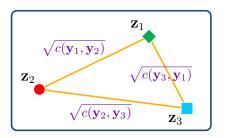


embedded space  $\mathcal{Z}$ 

#### Training Stage

- ▶ distances between embedded vectors ⇔ cost information
- ▶ larger (smaller) distance  $d(\mathbf{z}_i, \mathbf{z}_i) \Leftrightarrow \text{higher (lower) cost } c(\mathbf{y}_i, \mathbf{y}_i)$

### **Cost-Sensitive Embedding**

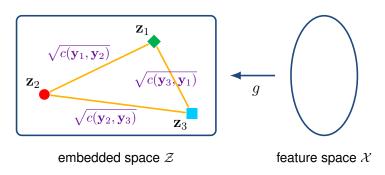


embedded space  $\mathcal Z$ 

#### **Training Stage**

- ▶ distances between embedded vectors ⇔ cost information
- ▶ larger (smaller) distance  $d(\mathbf{z}_i, \mathbf{z}_j) \Leftrightarrow$  higher (lower) cost  $c(\mathbf{y}_i, \mathbf{y}_j)$
- $d(\mathbf{z}_i, \mathbf{z}_j) \approx \sqrt{c(\mathbf{y}_i, \mathbf{y}_j)}$  by multidimensional scaling (manifold learning)

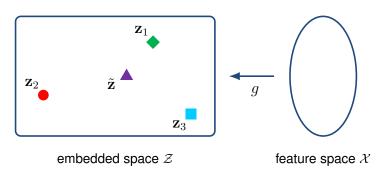
# **Cost-Sensitive Embedding**



### Training Stage

- ▶ distances between embedded vectors ⇔ cost information
- $\blacktriangleright \ \ \text{larger (smaller) distance} \ d(\mathbf{z}_i,\mathbf{z}_j) \Leftrightarrow \text{higher (lower) cost} \ c(\mathbf{y}_i,\mathbf{y}_j)$
- $d(\mathbf{z}_i, \mathbf{z}_j) \approx \sqrt{c(\mathbf{y}_i, \mathbf{y}_j)}$  by multidimensional scaling (manifold learning)

# **Cost-Sensitive Decoding**

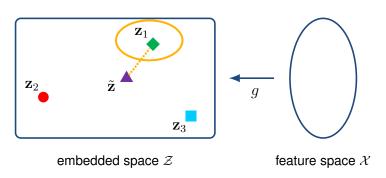


### **Predicting Stage**

• for testing instance  $\mathbf{x}$ , predicted embedded vector  $\tilde{\mathbf{z}} = g(\mathbf{x})$ 

ECML PKDD 2017

### Cost-Sensitive Decoding



### **Predicting Stage**

- for testing instance x, predicted embedded vector  $\tilde{\mathbf{z}} = q(\mathbf{x})$
- find nearest embedded vector  $\mathbf{z}_q$  of  $\tilde{\mathbf{z}}$
- ightharpoonup cost-sensitive prediction  $\tilde{\mathbf{y}} = \mathbf{y}_q$

### Theoretical Explanation

#### **Theorem**

$$c(\mathbf{y}, \tilde{\mathbf{y}}) \leq 5 \underbrace{\left( \left( d(\mathbf{z}, \mathbf{z}_q) - \sqrt{c(\mathbf{y}, \mathbf{y}_q)} \right)^2}_{\text{embedding error}} + \underbrace{\|\mathbf{z} - g(\mathbf{x})\|^2}_{\text{regression error}} \right)$$

# Theoretical Explanation

#### **Theorem**

$$c(\mathbf{y}, \tilde{\mathbf{y}}) \leq 5 \underbrace{\left( \left( d(\mathbf{z}, \mathbf{z}_q) - \sqrt{c(\mathbf{y}, \mathbf{y}_q)} \right)^2 + \underbrace{\|\mathbf{z} - g(\mathbf{x})\|^2}_{\text{regression error}} \right)}_{\text{regression error}}$$

#### Optimization

- ▶ embedding error → multidimensional scaling
- regression error → regressor g

# Theoretical Explanation

#### **Theorem**

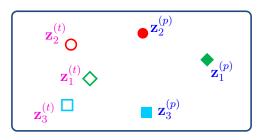
$$c(\mathbf{y}, \tilde{\mathbf{y}}) \leq 5 \underbrace{\left( \left( d(\mathbf{z}, \mathbf{z}_q) - \sqrt{c(\mathbf{y}, \mathbf{y}_q)} \right)^2 + \underbrace{\|\mathbf{z} - g(\mathbf{x})\|^2}_{\text{regression error}} \right)}_{\text{regression error}}$$

#### Optimization

- ▶ embedding error → multidimensional scaling
- ▶ regression error  $\rightarrow$  regressor g

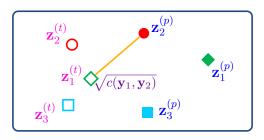
### Challenge

- asymmetric cost function vs. symmetric distance?
- $c(\mathbf{y}_i, \mathbf{y}_j) \neq c(\mathbf{y}_j, \mathbf{y}_i) \text{ VS. } d(\mathbf{z}_i, \mathbf{z}_j)$



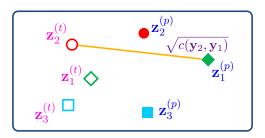
embedded space  $\mathcal{Z}$ 

lacktriangle two roles of  $\mathbf{y}_i$ : ground truth role  $\mathbf{y}_i^{(t)}$  and prediction role  $\mathbf{y}_i^{(p)}$ 



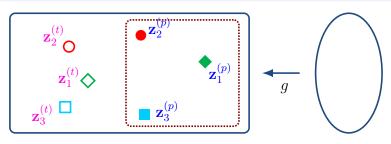
#### embedded space $\mathcal{Z}$

- ightharpoonup two roles of  $\mathbf{y}_i$ : ground truth role  $\mathbf{y}_i^{(t)}$  and prediction role  $\mathbf{y}_i^{(p)}$
- $\blacktriangleright \ \sqrt{c(\mathbf{y}_i,\mathbf{y}_j)} \Rightarrow \mathsf{predict} \ \mathbf{y}_i \ \mathsf{as} \ \mathbf{y}_j \Rightarrow \mathsf{for} \ \mathbf{z}_i^{(t)} \ \mathsf{and} \ \mathbf{z}_j^{(p)}$



#### embedded space $\mathcal{Z}$

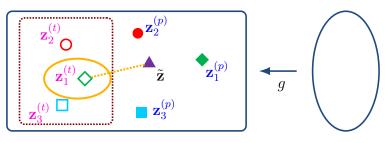
- ightharpoonup two roles of  $\mathbf{y}_i$ : ground truth role  $\mathbf{y}_i^{(t)}$  and prediction role  $\mathbf{y}_i^{(p)}$
- $\blacktriangleright \ \sqrt{c(\mathbf{y}_i,\mathbf{y}_j)} \Rightarrow \mathsf{predict} \ \mathbf{y}_i \ \mathsf{as} \ \mathbf{y}_j \Rightarrow \mathsf{for} \ \mathbf{z}_i^{(t)} \ \mathsf{and} \ \mathbf{z}_j^{(p)}$
- $ightharpoonup \sqrt{c(\mathbf{y}_j,\mathbf{y}_i)} \Rightarrow \operatorname{predict} \mathbf{y}_j \text{ as } \mathbf{y}_i \Rightarrow \operatorname{for} \mathbf{z}_i^{(p)} \text{ and } \mathbf{z}_j^{(t)}$



embedded space  $\mathcal{Z}$ 

feature space  $\mathcal{X}$ 

- lacktriangle two roles of  $\mathbf{y}_i$ : ground truth role  $\mathbf{y}_i^{(t)}$  and prediction role  $\mathbf{y}_i^{(p)}$
- $ightharpoonup \sqrt{c(\mathbf{y}_i,\mathbf{y}_j)} \Rightarrow \mathsf{predict} \ \mathbf{y}_i \ \mathsf{as} \ \mathbf{y}_j \Rightarrow \mathsf{for} \ \mathbf{z}_i^{(t)} \ \mathsf{and} \ \mathbf{z}_j^{(p)}$
- $ightharpoonup \sqrt{c(\mathbf{y}_j, \mathbf{y}_i)} \Rightarrow \operatorname{predict} \mathbf{y}_j \text{ as } \mathbf{y}_i \Rightarrow \operatorname{for} \mathbf{z}_i^{(p)} \text{ and } \mathbf{z}_j^{(t)}$
- ightharpoonup learn **regressor** g from  $\mathbf{z}_i^{(p)}, \mathbf{z}_2^{(p)}, ..., \mathbf{z}_L^{(p)}$



embedded space  ${\mathcal Z}$ 

feature space  ${\cal X}$ 

- lacktriangle two roles of  $\mathbf{y}_i$ : ground truth role  $\mathbf{y}_i^{(t)}$  and prediction role  $\mathbf{y}_i^{(p)}$
- $ightharpoonup \sqrt{c(\mathbf{y}_i,\mathbf{y}_j)} \Rightarrow \mathsf{predict} \ \mathbf{y}_i \ \mathsf{as} \ \mathbf{y}_j \Rightarrow \mathsf{for} \ \mathbf{z}_i^{(t)} \ \mathsf{and} \ \mathbf{z}_j^{(p)}$
- $ightharpoonup \sqrt{c(\mathbf{y}_j,\mathbf{y}_i)} \Rightarrow \operatorname{predict} \mathbf{y}_j \text{ as } \mathbf{y}_i \Rightarrow \operatorname{for} \mathbf{z}_i^{(p)} \text{ and } \mathbf{z}_j^{(t)}$
- ightharpoonup learn **regressor** g from  $\mathbf{z}_i^{(p)}, \mathbf{z}_2^{(p)}, ..., \mathbf{z}_L^{(p)}$
- ► find nearest embedded vector of  $\tilde{\mathbf{z}}$  from  $\mathbf{z}_1^{(t)}, \mathbf{z}_2^{(t)}, ..., \mathbf{z}_L^{(t)}$

### Cost-Sensitive Label Embedding with Multidimensional Scaling

#### Training Stage of **CLEMS**

- $\blacktriangleright$  given training instances  $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$  and cost function c
- $\blacktriangleright$  determine two roles of embedded vectors  $\mathbf{z}_i^{(t)}$  and  $\mathbf{z}_i^{(p)}$  for label vector  $\mathbf{y}_i$
- lacktriangle embedding function  $\Phi\colon \mathbf{y}_i o \mathbf{z}_i^{(p)}$
- $\blacktriangleright \text{ learn a regressor } g \text{ from } \{(\mathbf{x}^{(n)}, \Phi(\mathbf{y}^{(n)}))\}_{n=1}^N$

### Cost-Sensitive Label Embedding with Multidimensional Scaling

#### Training Stage of **CLEMS**

- $\blacktriangleright$  given training instances  $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$  and cost function c
- lacktriangle determine two roles of embedded vectors  $\mathbf{z}_i^{(t)}$  and  $\mathbf{z}_i^{(p)}$  for label vector  $\mathbf{y}_i$
- embedding function  $\Phi \colon \mathbf{y}_i \to \mathbf{z}_i^{(p)}$
- $\blacktriangleright \text{ learn a regressor } g \text{ from } \{(\mathbf{x}^{(n)}, \Phi(\mathbf{y}^{(n)}))\}_{n=1}^{N}$

#### Predicting Stage of **CLEMS**

- given the testing instance x
- ightharpoonup obtain the predicted embedded vector by  $\tilde{\mathbf{z}} = g(\mathbf{x})$
- decoding  $\Psi(\cdot) = \Phi^{-1}(\text{nearest neighbor}) = \Phi^{-1}(\operatorname{argmin} d(\mathbf{z}_i^{(t)}, \cdot))$
- prediction  $\tilde{\mathbf{y}} = \Psi(\tilde{\mathbf{z}})$

### **Experiments**

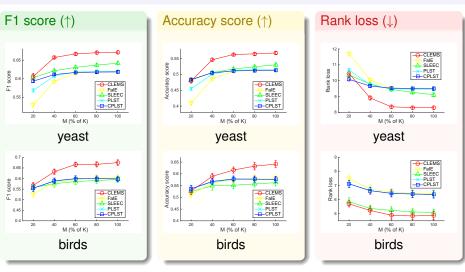
#### Settings

- 12 public datasets
- ▶ 50% for training, 25% for validation, and 25% for testing
- tune parameters by validation
- evaluation criteria
  - ▶ F1 score  $\frac{2\|\mathbf{y} \cap \tilde{\mathbf{y}}\|_1}{\|\mathbf{y}\|_1 + \|\tilde{\mathbf{y}}\|_1}$  (↑)
  - Accuracy score  $\frac{\|\mathbf{y} \cap \tilde{\mathbf{y}}\|_1}{\|\mathbf{y} \cup \tilde{\mathbf{y}}\|_1}$  (†)
  - ▶ Rank loss  $\sum_{\mathbf{y}[i]>\mathbf{y}[j]} (\llbracket \tilde{\mathbf{y}}[i] < \tilde{\mathbf{y}}[j] \rrbracket + \frac{1}{2} \llbracket \tilde{\mathbf{y}}[i] = \tilde{\mathbf{y}}[j] \rrbracket)$  (↓)
- average results of 20 experiments

#### Competitors

- label embedding algorithms
- cost-sensitive algorithms

# Comparison with Label Embedding Algorithms



CLEMS is the best across different criteria and dimensions

# Comparison with Cost-Sensitive Algorithms

Table: Performance across different evaluation criteria

data	F1 score (↑)			Accuracy score (↑)		Rank loss (↓)			
	CLEMS	CFT	PCC	CLEMS	CFT	PCC	CLEMS	CFT	PCC
emot.	0.676	0.640	0.643	0.589	0.557	_	1.484	1.563	1.467
scene	0.770	0.703	0.745	0.760	0.656	_	0.672	0.723	0.645
yeast	0.671	0.649	0.614	0.568	0.543	_	8.302	8.566	8.469
birds	0.677	0.601	0.636	0.642	0.586	_	4.886	4.908	3.660
med.	0.814	0.635	0.573	0.786	0.613	_	5.170	5.811	4.234
enron	0.606	0.557	0.542	0.491	0.448	-	29.40	26.64	25.11
lang.	0.375	0.168	0.247	0.327	0.164	_	31.03	34.16	19.11
flag	0.731	0.692	0.706	0.615	0.588	_	2.930	3.075	2.857
slash	0.568	0.429	0.503	0.538	0.402	_	4.986	5.677	4.472
CAL.	0.419	0.371	0.391	0.273	0.237	_	1247	1120	993
arts	0.492	0.334	0.349	0.451	0.281	-	9.865	10.07	8.467
EUR.	0.670	0.456	0.483	0.650	0.450	_	89.52	129.5	43.28

- **▶** generality for CSMLC: CLEMS = CFT > PCC
  - ▶ PCC requires an efficient inference rule
- ▶ performance: CLEMS ≈ PCC > CFT
- ▶ speed: CLEMS ≈ PCC > CFT

### Conclusion

- algorithm design: cost-sensitive label embedding algorithm (CLEMS)
  - embed the cost information in distance by multidimensional scaling
  - nearest-neighbor based decoding function
  - mirroring trick for asymmetric cost functions
- theoretical explanation:
  - prove the upper bound of the predicted cost for CLEMS
- empirical performance:
  - CLEMS outperforms existing label embedding algorithms
  - CLEMS is better than state-of-the-art cost-sensitive algorithms

14 / 14

### Conclusion

- algorithm design: cost-sensitive label embedding algorithm (CLEMS)
  - embed the cost information in distance by multidimensional scaling
  - nearest-neighbor based decoding function
  - mirroring trick for asymmetric cost functions
- theoretical explanation:
  - prove the upper bound of the predicted cost for CLEMS
- empirical performance:
  - CLEMS outperforms existing label embedding algorithms
  - CLEMS is better than state-of-the-art cost-sensitive algorithms

#### Thank you! Any question?