

# Advanced Machine Learning

## Multi-Target Prediction: Introduction



### Learning goals

- Understand the practical relevance of multi-target prediction problems
- Know relevant special cases of multi-target prediction
- Understand the difference between inductive and transductive learning problems

		Tennis	Football	Biking	Movies	TV	Belgium
01101	Text1	0	1	0	0	1	1
00111	Text2	1	0	0	0	0	1
01110	Text3	0	0	0	1	1	0
10001	Text4	0	0	1	0	1	0
01011	Text5	1	0	0	1	0	0
11110	Text6	?	?	?	?	?	?

# MULTI-TARGET PREDICTION: MOTIVATION

- Conventional supervised learning: Label space  $\mathcal{Y}$  is 1-D.
- Multi-target prediction (MTP): multiple targets of mixed types (binary, nominal, ordinal, real-valued).
- Learn one model per target independently?  $\rightsquigarrow$  Targets can be *statistically dependent*.
- Multi-label Emotions Dataset: 4 emotions of a music piece. Multiple emotions may be attributed to a single piece. Mutual information of the labels are:

	Calm	Quiet	Sad	Angry
Calm	1.000	0.073	0.018	<b>0.290</b>
Quiet	0.073	1.000	<b>0.241</b>	<b>0.164</b>
Sad	0.018	<b>0.241</b>	1.000	0.067
Angry	<b>0.290</b>	<b>0.164</b>	0.067	1.000

- It might be better to tackle targets *simultaneously*.



# MULTI-TARGET PREDICTION: CHARACTERISTICS

Characterized by instances  $\mathbf{x} \in \mathcal{X}$  and targets  $m \in \{1, 2, \dots, l\}$  with following properties:







- A training set  $\mathcal{D} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^n$ , where  $\mathbf{y}^{(i)} = (y_1^{(i)}, \dots, y_l^{(i)})$ , with  $y_m^{(i)} \in \mathcal{Y}_m$  is label for target  $m$ .
- $n$  instances and  $l$  targets  $\rightsquigarrow$  Labels  $y_m^{(i)}$  can be arranged in an  $n \times l$  matrix  $\mathbf{Y}$ . Note  $\mathbf{Y}$  may have missing values.
- Target spaces  $\mathcal{Y}_m$  can be nominal, ordinal or real-valued.
- Goal: predict scores for any pair  $(\mathbf{x}, m) \in \mathcal{X} \times \{1, 2, \dots, l\}$ .

In conventional MTP setting: no available side information for targets.



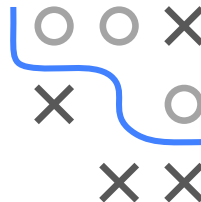
# MULTIVARIATE REGRESSION

Target space  $\mathcal{Y}_m = \mathbb{R} \forall m \in \{1, 2, \dots, l\}$ .

		Mol1	Mol2	Mol3	Mol4	Mol5	Mol6
01101		1,3	0,2	1,4	1,7	3,5	1,3
00111		2	1,7	1,5	7,5	8,2	7,6
01110		0,2	0	0,3	0,4	1,2	2,2
10001		3,1	1,1	1,3	1,1	1,7	5,2
01011		4,7	2,1	2,5	1,5	2,3	8,5
11110		?	?	?	?	?	?

Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).

Example: Predict binding strength between proteins (rows) and molecules (columns).



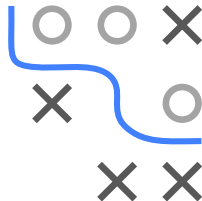
# MULTI-LABEL CLASSIFICATION

Target space  $\mathcal{Y}_m = \{0, 1\} \forall m \in \{1, 2, \dots, l\}$

		Tennis	Football	Biking	Movies	TV	Belgium
01101	Text1	0	1	0	0	1	1
00111	Text2	1	0	0	0	0	1
01110	Text3	0	0	0	1	1	0
10001	Text4	0	0	1	0	1	0
01011	Text5	1	0	0	1	0	0
11110	Text6	?	?	?	?	?	?

Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).

Example: Assign documents (rows) to category tags (columns).



# LABEL RANKING

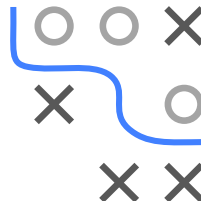
In *label ranking*, each instance is associated with a ranking of targets.

$\mathcal{Y}_m = \{1, \dots, l\} \forall m$ , and labels (i.e., ranks)  $y_m^{(i)} \neq y_k^{(i)} \forall m \neq k$ .

		Tennis	Football	Biking	Skating	Running	Walking
01101	User 1	2	1	4	3	5	6
00111	User 2	1	4	3	5	6	2
01110	User 3	4	5	1	2	3	6
10001	User 4	4	3	2	6	1	5
01011	User t5	1	3	5	2	6	4
11110	User 6	?	?	?	?	?	?







Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).

Example: Predict for users (rows) their preferences over specific activities (columns).

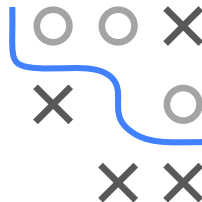


# MULTI-TASK LEARNING

- **Not all targets are relevant for all instances.** E.g., a student may only attend one school, other labels are **irrelevant**.
- Label space is homogenous across columns of  $\mathbf{Y}$ , e.g.,  $\mathcal{Y}_m = \{0, 1\}$  or  $\mathcal{Y}_m = \mathbb{R}$  for all  $m$ .

		School1	School2	School3
01101		7		
00111		9		
01110			5	
10001			8	
01011				9
11110		?	?	?

Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).



Example: Predict for students (rows) the final grades for a specific high-school course (columns).

## REMARKS

- It is also possible when the  $m$ -th task is multiclass classification. That is,  $f(\mathbf{x})_m \in \mathbb{R}^{g_m}$  is the probability predictions for  $g_m$  classes.  
~> The techniques for multi-target learning are also applicable under this setting, notation becomes cumbersome.
- Target space can be inhomogeneous, e.g.  $\mathcal{Y}_m = \{0, 1\}$  and  $\mathcal{Y}_k = \mathbb{R}$ .  
~> A mixture of multi-label classification and multivariate regression.





# SIDE INFORMATION ON TARGETS

- Sometimes, additional side information about targets is available.

- Extra representation for target molecules in drug design (*structured representation*).

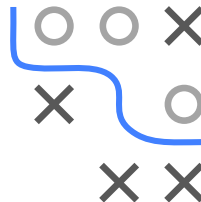
		Mol1	Mol2	Mol3	Mol4	Mol5	Mol6
01101		1,3	0,2	1,4	1,7	3,5	1,3
00111		2	1,7	1,5	7,5	8,2	7,6
01110		0,2	0	0,3	0,4	1,2	2,2
10001		3,1	1,1	1,3	1,1	1,7	5,2
01011		4,7	2,1	2,5	1,5	2,3	8,5

11110		?	?	?	?	?	?
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01101	Text1	0	0	0	0	0	1
00111	Text2	0	0	1	0	1	1
01110	Text3	0	0	0	1	1	0
10001	Text4	0	0	1	0	1	0
01011	Text5	1	0	0	1	0	0







11110	Text6	?	?	?	?	?	?
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- Taxonomy on document categories (*hierarchy*).

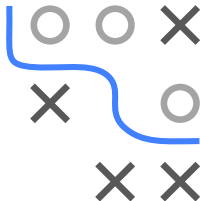
## SIDE INFORMATION ON TARGETS / 2

- Information about schools (geographical location, school reputation) in student mark forecasting (*feature representation*).

		0011	1100	0110
		School1	School2	School3
01101		7		
00111		9		
01110			5	
10001			8	
01011				9
11110		?	?	?

Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).

- Such problems are referred to as dyadic or link prediction.
- Labels  $y_m^{(i)}$  can be arranged in a matrix  $\mathbf{Y}$ , which is often sparse.
- Thus, *dyadic prediction* can be seen as *multi-target prediction with target features*.



# INDUCTIVE VS. TRANSDUCTIVE LEARNING

- In previous problems,
  - 1 predictions need to be generated for novel instances,
  - 2 targets are known beforehand and observed during training.
- These problems are *inductive* w.r.t. instances and *transductive* w.r.t. targets.



- Side information is important for generalizing to novel targets.
  - a novel target molecule in the drug design,
  - a novel tag in the document annotation,

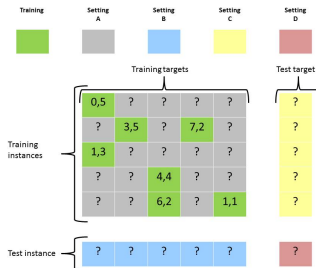
$g(\cdot, \cdot) : \text{target similarity}$

	Mol1	Mol2	Mol3	Mol4	Mol5	Mol6	Mol7
01101	1,3	0,2	1,4	1,7	3,5	1,3	?
00111	2	1,7	1,5	7,5	8,2	7,6	?
01110	0,2	0	0,3	0,4	1,2	2,2	?
10001	3,1	1,1	1,3	1,1	1,7	5,2	?
01011	4,7	2,1	2,5	1,5	2,3	8,5	?
11110	?	?	?	?	?	?	?

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# SUBDIVISION OF DIFFERENT LEARNING SETTINGS

- Setting A — transductive w.r.t. targets and instances. Goal: predict missing values of score matrix (*matrix completion*).
- Setting B — transductive w.r.t. targets and inductive w.r.t. instances (*classical supervised learning*).
- Setting C — inductive w.r.t. targets and transductive w.r.t. instances.  
~> Some targets are unobserved during training but may appear at prediction time.
- Setting D — inductive w.r.t. both targets and instances (*zero-shot learning*).



Waegeman et al. (2019), Multi-target prediction: A unifying view on problems and methods ([URL](#)).

