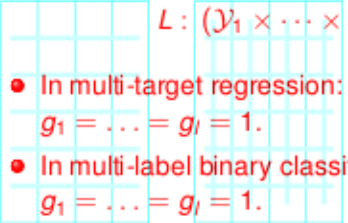
Advanced Machine Learning

Multi-Target Prediction: Loss Functions



Learning goals

- Get to know loss functions for multi-target prediction problems
- Understand the difference between instance-wise and decomposable losses
- Know risk minimizer for Hamming and subset 0/1 loss

MULTIVARIATE LOSS FUNCTIONS

- In MTP: For a feature vector $\mathbf{x}$, predict a tuple of scores $f(\mathbf{x}) = (f(x)_1, f(x)_2, \dots, f(x)_l)^\top$ for l targets with a function (hypothesis) $f : \mathcal{X} \to \mathbb{R}^{g_1} \times \dots \times \mathbb{R}^{g_l}$.
- Following loss minimization in machine learning, we need a *multivariate loss function*

$$L : (\mathcal{Y}_1 \times \dots \times \mathcal{Y}_l) \times (\mathbb{R}^{g_1} \times \dots \times \mathbb{R}^{g_l}) \to \mathbb{R}.$$

- In multi-target regression: $\mathcal{Y}_1 = \dots = \mathcal{Y}_l = \mathbb{R}$, and $g_1 = \dots = g_l = 1$.
- In multi-label binary classification: $\mathcal{Y}_1 = \dots = \mathcal{Y}_l = \{0, 1\}$, and $g_1 = \dots = g_l = 1$.

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- We treat two categories: Decomposable and instance-wise
- L is decomposable over targets if
$$L(\mathbf{y}, f) = \frac{1}{l} \sum_{m=1}^{l} L_m(y_m, f(\mathbf{x})_m)$$
with single-target losses L_m.
- Example: *Squared error loss* (in multivariate regression):
$$L_{\text{MSE}}(\mathbf{y}, f) = \frac{1}{l} \sum_{m=1}^{l} (y_m - f(\mathbf{x})_m)^2.$$
- Can also be used for cases with missing entries.

INSTANCE-WISE LOSSES

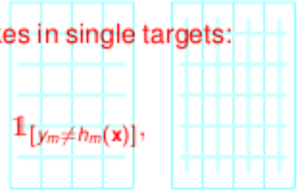
- *Hamming loss* averages over mistakes in single targets:

$$L_H(\mathbf{y}, \mathbf{h}) = \frac{1}{l} \sum_{m=1}^{l} \mathbb{1}_{[y_m \neq h_m(\mathbf{x})]},$$

where $h_m(\mathbf{x}) := [f(\mathbf{x})_m \geq c_m]$ is the threshold function for target m with threshold c_m.

- Hamming loss is identical to the average *0/1 loss* and is decomposable.
- The *subset 0/1 loss* checks for entire correctness and is not decomposable:

$$L_{0/1}(\mathbf{y}, \mathbf{h}) = \mathbb{1}_{[\mathbf{y} \neq \mathbf{h}]} = \max_m \mathbb{1}_{[y_m \neq h_m(\mathbf{x})]}$$



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HAMMING VS. SUBSET 0/1 LOSS

- The risk minimizer for the Hamming loss is the *marginal mode*:

$$f^*(\mathbf{x})_m = \arg\max_{y_m \in \{0,1\}} \Pr(y_m \mid \mathbf{x}), \quad m = 1, \dots, l,$$

  while for the subset 0/1 loss it is the *joint mode*:

$$f^*(\mathbf{x}) = \arg\max_{\mathbf{y}} \Pr(\mathbf{y} \mid \mathbf{x}).$$

- Marginal mode vs. joint mode:

$\mathbf{y}$	$\Pr(\mathbf{y})$
0 0 0 0	0.30
0 1 1 1	0.17
1 0 1 1	0.18
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1 1 1 0	0.18

Marginal mode: 1 1 1 1
Joint mode: 0 0 0 0

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