## Multi Instance Multi Label

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### Machine Learning

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# Binary classification

Goal: To produce a classifier able to decide whether an object belongs to one or more classes.

Idea: Supervised Learning: Given a dataset of already classified examples, the classifier *learns* a function that solves classification problem.

- A vector  $x \in \mathbb{R}^f$  represents an object using f relevant features.
- A vector  $y \in \{-1, +1\}^I$  indicates wether the example belong to each of the I label classes.

The input of a classification problem is a dataset  $D = \{X, Y\}$  where  $X \in \mathbb{R}^{n \times f}$  is a set of examples and  $Y \in \mathbb{R}^{n \times l}$  is a set of labels. While learning the target function, the dataset is divided in *training set* and *test set*.

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• For 1-class problems we have to compute the *maximum-margin* hyperplane  $w^Tx + b$  which best separates positive examples from negative examples.

Optimization problem is:

$$argmin_w \frac{1}{2} ||w||^2$$

$$y^{(i)} (w^T x^{(i)} + b) \ge 1 \ \forall i \in [1, n]$$

• The examples may not be linearly serparable and so the problem would not have any solutions because constraints are not satisfied. Then we introduce slack variables  $\xi$ 

Optimization problem becames:

$$\begin{aligned} & argmin_{w,\xi} \frac{1}{2} ||w||^2 + C \sum_{i=1} n \xi^{(i)} \\ & y^{(i)} (w^T x^{(i)} + b) \ge 1 - \xi^{(i)} \ \forall i \in [1, n] \\ & \xi^{(i)} \ge 0 \ \forall i \in [1, n] \end{aligned}$$

#### Motivation:

- Sometimes a complex item can be well represented by a set of instances
- A single instance may belong or not to a class
- An example is positive if at least one of its instances is positive, it's negative otherwise
- Dataset labels are assigned to examples, not to instances
- We have a semi-supervised learning problem

### Notation

Dataset is now a set of bags, where each bag is a set of instances:

$$D = \{(X^{(i)}, Y^{(i)}) | i \in [1, n]\}$$

$$X^{(i)} = \{x_k^{(i)} | k \in [1, k_i], x_k \in \mathbb{R}^f\}$$

Notice that each bag can be made of any number of instances, but every instance has a fixed number of features f.

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The first naive approach makes the following label assignment:

- If an instance belongs to a negative bag, sets its label is (to?) -1
- If an instance belongs to a positive bag (wrongly) sets its label to +1 che vuol dire?

The resulting problem can be solved using a regular SVM, treating each instance as a whole document.

Using this approach makes almost useless multi-instance formulation.

Instances label assignment:

- ullet If an instance belongs to a negative bag we can say that its label is -1
- If an instance belongs to a positive bag we don't know for sure its label

This leads to 2 new constraints in SVM problem:

$$y_k^{(i)} = -1$$
 if  $Y^{(i)} = -1$ 

$$\sum_{k=1}^{k_i} \frac{y_k^{(i)} + 1}{2} \ge 1 \ \textit{if} \ \ Y^{(i)} = +1$$

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Our SVM problem becames the following:

$$\begin{aligned} \min_{Y} \min_{w,\xi} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \xi^{(i)} \\ y_k^{(i)} (w^T x_k^{(i)} + b) &\geq 1 - \xi^{(i)} \ \forall i \in [1, n], k \in [1, k_i] \\ \xi^{(i)} &\geq 0 \ \forall i \in [1, n] \\ y_k^{(i)} &= -1 \ \text{if} \ Y^{(i)} = -1 \\ \sum_{k=1}^{k_i} \frac{y_k^{(i)} + 1}{2} &\geq 1 \ \text{if} \ Y^{(i)} = +1 \end{aligned}$$

That is an intractable mixed optimization problem

A feasible algorithm that finds a non optimal solution is the following:

```
MI-SVM (X, Y)

1 y_k^{(i)} = -1 if Y^{(i)} = -1

2 y_k^{(i)} = +1 if Y^{(i)} = +1

3 do

4 Solve regular SVM finding w, b

5 y_k^{(i)} = sign(w^T x_k^{(i)} + b) if Y^{(i)} = +1

6 Adjust each positive bag to satisfy constraints

7 while (y_k^{(i)}) change
```

This approach uses directly the dataset in its bag form:

$$argmin_{w,\xi} \frac{1}{2} ||w||^2 + C \sum_{i=1}^n \xi^{(i)}$$

$$y^{(i)} (max_k w^T x_k^{(i)} + b) \ge 1 - \xi^{(i)} \ \forall i \in [1, n]$$

$$\xi^{(i)} \ge 0 \ \forall i \in [1, n]$$

This is possible by selecting a witness from each bag instances.

# Algorithm

A feasible algorithm that finds a solution is the following:

**1** 
$$x_s^{(i)} = avg(x_k^{(i)}) \ \forall i \in [1, n]$$

- do
  - $oldsymbol{0}$  Solve regular SVM finding w, b, balancing lagrange multipliers
  - **2** Find new  $x_s^{(i)}$  by selecting the best one for each positive bag
- while witnesses change

## Multi label classification

#### Motivation:

- Sometimes a complex item can be well represented by a set of labels
- Helps single label classification when the concept is more complicated or general

#### Solutions:

- Problem transformation
- Algorithm adaptation

## **Notation**

A set of labels  $L = \{y_1, y_2, ... y_l\}$  is given.

Each object contained in the dataset is associated with a set of labels:

$$D = \{ (X_i, Y_i | i \in [1, n] \}$$

$$X_i \in \mathbb{R}^f$$

$$Y_i = \{ y_{i,h} | h \in [1, h_i], y_{i,h} \in L, h_i \le I \}$$

## Problem transformation

Attempt to convert the multilabel problem in a regular binary task. Two lossy methods:

- Randomly discard each label information except one from each instance
- Remove instances that have actually more than one label

#### Other solutions:

- Train a binary classifier for each existing combination of labels
- Train a binary classifier for each label (used in this work)

## Algorithm adaptation

Regular algorithms are modified to support multi-label tasks.

Sometimes they use problem transformation at the core.

An example using SVM-related approach based on ranking and label set size prediction.

## Introduction to MIML

MIML problems combine motivations of multi instance and multi label ones.

Given a set of labels 
$$L = \{y_1, y_2, ... y_l\}$$
 
$$D = \{(X_i, Y_i) | i \in [1, n]\}$$
 
$$X_i = \{x_{i,k} | k \in [1, k_i], x_{i,k} \in \mathbb{R}^f\}$$
 
$$Y_i = \{y_{i,h} | h \in [1, h_i], y_{i,h} \in L, h_i \leq l\}$$

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## SVM Solution

To allow regular SVMs to solve this problem, we use *problem transformation*.

There are 2 possibilities:

- MIML → MISL → SISL (used in this work)
- MIMI  $\rightarrow$  SIMI  $\rightarrow$  SISI

# Multi label to single label

Excluding lossy approaches, the idea is to train a multi-instance (single label) classifier for each label.

Given a MIML dataset  $D = \{(X_i, Y_i) | i \in [1, n]\}$  we produce I datasets as follows:

$$D_{y_j} = \{(X_i, Y_{y_j}) | i \in [1, n]\} \ \forall j \in [1, L]$$

Where

$$Y_{y_j} = \begin{cases} +1 & \text{if } y_j \in Y_i \\ -1 & \text{otherwise} \end{cases}$$

Then we train L regular multi-instance SVMs and collect their results.

## Multi instance to single instance

Given one of MISL datasets produced at previous step, we compared the 3 methods previously exposed:

- SIL
- MI-SVM
- mi-SVM

They all use a standard SISL SVM as subroutine.