

Multi Instance Multi Label

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- Introduction

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 $y \in \{-1, +1\}^l$ indicates whether the example belongs to each of the l 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*.

SVM idea

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

Optimization problem is:

$$\operatorname{argmin}_w \frac{1}{2} \|w\|^2$$

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

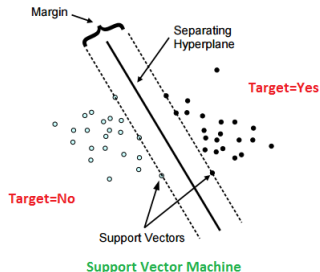


Figure 1: Solution of maximum-margin hyperplane

SVM idea

- The examples may not be linearly separable and so the problem would not have any solutions because constraints are not satisfied. Then we introduce slack variables ξ

Optimization problem becomes:

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

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

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

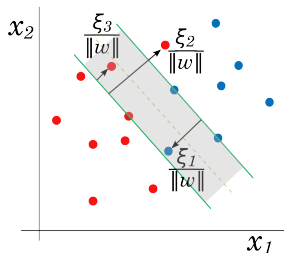


Figure 2: Solution with slacks

Multi instance classification

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

[1]

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

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

$$X_i = \{x_{i,k} | k \in [1, k_i], x_{i,k} \in \mathbb{R}^f\}$$

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

The first naive approach makes the following label assignment:

- If an instance belongs to a negative bag, sets its label to -1
- If an instance belongs to a positive bag, sets its label to $+1$

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:

- 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:

$$y_{i,k} = -1 \text{ if } Y_i = -1$$

$$\sum_{k=1}^{k_i} \frac{y_{i,k} + 1}{2} \geq 1 \text{ if } Y_i = +1$$

Our SVM problem becomes the following:

$$\min_Y \min_{w, \xi} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i$$

$$y_{i,k}(w^T x_{i,k} + b) \geq 1 - \xi_i \quad \forall i \in [1, n], k \in [1, k_i]$$

$$\xi_i \geq 0 \quad \forall i \in [1, n]$$

$$y_{i,k} = -1 \text{ if } Y_i = -1$$

$$\sum_{k=1}^{k_i} \frac{y_{i,k} + 1}{2} \geq 1 \text{ if } Y_i = +1$$

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       $y_k^{(i)} = \text{sign}(w^T x_k^{(i)} + b)$  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:

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

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

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

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

A feasible algorithm that finds a solution is the following:

MI-SVM(X, Y)

```
1   $\bar{x}_i = \text{avg}(x_{i,k}) \ \forall x_{i,k} \in X_i$  positive bag
2  do
3      Assign  $\bar{\alpha}_i \in [0, C]$  to each  $\bar{x}_i$ 
4      Assign  $\alpha_{i,j}$  with  $\sum_{j=1}^{k_i} \alpha_{i,j} \in [0, C] \ \forall x_{i,k} \in X_i$  negative bag
5      Solve regular SVM finding  $w, b$ 
6      Find new  $\bar{x}_i$  by selecting the best one for each positive bag
7  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

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

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

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

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

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

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)

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.

Another multi label approach

[2]

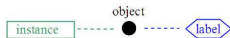
Introduction to MIML

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

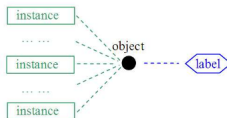
Given a set of labels $L = \{y_1, y_2, \dots, y_l\}$

$$X_i = \{x_{i,k} | k \in [1, k_i], x_{i,k} \in \mathbb{R}^f\} \quad Y_i = \{y_{i,h} | h \in [1, h_i], y_{i,h} \in L, h_i \leq l\}$$

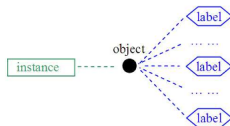
$$D = \{(X_i, Y_i) | i \in [1, n]\}$$



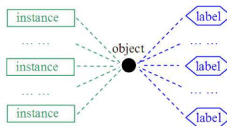
(a) Traditional supervised learning



(b) Multi-instance learning



(c) Multi-label learning



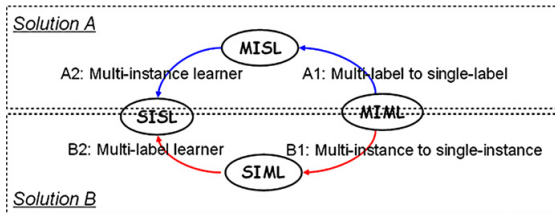
(d) Multi-instance multi-label learning

SVM Solution

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

There are 2 possibilities:

- MIML \rightarrow MISL \rightarrow SISL (used in this work)
- MIML \rightarrow SIML \rightarrow SISL



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 L datasets as follows:

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

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.

- [1] S. Andrews, I. Tsochantaridis, and T. Hofmann. Support vector machines for multiple-instance learning. *S. Becker, S. Thrun, K. Obermayer (Eds.), Advances in Neural Information Processing Systems*, 2003.
- [2] A. Elisseeff and J. Weston. A kernel method for multi-labelled classification. *Advances in neural information processing systems*, 2002.
- [3] Zhi-Hua Zhou, Min-Ling Zhang, Sheng-Jun Huang, and Yu-Feng Li. Multi-instance multi-label learning. *Artificial Intelligence*, 176(1):2291–2320, 2012.