Multi-Instance Learning Revisited
（多示例学习回顾）

Zhi-Hua Zhou

http://cs.nju.edu.cn/zhouzh/
Email: zhouzh@nju.edu.cn

LAMDA Group
National Key Laboratory for Novel Software Technology,
Nanjing University, China
The talk involves some joint work with my students:

Min-Ling Zhang (张敏灵)
Yu-Feng Li (李宇峰)
Jun-Ming Xu (眭俊明)
Yu-Yin Sun (孙雨音)
Xiao-Bing Xue (薛晓冰)

... ...

And my collaborators:

James Kwok
Ivor Tsang

... ...
Origin
The Motivating Problem

Originated from the research on drug activity prediction [Dietterich et al. AIJ97]

- Drugs are small molecules working by binding to the target area
- For molecules qualified to make the drug, one of its shapes could tightly bind to the target area
The Motivating Problem (con't)

- A molecule may have many alternative shapes

Reprinted from [Dietterich et al., AIJ97]

The difficulty:

Biochemists know that whether a molecule is qualified or not, but do not know which shape responses for the qualification
To Represent the Molecule

Each shape can be represented by a feature vector, i.e., an instance…

Thus, a molecule is a **bag** of instances

- A bag is positive if it contains at least one positive instance; otherwise it is negative
- The labels of the training bags are known
- The labels of the instances in the training bags are unknown
Formal Definition of MIL

Given a data set \( \{(X_1, y_1), \ldots, (X_i, y_i), \ldots, (X_N, y_N)\} \), where \( X_i = \{x_{i1}, \ldots, x_{ij}, \ldots, x_{in} \} \subseteq \mathcal{X} \) is called a bag and \( y_i \in \mathcal{Y} = \{-1, +1\} \) is the label of \( X_i \), the goal is to predict the labels of unseen bags.

\( X_i \) is a positive bag (thus \( y_i = +1 \)) if there exists \( g \in \{1, \ldots, n\} \), \( x_{ig} \) is positive. Yet the value of the index \( g \) is unknown.

\( x_{ij} \in \mathcal{X} \) is an instance \([x_{ij1}, \ldots, x_{ijl}, \ldots, x_{ijd}]^{'}\), \( x_{ijl} \) is the value of \( x_{ij} \) at the \( l \)-th attribute.
Can we solve this problem with traditional supervised learning?

Possible solution 1: Assign the bag labels to instances

Maybe most instances in the positive bag are actually negative.
Possible solution 2: Concatenate the instances in a bag

Moreover, different bags may contain different number of instances

Which order should be used?
The APR Algorithms

Three APR (Axis-Parallel Rectangle) algorithms

Iterated-discrim APR

• Iterated-discrim APR achieves the best performance on the MUSK data (92.4% / 89.2%)

• BP neural network and C4.5 decision tree cannot work well

  BP (75.0% / 67.7%)

  C4.5 (68.5% / 58.8%)

Figure reprinted from [Dietterich et al., AIJ97]
Comparing with Traditional Supervised Learning

Traditional (single-instance) supervised learning

Multi-instance learning
Why MIL is Appealing?

Many tasks can be modeled as an MIL task

$[a_1, a_2, \ldots, a_m]^T$

$[b_1, b_2, \ldots, b_m]^T$

$\ldots$

$[u_1, u_2, \ldots, u_m]^T$

image $\rightarrow$ bag

regions in the image $\rightarrow$ instances in the bag
Applications
MIL Applications

✓ Drug prediction [Dietterich et al., AIJ97]
✓ Image categorization [Maron & Ratan, ICML’98; Chen & Wang, JMLR04; Chen et al., PAMI06]
✓ Image retrieval [Zhang et al., ICDE’02; Zhou et al., AJCAI’05]
✓ Text categorization [Andrews et al., NIPS’02; Settles et al., NIPS’07]
✓ Computer security [Ruffo, Thesis00]
✓ Web mining [Zhou et al., APIN05]
✓ Face detection [Viola et al., NIPS’05; Zhang & Viola, NIPS’07]
✓ Computer-aided medical diagnosis [Fung et al., NIPS’06]
✓ ... ...
Figure 6: Results for the waterfall concept using the **single blob with neighbors** concept with $+10\text{fp}$. Top row: Initial training set—5 positive and 5 negative examples. Second row: Additional false positives. Last three rows: Top 30 matches retrieved from the large test set. The red squares indicate where the closest instance to the learned concept is located.

Figure reprinted from [Maron & Ratan, ICML'98]
Application: Image Retrieval

User-selected positive examples

User-selected negative examples

Final retrieval from test set (top 16 images)

Figure 6. A sample run with 3 rounds of training: retrieving cars

Figure 7. Precision-recall curve for Figure 6

Figures reprinted from [Yang & Lozano-Pérez, ICDE’00]
Application: Stock Selection

**Goal:** To choose stocks perform well for fundamental reasons

**Positive bag:** 100 stocks with the highest return in every month

**Negative bag:** the bottom 5 stocks in every month

Figure 6: Black bars show Diverse Density’s average return on a decile, and the white bars show GMO’s predictor’s return.

Figures reprinted from [Maron & Lozano-Pérez, NIPS’97]
Application: Webpage Recommendation

A web index page linking to \( m \) pages, i.e. a bag containing \( m \) instances, can be represented as 
\[
\{[t_{11}, t_{12}, \ldots, t_{1n}], [t_{21}, t_{22}, \ldots, t_{2n}], \ldots, [t_{m1}, t_{m2}, \ldots, t_{mn}]\}
\]

The label of the bag is positive if the web index page interested the user; otherwise the label is negative.

Fig. 1. The web index page is regarded as a bag, while its linked pages are regarded as the instances in the bag.

Figure reprinted from [Zhou et al., APIN05]
Application: Face Detection

By incorporating MIL, the detection rate of the famous Viola-Jones face detector improves by nearly 15% (at a 10% false positive rate)

Figure 2: Some of the subwindows in one positive bag.

Figures reprinted from [Viola et al., NIPS’05]

http://cs.nju.edu.cn/zhouzh/
Learnability
Learnability - Earlier Results

- [Long & Tan, COLT'96; MLJ98]
  - If the instances in the bags are independently drawn from product distribution, then the APR is PAC-learnable
  - A polynomial-time theoretical algorithm

- [Auer et al., JCSS98]
  - If the instances in the bags are not independent, then APR learning under MIL is NP-hard
  - A theoretical algorithm that does not require product distribution but with smaller sample complexity than that of Long and Tan's algorithm. Later transformed to MULTINST [Auer, ICML'97]

- [Blum & Kalai, MLJ98]
  - A reduction from the problem of PAC-learning under MIL to PAC-learning with one-sided random classification noise
  - A theoretical algorithm with smaller sample complexity than that of Auer et al.'s algorithm
Learnability - Summary of Main Results

<table>
<thead>
<tr>
<th></th>
<th>Sample</th>
<th>Time</th>
<th>Assumption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Long &amp; Tan</td>
<td>(\tilde{O}(\frac{d^2 r^6}{\varepsilon^{10}}))</td>
<td>(\tilde{O}(\frac{d^5 r^{12}}{\varepsilon^{20}}))</td>
<td>Instances in bag are independent, and drawn from production distribution</td>
</tr>
<tr>
<td>Auer et al.</td>
<td>(\tilde{O}(\frac{d^2 r^2}{\varepsilon^2}))</td>
<td>(\tilde{O}(\frac{d^3 r^2}{\varepsilon^2}))</td>
<td>Instances in bag are independent</td>
</tr>
<tr>
<td>Blum &amp; Kalai</td>
<td>(\tilde{O}(\frac{d^2 r^2}{\varepsilon^2}))</td>
<td>(\tilde{O}(\frac{d^3 r^2}{\varepsilon^2}))</td>
<td>Instances in bag are independent</td>
</tr>
</tbody>
</table>
Learnability - Important Insights

The heterogeneous case: MIL is hard [Auer et al., JCSS98]

- PAC-learning disjunctions of $r$ APR over $R^d$ is as hard as learning DNF formulas with $r$ clauses over $d$ variables
- A polynomial-time algorithm exists only if $RP = NP$

The homogeneous case: If instances are independent, MIL is easy [Blum & Kalai, MLJ98]

- There is a polynomial-time reduction from MIL to the problem of classification with random label noise

Heterogeneous: Each instance in the bag is classified by a different rule

Homogeneous: All instances are classified by the same rule
Learnability - A Recent Result

The homogeneous case, when instances are statistically dependent [Sabato & Tishby, COLT’08]:

- At least for $\neq \text{OR}$, MIL is PAC-learnable for arbitrary distribution over bags
- VC-dim grows logarithmically with $r$. 

Algorithms
Representative Algorithms - Diverse Density

(a) The different shapes that a molecule can take on are represented as a path. The intersection point of positive paths is where they took on the same shape.

(b) Samples taken along the paths. Section B is a high density area, but point A is a high Diverse Density area.

Figure 1: A motivating example for Diverse Density

To search for the point with the maximal diverse density by gradient search, every instance in positive bags is used as a start point for search.

Figures reprinted from [Maron & Lozano-Pérez, NIPS'97]
To search for the maximal margin hyperplane
the margin of a “positive bag” is
the margin of its “most positive” instance

\[ \text{MI-SVM} \quad \min_{w,b,\xi} \frac{1}{2} \|w\|^2 + C \sum_I \xi_I \]
\[ \text{s.t.} \quad \forall I : Y_I \max_{i \in I} (\langle w, x_i \rangle + b) \geq 1 - \xi_I, \xi_I \geq 0. \]
Representative Algorithms - MI-Kernel

Based on set kernel:

$$K(Bag_1, Bag_2) = \sum_{i=1}^{M} \sum_{j=1}^{N} k(x_{1i}, x_{2j})$$

$k$ is Gaussian RBF kernel

[Gärtner et al., ICML'02]
Many MIL Algorithms

- **Diverse Density** [Maron & Lozano-Perez, NIPS’97], **EM-DD** [Zhou & Goldman, NIPS’01]
- **K-Nearest Neighbor:** Citation-kNN [Wang & Zucker, ICML’00]
- **Decision trees:** RELIC [Ruffo, Thesis00], MITI [Blockeel et al., ICML’05]
- **Neural networks:** BP-MIP [Zhou & Zhang, ICIIT’02], RBF-MIP [Zhang & Zhou, NPL06]
- **Rule learning algorithm:** RIPPER-MI [Chevaleyre & Zucker, CanadianAI’01]
- **Ensemble methods:** MI-Ensemble [Zhou & Zhang, ECML’03], MI-Boosting [Xu & Frank, PAKDD’04], MIL-Boosting [Auer & Ortner, ECML’04]
- **Logistic regression algorithm:** MI-LR [Ray & Craven, ICML’05]
- ... ...
Kernel/SVM Methods

- MI-Kernel  [Gärtner et al., ICML'02]
- mi-SVM and MI-SVM [Andrews et al., NIPS'02]
- DD-SVM [Chen & Wang, JMLR04]
- CCCP SVM [Cheung & Kwok, ICML'06]
- marginalized Kernel [Kwok & Cheung, IJCAI'07]
- MissSVM [Zhou & Xu, ICML'07]
- PPMM Kernel [Wang et al., ICML'08]
- ... ...
Adapting SIL Algorithms to MIL

A general routine:

Supervised learning algorithms can be adapted to multi-instance learning, by shifting their focuses from the discrimination on instances to the discrimination on bags

[Zhou & Zhang, ECML’03; JCST06]
A New General Solution

adapt single-instance learners to multi-instance representation

Multi-instance representation

adapt multi-instance representation to single-instance learners

Single-instance learner
Example: The CCE Algorithm

CCE (Constructive Clustering based Ensemble) [Zhou & Zhang, KAIS07]

The key: Re-represent bags as single-instances

Classifier 1

Instance in bag₁: [2,3,1]
Instance in bag₂: [1,1,3]

Classifier 2

Instance in bag₁: [5,1]
Instance in bag₂: [2,3]

Classifier N

Instance in bag₁: [4,2]
Instance in bag₂: [1,4]

Ensemble
It is worth noting that:

Most existing MIL algorithms assume i.i.d. instances
A Recent Study

[Zhou & Xu, ICML’07] disclosed that if instances in bags were assumed as i.i.d. samples, MIL is just a special case of semi-supervised learning.

The definition of MIL [Dietterich et al., AIJ97] implies that:

- **Negative bags contain only negative instances**
  Thus, we can regard instances from negative bags as labeled negative examples.

- **Positive bags can contain positive as well as negative instances**
  Thus, we can regard instances from positive bags as unlabeled examples with positive constraints.
An semi-supervised learning task:

**Definition 1** Given a set of labeled negative examples \(((x_1, -1), (x_2, -1), \ldots, (x_{TL}, -1))\) and a set of unlabeled instances \(\{x_{TL+1}, \ldots, x_T\}\), to learn a function \(F^s: \mathcal{X} \rightarrow \{-1, +1\}\) subject to: For \(i = q + 1, \ldots, m\), at least one instance in \(\{x_{s_i}, \ldots, x_{e_i}\}\) is positive.

The task can be solved by semi-supervised SVM algorithm:

MissSVM (**Multi-instance learning by semi-supervised SVM**) 
- Our main focus is not the proposal of a new algorithm (although we do propose a new algorithm)
- Instead of designing elaborate method, we try to use typical and simple SSL technique
The MissSVM Algorithm - [Zhou & Xu, ICML’07]

The optimization problem for popular semi-supervised support vector machine:

\[
\min_f \frac{1}{2} \|f\|^2_H + \lambda \sum_{t=1}^{T_L} H_1(y_t f(x_t)) + \delta \sum_{t=T_L+1}^{T} D(f(x_t))
\]

where \( H_1(z) = \max\{0, 1 - z\} \) is hinge loss

\[
D(z) = \min\{H_1(z), H_1(-z)\} \quad [\text{Bennett & Demiriz, NIPS’98}]
\]

Considering the positive constraints, the term should be added:

\[
\sum_{i=q+1}^{m} H_1\left(\max_{t=s_i, \ldots, c_i} f(x_t)\right)
\]
The MissSVM Algorithm (con’t)

Thus, the optimization problem can be written as:

\[
\min_{f \in \mathcal{H}, \eta, \theta, \varepsilon, \xi} \frac{1}{2} \|f\|_{\mathcal{H}}^2 + \lambda \eta' 1 + \gamma \theta' 1 + \delta \min(\varepsilon, \xi)' 1
\]

\[
\begin{align*}
& (-1)f(x_t) + \eta_t \geq 1, \ \eta_t \geq 0, \ t = 1, 2, \ldots, T_L; \\
& \max_{t = s_i, \ldots, e_i} f(x_t) + \theta_{i-q} \geq 1, \ \theta_{i-q} \geq 0, \\
& \text{s.t.} \\
& f(x_t) + \varepsilon_{t-T_L} \geq 1, \ \varepsilon_{t-T_L} \geq 0, \ t = T_L + 1, \ldots, T; \\
& (-1)f(x_t) + \xi_{t-T_L} \geq 1, \ \xi_{t-T_L} \geq 0, \ t = T_L + 1, \ldots, T.
\end{align*}
\]

- \( \eta = [\eta_1, \ldots, \eta_{T_L}]' \) - slack variables for errors on instances from negative bags
- \( \theta = [\theta_1, \ldots, \theta_p]' \) - slack variables for errors on positive bags
- \( \varepsilon = [\varepsilon_1, \ldots, \varepsilon_{T_U}]' \) and \( \xi = [\xi_1, \ldots, \xi_{T_U}]' \) - slack variables for errors on instances from positive bags
- \( \lambda, \gamma \) and \( \delta \) - parameters
The MissSVM Algorithm (con’t)

Let $K$ denote a $T \times T$ kernel matrix and let $k_t$ denote the $t$-th column:

$$\min_{\alpha, \eta, \theta, \varepsilon, \xi, b} \frac{1}{2} \alpha' K \alpha + \lambda \eta' 1 + \gamma \theta' 1 + \delta \min(\varepsilon, \xi)' 1$$

subject to

$$(-1)(k'_t \alpha + b) + \eta_t \geq 1, \quad \eta_t \geq 0,$$

$$\max_{t=s_i, \cdots, c_i} (k'_t \alpha + b) + \theta_{i-q} \geq 1, \quad \theta_{i-q} \geq 0,$$

$$i = q + 1, \cdots, m;$$

$$(k'_t \alpha + b) + \varepsilon_{t-T_L} \geq 1, \quad \varepsilon_{t-T_L} \geq 0,$$

$$t = T_L + 1, \cdots, T;$$

$$(-1)(k'_t \alpha + b) + \xi_{t-T_L} \geq 1, \quad \xi_{t-T_L} \geq 0,$$

$$t = T_L + 1, \cdots, T.$$

After replacing the gradients of the non-smooth $\min$ and $\max$ by their subgradients, CCCP (Constrained Convex-Concave Procedure) [Smola et al., AISTATS’05] can be used to solve this optimization problem.
Shouldn’t Assume I.I.D. Instances

From the aspect of the nature of MIL task:

It is often not reasonable to assume independent instances since the instances were generally extracted from the same object.

From the aspect of MIL techniques:

If i.i.d. instances were assumed, MIL problems can be solved by adapting SSL techniques, and therefore we do not need to study dedicated MIL techniques.
Can we do MIL without assuming i.i.d. instances?
An Inspirational Example

Figure 1. Example images with six marked patches each corresponding to an instance.
An Inspirational Example (con’t)

Figure 2. If we do not consider the relations among the instances, the three bags are similar to each other since they have identical number of very similar instances.

Figure reprinted from [Zhou et al., ICML’09]
An Inspirational Example (con’t)

Figure 3. If we consider the relations among the instances, the first two bags are more similar than the third bag. Here, the solid lines highlight the high affinity among similar instances.
1) Map each bag into a graph (e.g., $\varepsilon$-graph)
The MIGraph Method (con’t)

2) A graph kernel to distinguish positive/negative graphs

*Figure 4. Illustration of the graph kernel in MIGraph*
We define both $k_{nd}$ and $k_{ed}$ as Gaussian RBF kernel.

**Complexity of MIGraph:** $O(n_in_j + m_im_j)$
1) Instead of constructing a graph explicitly, we consider an affinity matrix for each bag

\[ \begin{bmatrix}
1 & 1 & \cdots & 0 \\
1 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 1 
\end{bmatrix} \]

\[ \begin{bmatrix}
d_{11} & d_{12} & \cdots & d_{1M} \\
d_{21} & d_{22} & \cdots & d_{2M} \\
\vdots & \vdots & \ddots & \vdots \\
d_{M1} & d_{M2} & \cdots & d_{MM} 
\end{bmatrix} \]
The miGraph Method (con’t)

2) A kernel to distinguish positive/negative graphs

\[ k_g(X_i, X_j) = \sum_{a=1}^{n_i} \sum_{b=1}^{n_j} W_{i\alpha} W_{j\beta} k(x_{i\alpha}, x_{j\beta}) \]

\[ W_{i\alpha} = 1/\sum_{u=1}^{n_i} w_{i\alpha u} \]

Complexity of miGraph: \( O(n_i n_j) \)

The node kernel as similar as in MIGraph, realized with Gaussian RBF kernel
Four Kinds of Tasks

1. Benchmark tasks
2. Image categorization
3. Text categorization
4. Multi-instance regression

We have re-implemented MI-Kernel since the comparison with MI-Kernel will clearly show whether it is helpful to treat instances as non-i.i.d. samples.

The performance of MI-Kernel in our implementation is better than that reported in [Gärtner et al., ICML’02].
The Implication

When designing MIL algorithms, we should not treat instances in bags as i.i.d. samples!!

A new way to the design of MIL algorithms. Many things can be done along this way, e.g.,

✓ Better graph/kernel
✓ Extend to other MIL methods/settings
✓ Alternative non-i.i.d. strategies
✓ ... ...

http://cs.nju.edu.cn/zhouch/
Can we identify the “key instances”? 
Locating ROI in CBIR

Return relevant images with marked ROI
Potential usage: medical, military, etc.

Fig. 3. The ROI located by Diverse Density and CkNN-ROI. Each row shows five pairs of example images on the target concepts castle, firework, mountain, sunset, and waterfall, respectively. In each pair the first image is obtained with Diverse Density while the second one is obtained with CkNN-ROI.

DD can be used in scene classification, but can hardly in CBIR

Time per query:
• DD: 14,475 seconds (≈ 4 hours)
• CkNN-ROI: 0.32 second

The first attempt of locating ROI in CBIR

Figure reprinted from [Zhou et al., AJCAI’05]
Locating ROI in CBIR (con’t)

**MI-SVM** [Andrews et al., NIP’02]
- can identify key instances

The MI-SVM formulation is non-convex

**KI-SVM** [Li et al., ECML’09]:
- A Convex relaxation method
  - Inst-KI-SVM
  - Bag-KI-SVM

Improving efficiency by using cutting plane and label generation

Performance better than DD, CkNN-ROI and MI-SVM
Efficiency better than DD and MI-SVM
Multi-Instance Learning ... more details

Adapting SIL-learners to MIL-representation; MI-Ensemble:


Adapting MIL-representation to SIL-learners:


Code: http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/CCE.htm
Multi-Instance Learning ... more details

**MIL & SSL:**


  Code: [http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/MissSVM.htm](http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/MissSVM.htm)

**MIL without i.i.d. assumption:**


  Code: [http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miGraph.htm](http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miGraph.htm)

Identifying key instances:


Code: http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/KISVM.htm
Multi-Instance Learning ... more details

**MIL-based Webpage recommendation:**


**Multi-instance bag generator:**

Thanks!