

# Multi-Instance Learning Revisited

(多示例学习回顾)

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The talk involves some joint work with my students :

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*Yu-Yin Sun (孙雨音)*

*Xiao-Bing Xue (薛晓冰)*

... ..

And my collaborators:

*James Kwok*

*Ivor Tsang*

... ..

# Origin

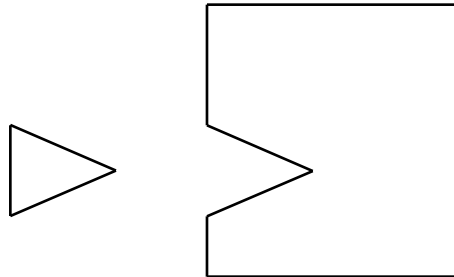
# The Motivating Problem

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Originated from the research on drug activity prediction

[Dietterich et al. AIJ97]

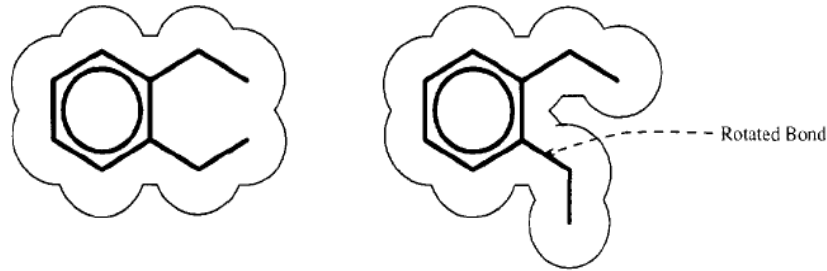
- Drugs are small molecules working by binding to the target area
- For molecules qualified to make the drug, one of its shapes could tightly bind to the target area



## The Motivating Problem (con't)

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- A molecule may have many alternative shapes



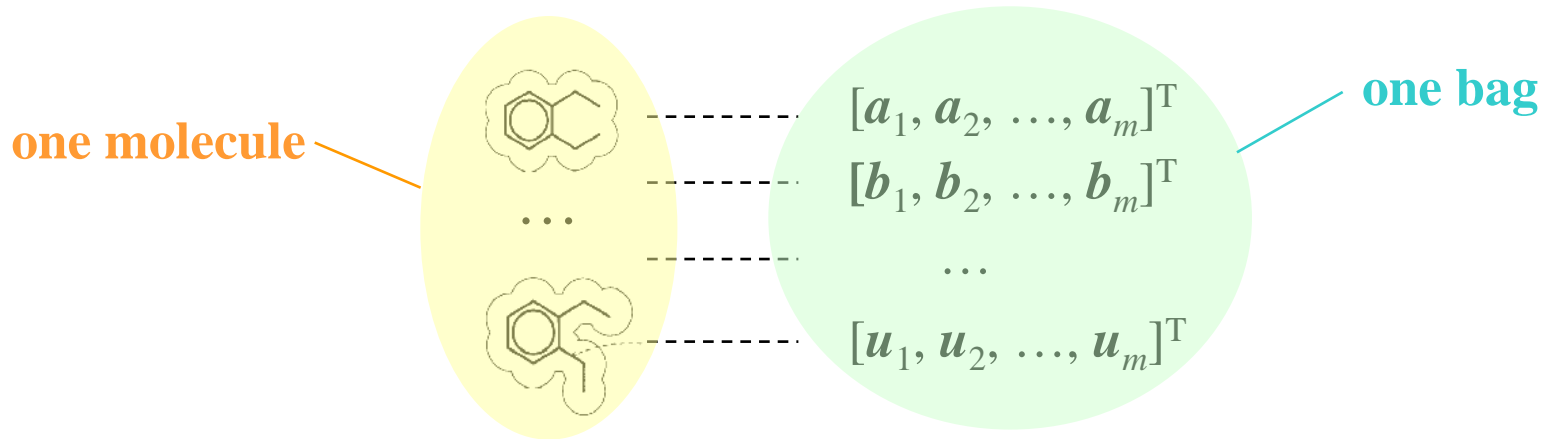
Reprinted from [Dietterich et al., AIJ97]

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

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Given a data set  $\{(X_1, y_1), \dots, (X_i, y_i), \dots, (X_N, y_N)\}$ , where  $X_i = \{x_{i1}, \dots, x_{ij}, \dots, x_{in_i}\} \subseteq \mathcal{X}$  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

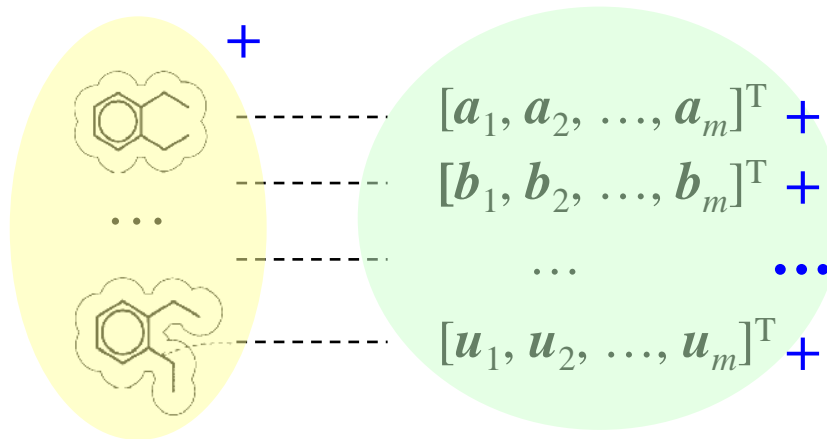
$X_i$  is a positive bag (thus  $y_i = +1$ ) if there exists  $g \in \{1, \dots, n_i\}$ ,  $x_{ig}$  is positive. Yet the value of the index  $g$  is unknown

$x_{ij} \in \mathcal{X}$  is an instance  $[x_{ij1}, \dots, x_{ijl}, \dots, x_{ijd}]'$ ,  $x_{ijl}$  is the value of  $x_{ij}$  at the  $l$ -th attribute

# Why Multi-Instance Learning?

Can we solve this problem with traditional supervised learning?

Possible solution ~~1~~: Assign the bag labels to instances

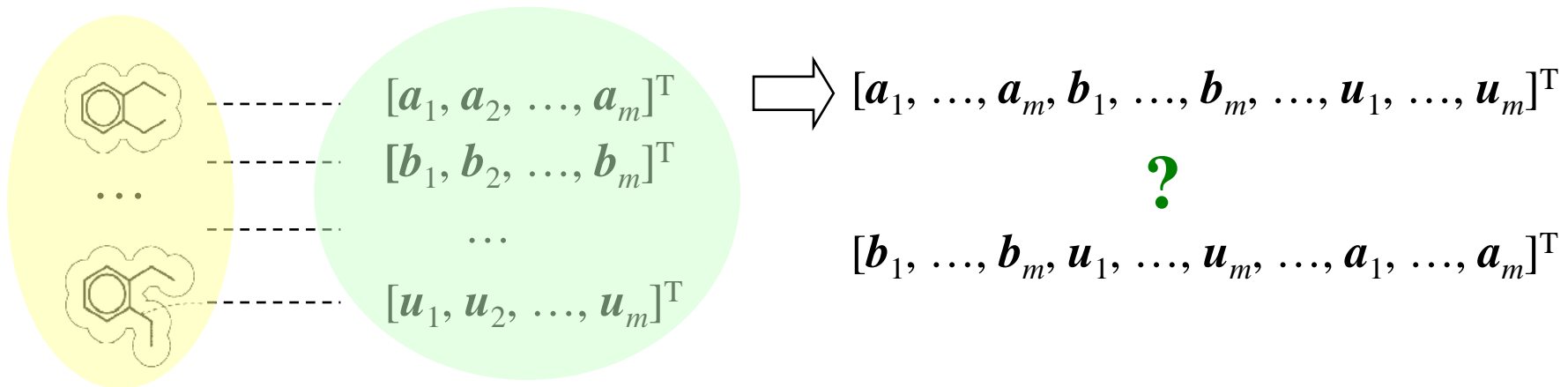


Maybe most instances in the positive bag are actually negative



## Why Multi-Instance Learning? (con't)

Possible solution ~~1~~ 2: Concatenate the instances in a bag



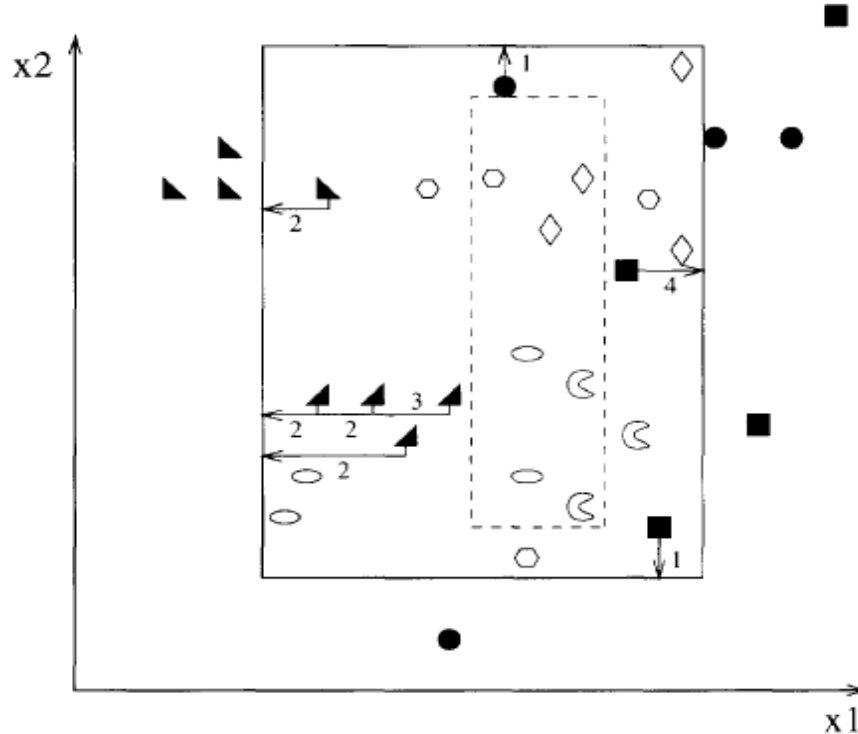
Which order should be used?

Moreover, different bags may contain different number of instances

# The APR Algorithms

## Three APR (Axis-Parallel Rectangle) algorithms

### Iterated-discrim APR



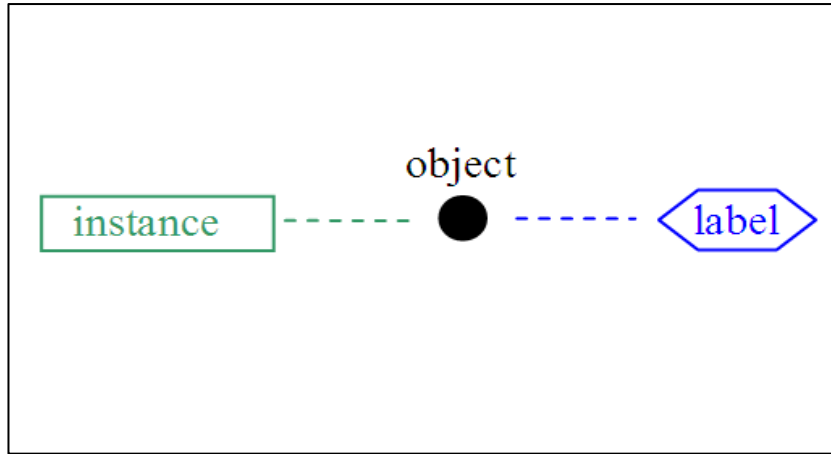
- Iterated-discrim APR achieves the best performance on the MUSK data (92.4% / 89.2%)
- BP neural network and C4.5 decision tree cannot work well

BP (75.0% / 67.7%)

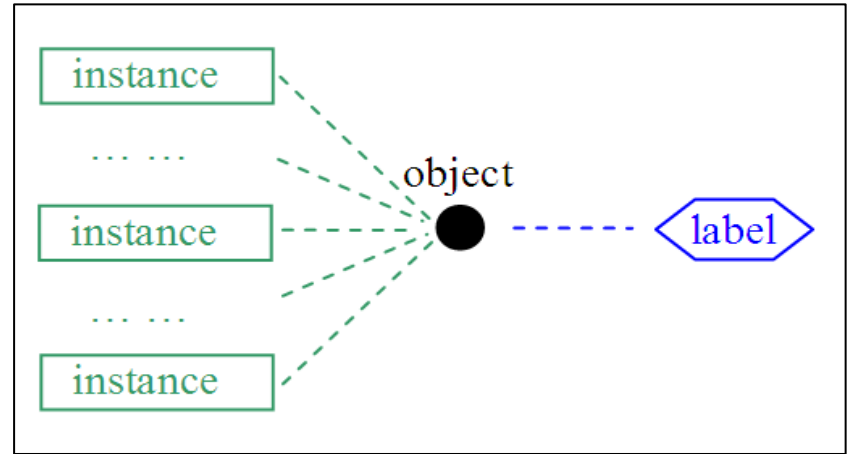
C4.5 (68.5% / 58.8%)

# Comparing with Traditional Supervised Learning

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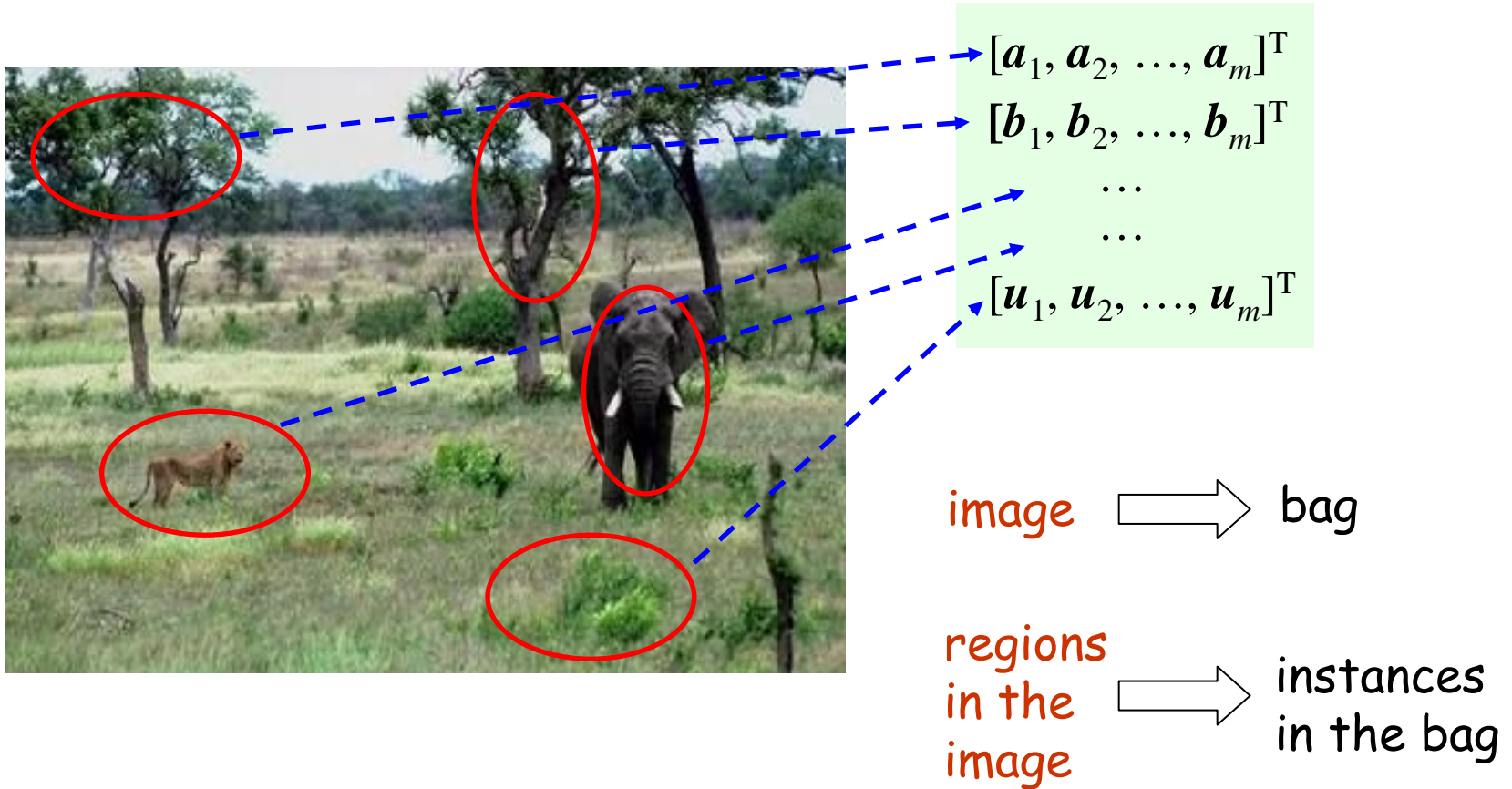
Traditional (single-instance)  
supervised learning



Multi-instance learning

# Why MIL is Appealing ?

Many tasks can be modeled as an MIL task



# Applications

# MIL Applications

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- ✓ 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]
- ✓ ... ..

# Application: Image Categorization

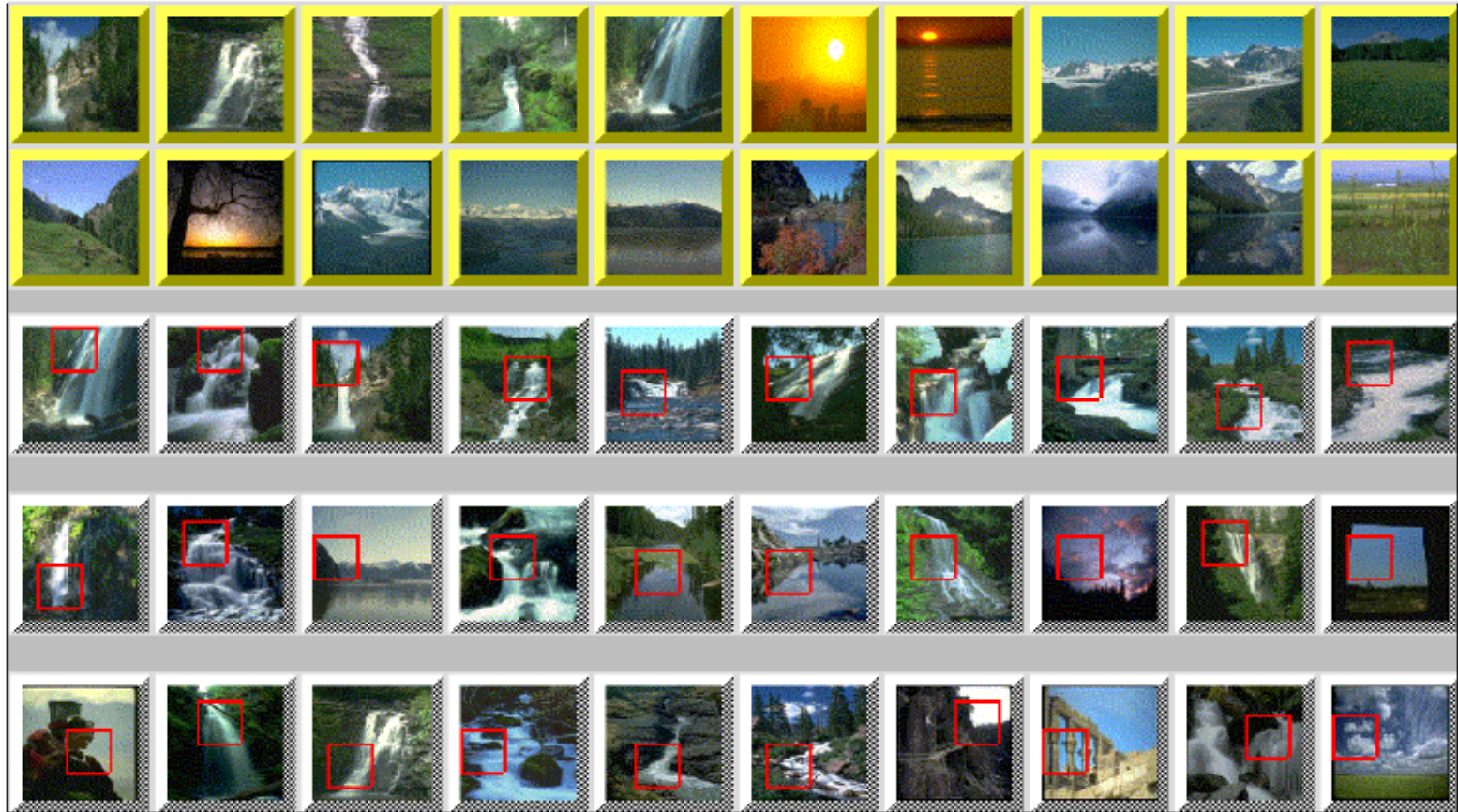


Figure 6: Results for the waterfall concept using the **single blob with neighbors** concept with **+10fp**. Top row: Initial training set—5 positive and 5 negative examples. Second Row: Additional false positives. Last three rows: Top 30 matches retrieved from the large test set. The red squares indicate where the closest instance to the learned concept is located.



# Application: Image Retrieval



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

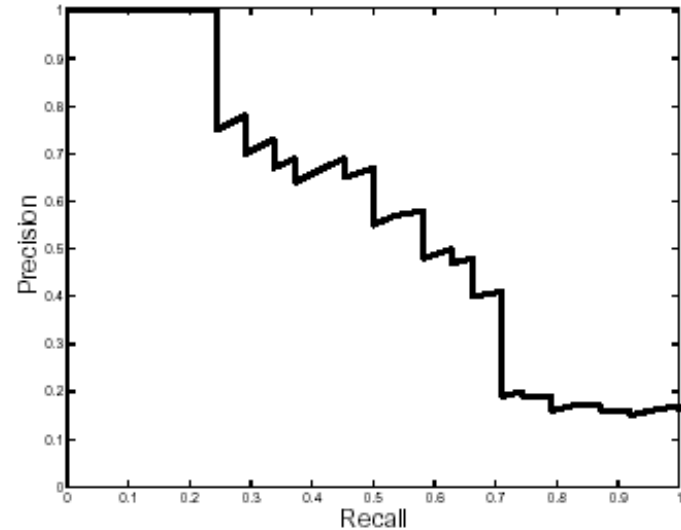


Figure 7. Precision-recall curve for Figure 6



# 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

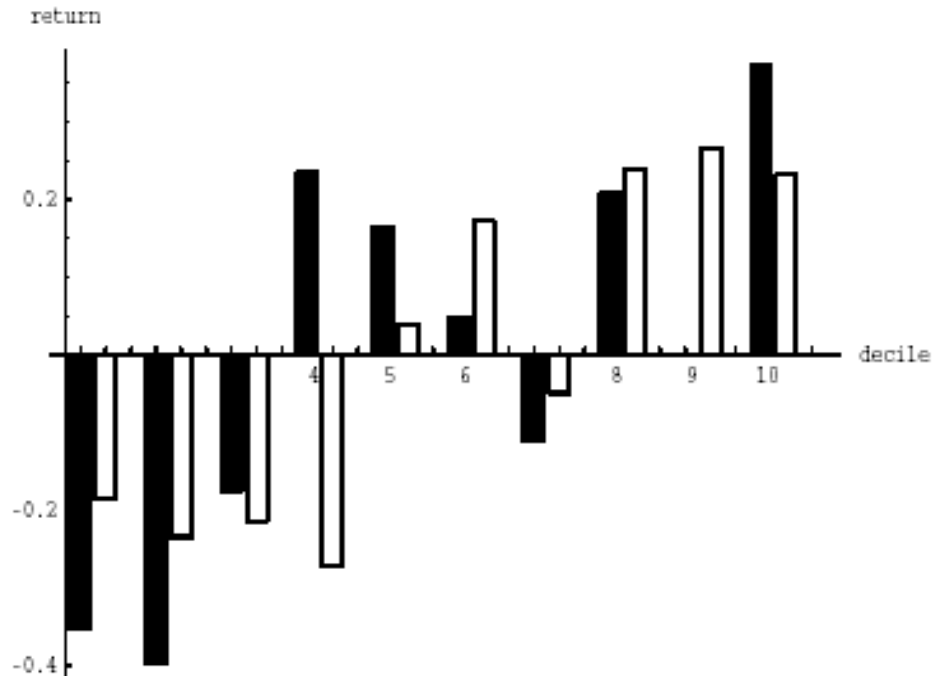


Figure 6: Black bars show Diverse Density's average return on a decile, and the white bars show GMO's predictor's return.

# Application: Webpage Recommendation



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

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

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

# Application: Face Detection

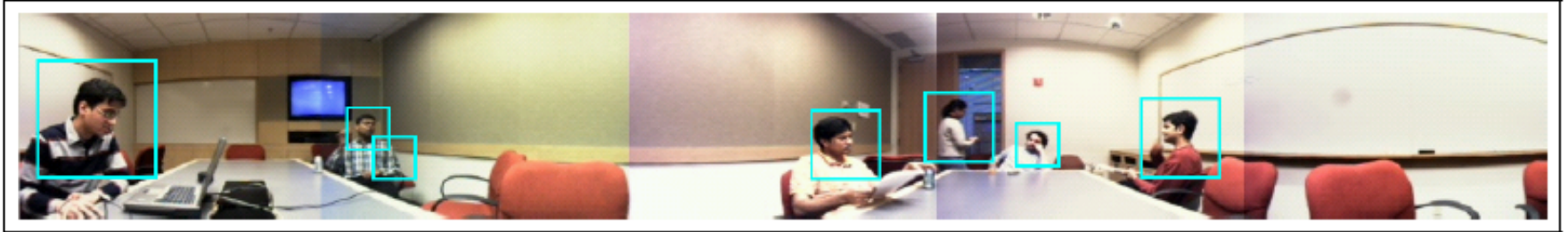


Figure 4: One example from the testing dataset and overlaid results.

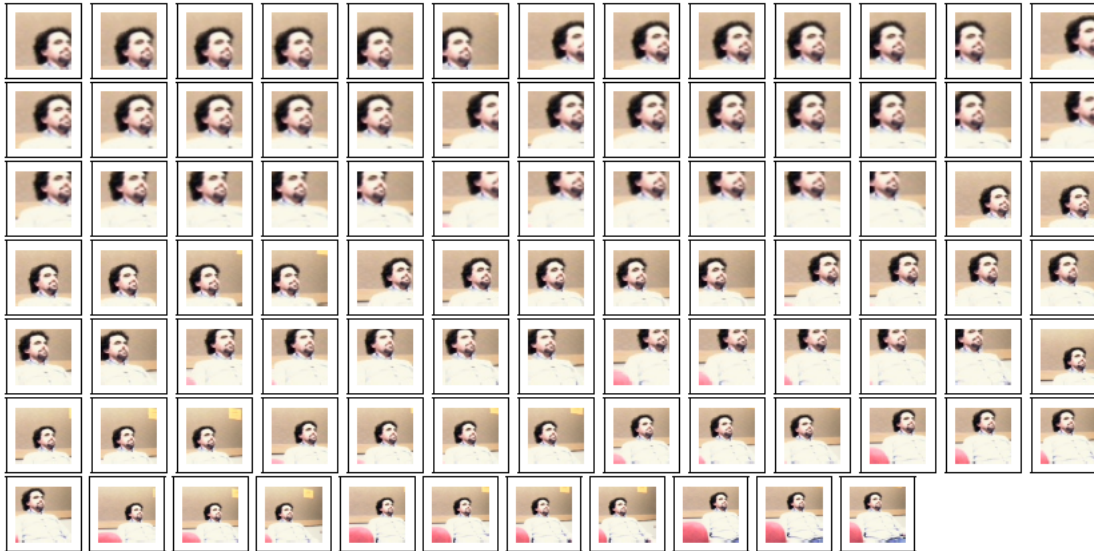


Figure 2: Some of the subwindows in one positive bag.

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

# Learnability

# Learnability - Earlier Results

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- [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

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	Sample	Time	Assumption
Long & Tan	$\tilde{O}\left(\frac{d^2 r^6}{\epsilon^{10}}\right)$	$\tilde{O}\left(\frac{d^5 r^{12}}{\epsilon^{20}}\right)$	Instances in bag are independent, and drawn from production distribution
Auer et al.	$\tilde{O}\left(\frac{d^2 r^2}{\epsilon^2}\right)$	$\tilde{O}\left(\frac{d^3 r^2}{\epsilon^2}\right)$	Instances in bag are independent
Blum & Kalai	$\tilde{O}\left(\frac{d^2 r}{\epsilon^2}\right)$	$\tilde{O}\left(\frac{d^3 r^2}{\epsilon^2}\right)$	Instances in bag are independent

# Learnability - Important Insights

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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  $\mathcal{RP} = \mathcal{NP}$

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

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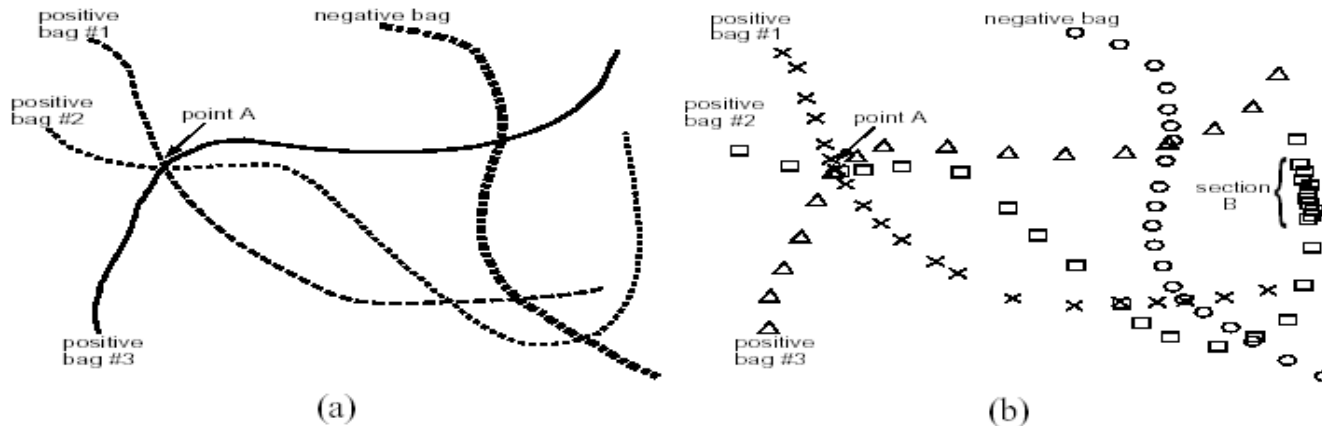
The homogeneous case, when instances are statistically dependent [Sabato & Tishby, COLT'08] :

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



# Algorithms

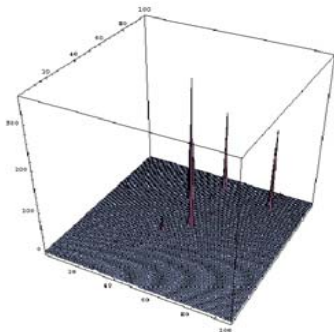
# Representative Algorithms - Diverse Density



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.

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

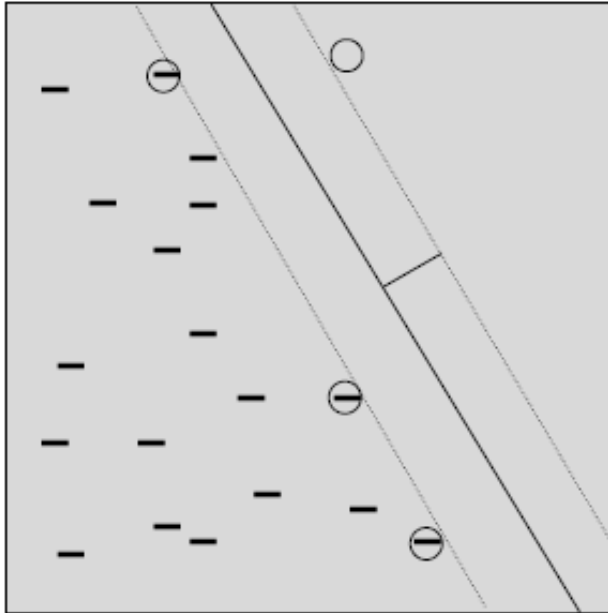
Figure 1: A motivating example for Diverse Density



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

# Representative Algorithms - MI-SVM



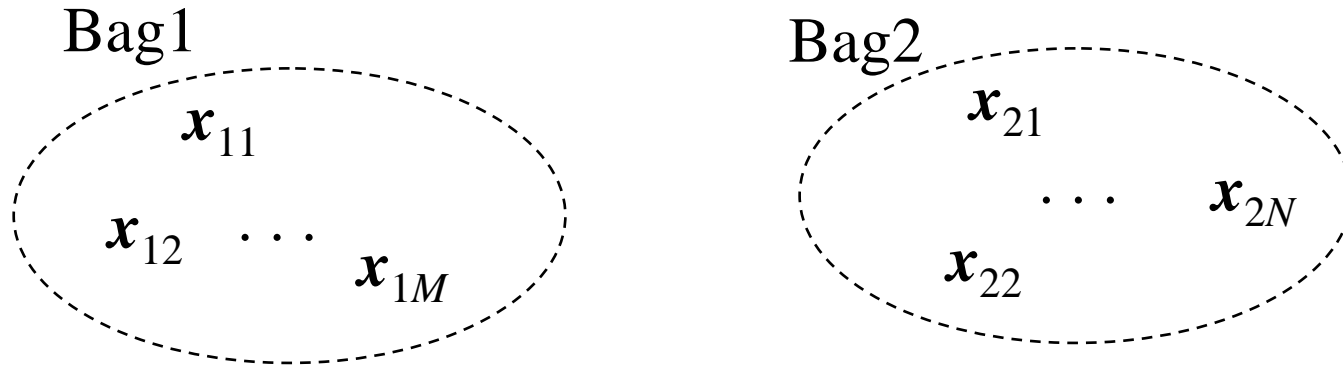
To search for the maximal margin hyperplane

the margin of a "positive bag" is the margin of its "most positive" instance

$$\begin{aligned}
 \text{MI-SVM} \quad & \min_{\mathbf{w}, b, \xi} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_I \xi_I \\
 \text{s.t.} \quad & \forall I : Y_I \max_{i \in I} (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_I, \quad \xi_I \geq 0.
 \end{aligned}$$

# Representative Algorithms - MI-Kernel

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Based on *set kernel* :

$$\mathbf{K}(\text{Bag1}, \text{Bag2}) = \sum_{i=1}^M \sum_{j=1}^N k(\mathbf{x}_{1i}, \mathbf{x}_{2j})$$

$k$  is Gaussian RBF kernel

[Gärtner et al., ICML'02]

# Many MIL Algorithms

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- ✓ 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

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- ✓ 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

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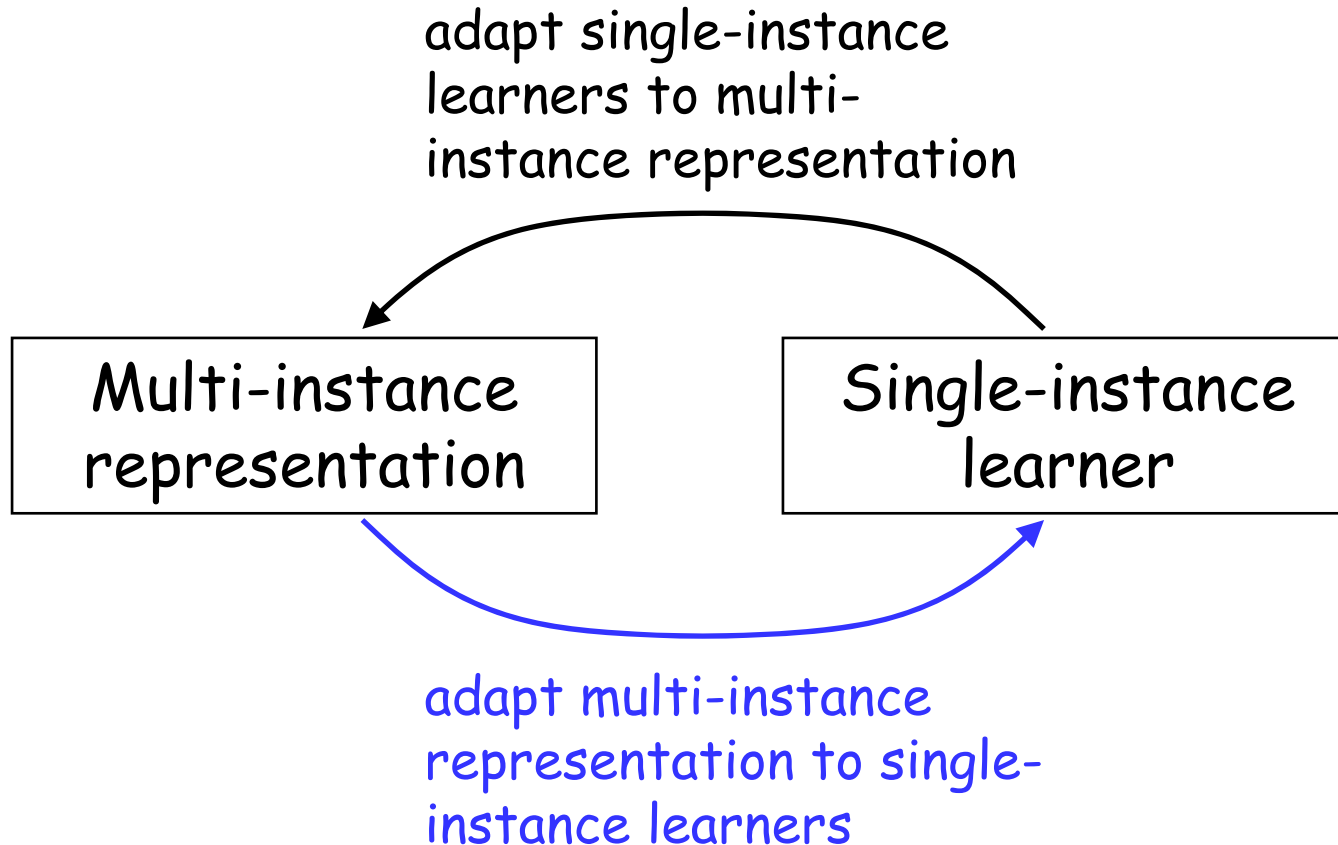
## A general routine :

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

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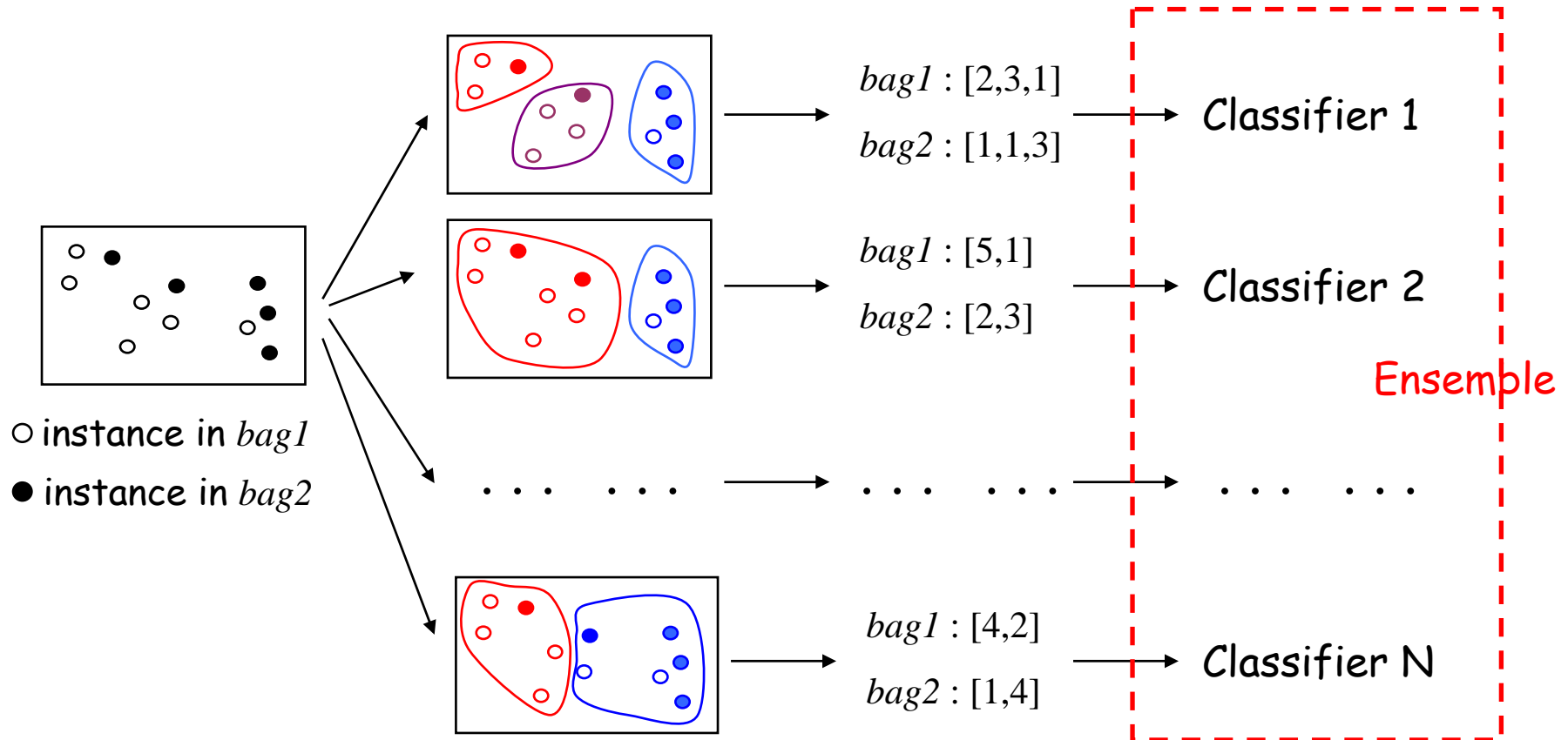




# Example: The CCE Algorithm

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

The key: Re-represent bags as single-instances



It is worth noting that:

Most existing MIL algorithms assume  
i.i.d. instances

## A Recent Study

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[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

# A Reformulation of MIL Task - [Zhou & Xu, ICML'07]

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An semi-supervised learning task:

**Definition 1** *Given a set of labeled negative examples  $\{(\mathbf{x}_1, -1), (\mathbf{x}_2, -1), \dots, (\mathbf{x}_{T_L}, -1)\}$  and a set of unlabeled instances  $\{\mathbf{x}_{T_L+1}, \dots, \mathbf{x}_T\}$ , to learn a function  $F^s : \mathcal{X} \rightarrow \{-1, +1\}$  subject to: For  $i = q + 1, \dots, m$ , at least one instance in  $\{\mathbf{x}_{s_i}, \dots, \mathbf{x}_{e_i}\}$  is positive.*

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

MissSVM (Multi-iinstance 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]

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

$$\min_f \frac{1}{2} \|f\|_{\mathcal{H}}^2 + \lambda \sum_{t=1}^{T_L} H_1(y_t f(\mathbf{x}_t)) + \delta \sum_{t=T_L+1}^T D(f(\mathbf{x}_t))$$

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:

$$\sum_{i=q+1}^m H_1 \left( \max_{t=s_i, \dots, e_i} f(\mathbf{x}_t) \right)$$

# The MissSVM Algorithm (con't)

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Thus, the optimization problem can be written as:

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

$$\text{s.t.} \left\{ \begin{array}{l} (-1)f(\mathbf{x}_t) + \eta_t \geq 1, \eta_t \geq 0, t = 1, 2, \dots, T_L; \\ \max_{t=s_i, \dots, e_i} f(\mathbf{x}_t) + \theta_{i-q} \geq 1, \theta_{i-q} \geq 0, \\ \qquad \qquad \qquad i = q + 1, \dots, m; \\ f(\mathbf{x}_t) + \varepsilon_{t-T_L} \geq 1, \varepsilon_{t-T_L} \geq 0, \\ \qquad \qquad \qquad t = T_L + 1, \dots, T; \\ (-1)f(\mathbf{x}_t) + \xi_{t-T_L} \geq 1, \xi_{t-T_L} \geq 0, \\ \qquad \qquad \qquad t = T_L + 1, \dots, T. \end{array} \right.$$

- $\eta = [\eta_1, \dots, \eta_{T_L}]'$  - slack variables for errors on instances from negative bags
- $\theta = [\theta_1, \dots, \theta_p]'$  - slack variables for errors on positive bags
- $\varepsilon = [\varepsilon_1, \dots, \varepsilon_{T_U}]'$  and  $\xi = [\xi_1, \dots, \xi_{T_U}]'$  - slack variables for errors on instances from positive bags
- $\lambda, \gamma$  and  $\delta$  - parameters

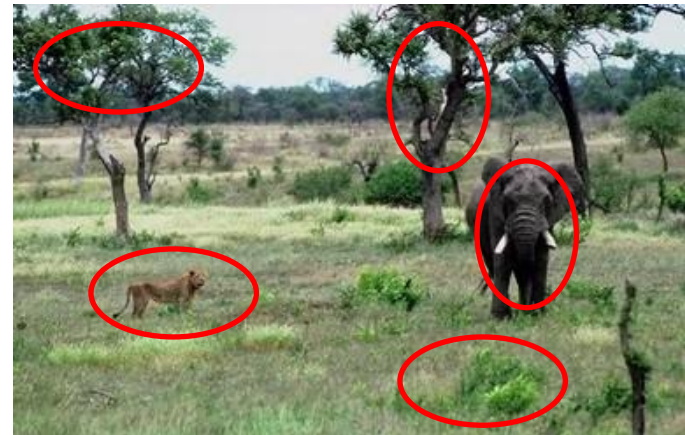


# Shouldn't Assume I.I.D. Instances

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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:

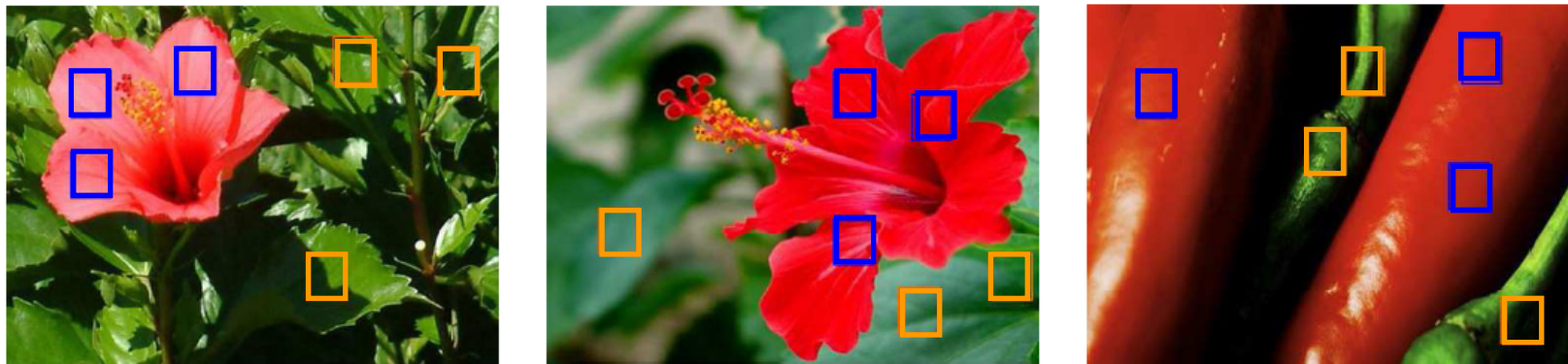
If i.i.d. instances were assumed, MIL problems can be solved by adapting SSL techniques, and therefore we do not need to study dedicated MIL techniques



Can we do MIL without assuming  
i.i.d. instances ?

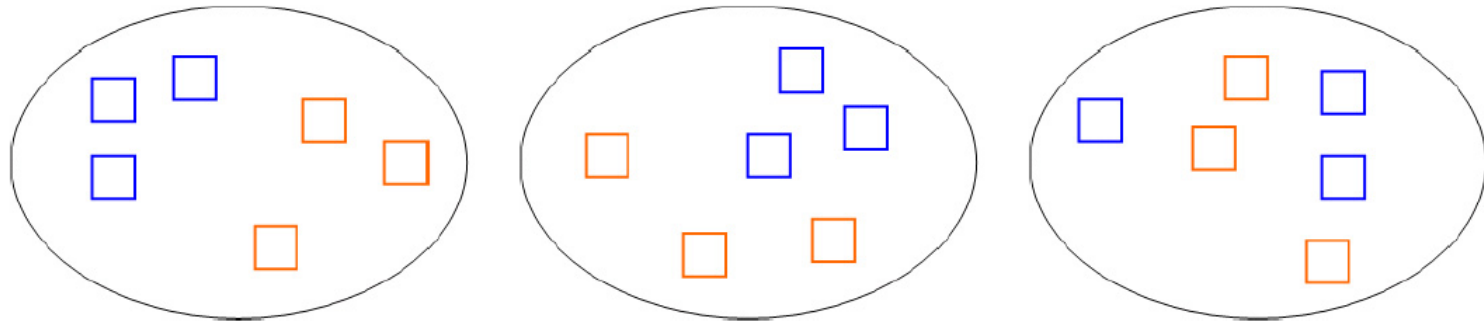
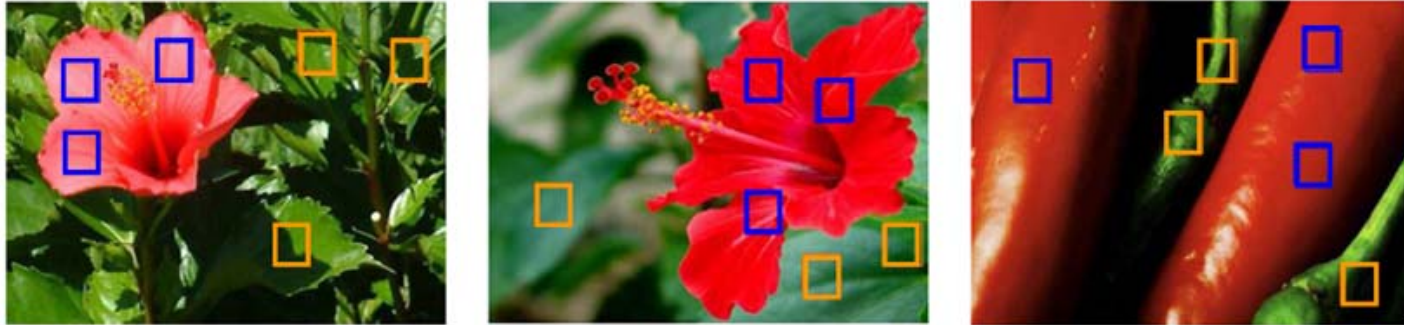
# An Inspirational Example

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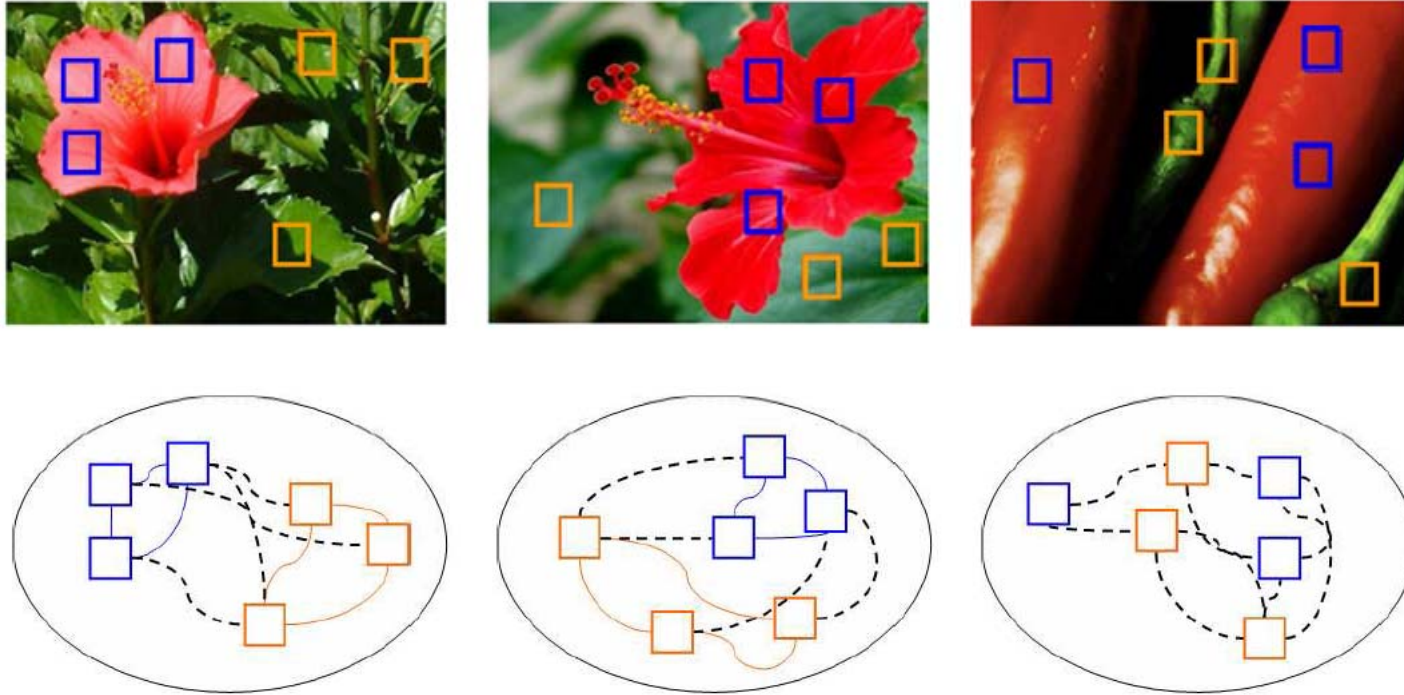
*Figure 1.* Example images with six marked patches each corresponding to an instance

## 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

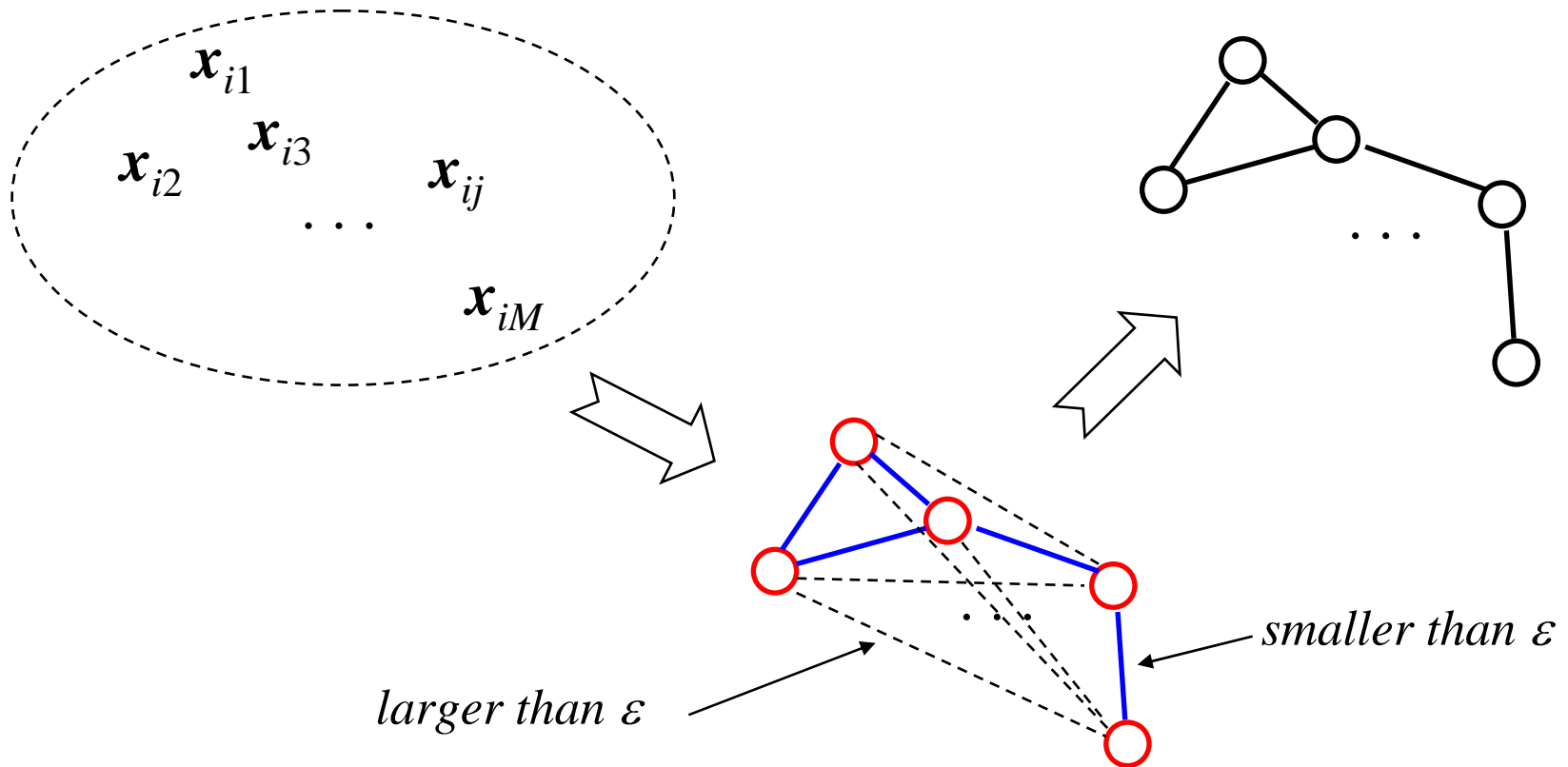
## An Inspirational Example (con't)



*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

# The MIGraph Method - [Zhou et al., ICML'09]

## 1) Map each bag into a graph (e.g., $\epsilon$ -graph)



## The MIGraph Method (con't)

### 2) A graph kernel to distinguish positive/negative graphs

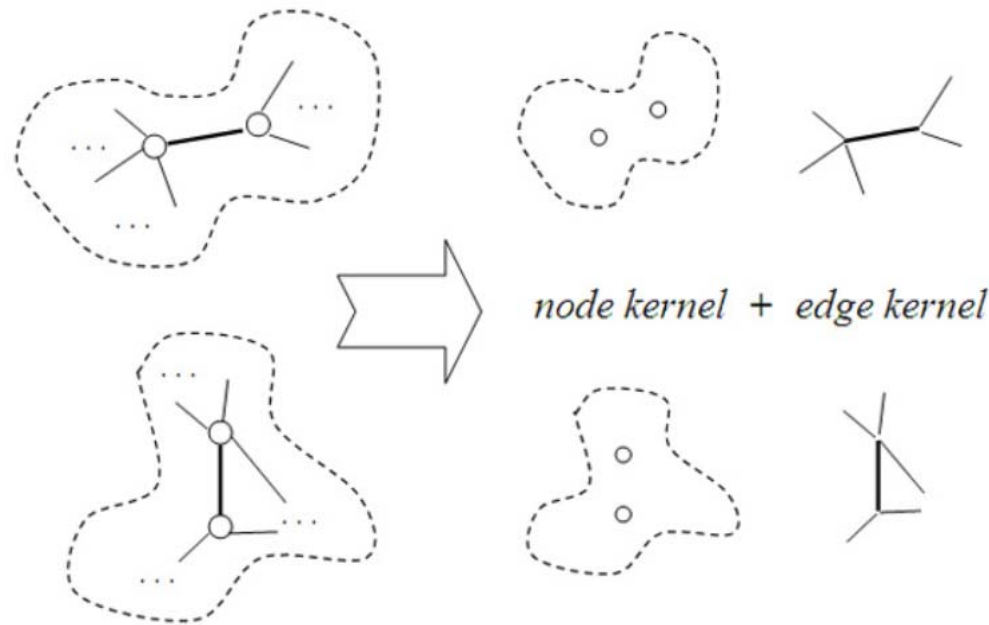
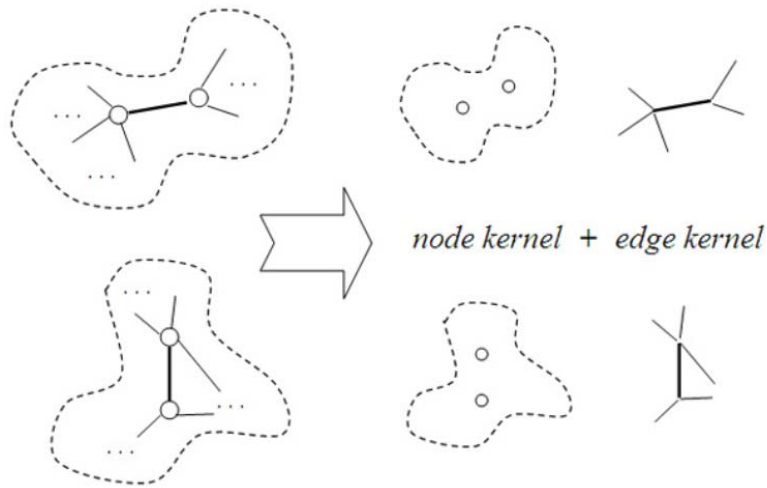


Figure 4. Illustration of the graph kernel in MIGraph

# The MIGraph Method (con't)



MI-Kernel [Gärtner et al., ICML'02]

$$\begin{aligned}
 k_G(X_i, X_j) &= \sum_{a=1}^{n_i} \sum_{b=1}^{n_j} k_{node}(\mathbf{x}_{ia}, \mathbf{x}_{jb}) \\
 &+ \sum_{a=1}^{m_i} \sum_{b=1}^{m_j} k_{edge}(\mathbf{e}_{ia}, \mathbf{e}_{jb})
 \end{aligned}$$

We define the edge connecting  $\mathbf{x}_{iu}$  and  $\mathbf{x}_{iv}$  as  $[d_u, p_u, d_v, p_v]'$

$d_u$  is the degree of  $\mathbf{x}_{iu}$        $p_u = w_{uv} / \sum w_{u,*}$

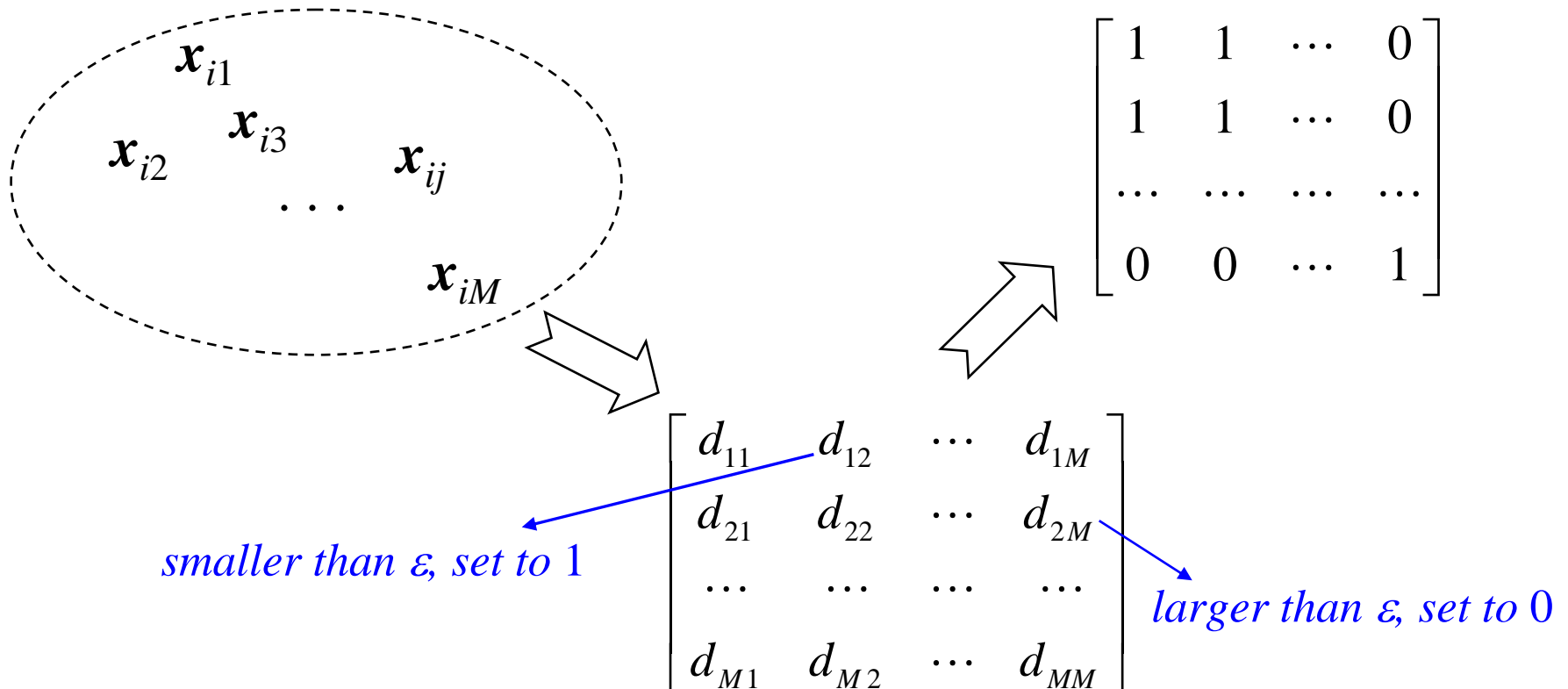
We define both  $k_{node}$  and  $k_{edge}$  as Gaussian RBF kernel

Complexity of MIGraph:  $O(n_i n_j + m_i m_j)$ .



# The miGraph Method - [Zhou et al., ICML'09]

1) Instead of constructing a graph explicitly, we consider an affinity matrix for each bag





# The miGraph Method (con't)

## 2) A kernel to distinguish positive/negative graphs

$$k_g(X_i, X_j) = \frac{\sum_{a=1}^{n_i} \sum_{b=1}^{n_j} W_{ia} W_{jb} k(\mathbf{x}_{ia}, \mathbf{x}_{jb})}{\sum_{a=1}^{n_i} W_{ia} \sum_{b=1}^{n_j} W_{jb}}$$

The node kernel as similar as in MIGraph, realized with Gaussian RBF kernel

$$W_{ia} = 1 / \sum_{u=1}^{n_i} w_{au}^i$$

1	1	...	0
1	1	...	0
...	...	...	...
0	0	...	1

Complexity of miGraph:  $O(n_i n_j)$

# Four Kinds of Tasks

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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

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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
- ✓ ... ..

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:

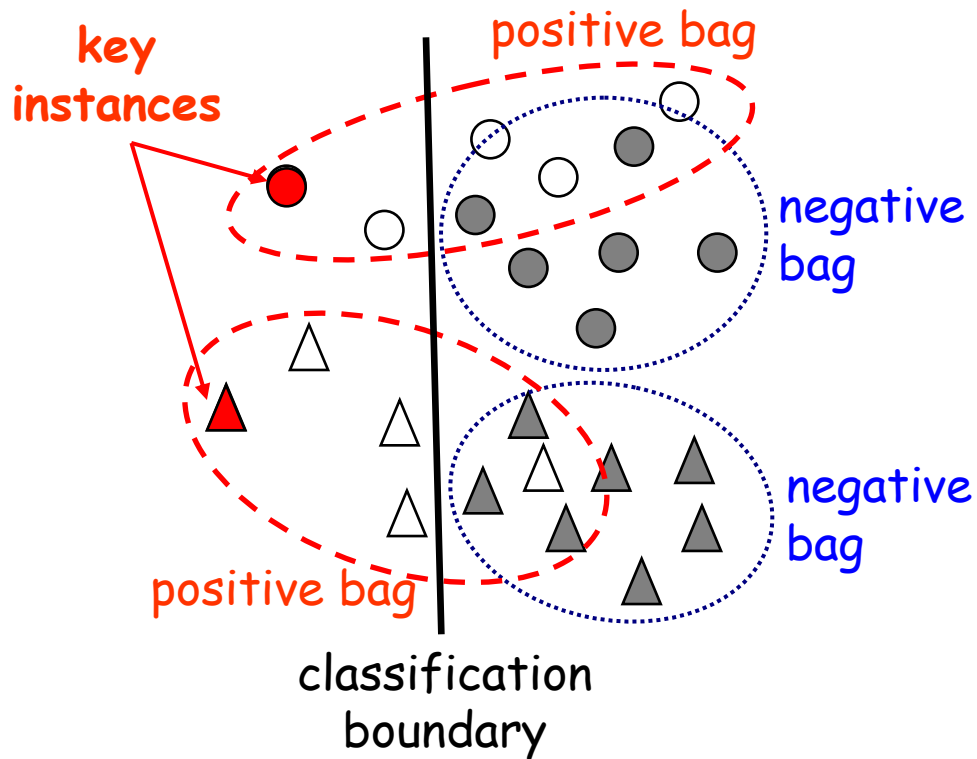
- DD :  
14,475  
seconds  
( $\approx$  4 hours)
- $CkNN$ -ROI:  
0.32 second

The first attempt of locating ROI in CBIR

# 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

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

- ✓ Z.-H. Zhou and M.-L. Zhang. Ensembles of multi-instance learners. In: Proceedings of the 14th European Conference on Machine Learning (ECML'03), Cavtat-Dubrovnik, Croatia, LNAI 2837, 2003, pp.492-502

Code: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/MIL-Ensemble.htm>

- ✓ Z.-H. Zhou. Multi-instance learning from supervised view. Journal of Computer Science and Technology, 2006, 21(5): 800-809

## Adapting MIL-representation to SIL-learners:

- ✓ Z.-H. Zhou and M.-L. Zhang. Solving multi-instance problems with classifier ensemble based on constructive clustering. Knowledge and Information Systems, 2007, 11(2): 155-170

Code: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/CCE.htm>

# Multi-Instance Learning ... more details

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## MIL & SSL:

- ✓ Z.-H. Zhou and J.-M. Xu. On the relation between multi-instance learning and semi-supervised learning. In: Proceedings of the 24th International Conference on Machine Learning (ICML'07), Corvallis, OR, 2007, pp.1167-1174.

Code: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/MissSVM.htm>

## MIL without i.i.d. assumption:

- ✓ Z.-H. Zhou, Y.-Y. Sun, and Y.-F. Li. Multi-instance learning by treating instances as non-i.i.d. samples. In: Proceedings of the 26th International Conference on Machine Learning (ICML'09), Montreal, Canada, 2009, pp.1249-1256. (CORR abs/0807.1997)

Code: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miGraph.htm>

Data: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/mil-text-data.htm>



# Multi-Instance Learning ... more details

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## Identifying key instances:

- ✓ Z.-H. Zhou, X.-B. Xue, and Y. Jiang. Locating regions of interest in CBIR with multi-instance learning techniques. In: Proceedings of the 18th Australian Joint Conference on Artificial Intelligence (AJCAI'05), Sydney, Australia, LNAI 3809, 2005, pp.92-101.
- ✓ Y.-F. Li, J. T. Kwok, I. W. Tsang, and Z.-H. Zhou. A convex method for locating regions of interest with multi-instance learning. In: Proceedings of the European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML PKDD'09), Bled, Slovenia, Part II, LNAI 5782, 2009, pp.15-30.

Code: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/KISVM.htm>

# Multi-Instance Learning ... more details

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## MIL-based Webpage recommendation:

- ✓ Z.-H. Zhou, K. Jiang, and M. Li. Multi-instance learning based web mining. Applied Intelligence, 2005, 22(2): 135-147

Data: <http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/milweb-datafile.htm>

## Multi-instance bag generator:

- ✓ Z.-H. Zhou, M.-L. Zhang, and K.-J. Chen. A novel bag generator for image database retrieval with multi-instance learning techniques. In: Proceedings of the 15th IEEE International Conference on Tools with Artificial Intelligence (ICTAI'03), Sacramento, CA, 2003, pp.565-569.

Thanks !