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The presentation involves some joint work with:

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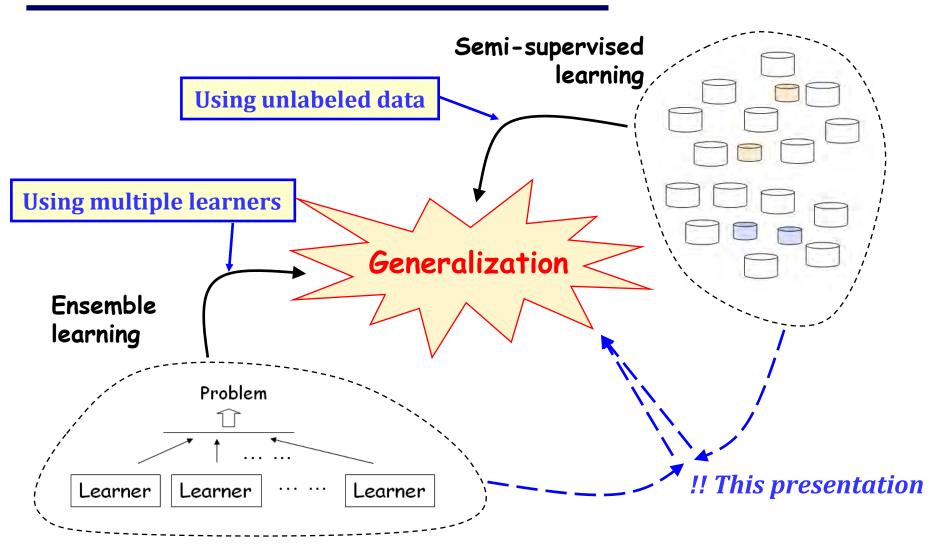
Min-Ling Zhang

De-Chuan Zhan

... ...



One Goal, Two Paradigms



Outline



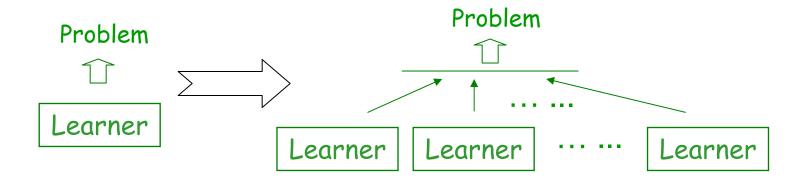
- > Ensemble Learning
- > Semi-Supervised Learning
- > Classifier Combination vs. Unlabeled Data





Ensemble learning is a machine learning paradigm where multiple (homogenous/heterogeneous) individual learners are trained for the same problem

e.g. neural network ensemble, decision tree ensemble, etc.



Many ensemble methods



Parallel methods

Bagging

Random Subspace

Random Forests

•

[L. Breiman, MLJ96]

[T. K. Ho, TPAMI98]

[L. Breiman, MLJ01]

Sequential methods

AdaBoost

[Y. Freund & R. Schapire, JCSS97]

· Arc-x4

[L. Breiman, AnnStat98]

LPBoost

[A. Demiriz et al., MLJ06]

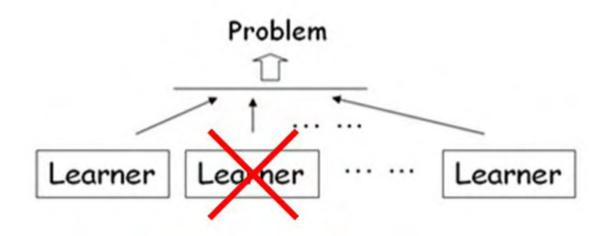
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Selective ensemble



Many Could be Better Than All:

When a number of base learners are available, ..., ensembling many of the base learners may be better than ensembling all of them [Z.-H. Zhou et al., IJCAI'01 & AIJ02]







Abundant studies on theoretical properties of ensemble methods

Appeared/ing in many leading statistical journals, e.g. <u>Annals of Statistics</u>

√ Agreement: Different ensemble methods may have different foundations



Diversity among the base learners is (possibly) the key of ensembles

$$E=E-A$$
 [A. Krogh & J. Vedelsby, NIPS'94]

The more accurate and the more diverse, the better

but, what is "diversity"? [L.I. Kuncheva & C.J. Whitaker, MLJ03]





Even for some theory-intrigued methods, ... still mysteries

E.g., Why AdaBoost does not overfit?

- Margin! [R.E. Schapire et al., AnnStat98]
- No! [L. Breiman, NCJ99]
 (contrary evidence: minimal margin)
- Wait ... [L. Reyzin & R.E. Schapire, ICML'06 best paper]
 (minimal Margin ?? Margin distribution)
- One more support [L. Wang et al., COLT'08]

For the whole story see:

Z.-H. Zhou & Y. Yu, **AdaBoost**. In: X. Wu and V. Kumar eds. <u>The Top Ten Algorithms in Data Mining</u>, Boca Raton, FL: Chapman & Hall, 2009

Great success of ensemble methods



- □ KDDCup'05: all awards ("Precision Award",

 "Performance Award", "Creativity Award") for "An ensemble search based method ..."
- □ KDDCup'06: 1st place of Task1 for "Modifying Boosted Trees to ..."; 1st place of Task2 & 2nd place of Task1 for "Voting ... by means of a Classifier Committee"
- □ KDD Time-series Classification Challenge 2007:

 1st place for "... Decision Forests and ..."



Great success of ensemble methods (con't)

- □ KDDCup'08: 1st place of Challenge1 for a method using Bagging; 1st place of Challenge2 for "... Using an Ensemble Method"
- □ KDDCup'09: 1st place of Fast Track for "Ensemble ..."; 2nd place of Fast Track for "... bagging ... boosting tree models ...", 1st place of Slow Track for "Boosting with classification trees and shrinkage"; 2nd place of Slow Track for "Stochastic Gradient Boosting"

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Great success of ensemble methods (con't)

□ Netflix Prize:

- ✓ 2007 Progress Prize Winner: *Ensemble*
- ✓ 2008 Progress Prize Winner: *Ensemble*
- ✓ 2009 \$1 Million Grand Prize Winner: Ensemble!!
- □ "Top 10 Data Mining Algorithms" (ICDM'06): AdaBoost
- □ Application to almost all areas



Recently, very few papers in top machine learning conferences

Why?

Easier tasks finished New challenges needed

Outline

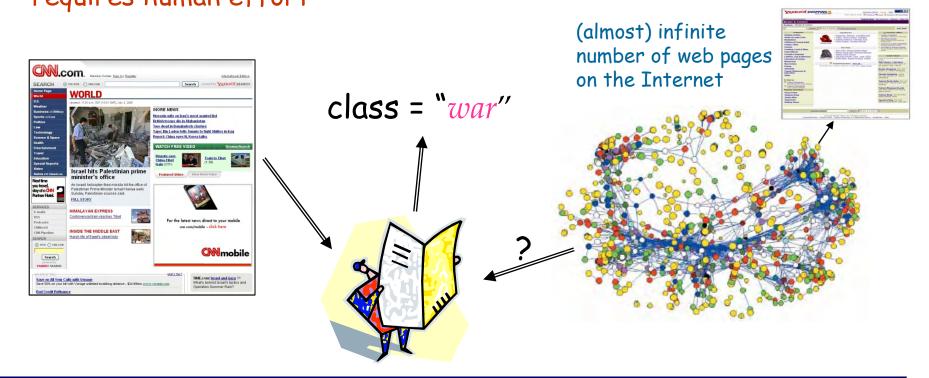


- > Ensemble Learning
- > Semi-Supervised Learning
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Labeled vs. Unlabeled



In many practical applications, unlabeled training examples are readily available but labeled ones are fairly expensive to obtain because labeling the unlabeled examples requires human effort





SSL: Why unlabeled data can be helpful?

Suppose the data is well-modeled by a mixture density:

$$f(x|\theta) = \sum_{l=1}^{L} \alpha_l f(x|\theta_l)$$
 where $\sum_{l=1}^{L} \alpha_l = 1$ and $\theta = \{\theta_l\}$

The class labels are viewed as random quantities and are assumed chosen conditioned on the selected mixture component $m_i \in \{1,2,...,L\}$ and possibly on the feature value, i.e. according to the probabilities $P[c_i | x_i, m_i]$

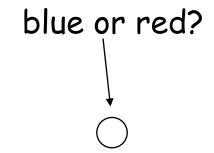
Thus, the optimal classification rule for this model is the MAP rule:

$$S(x) = \arg\max_{k} \sum_{j} P[c_{i} = k | m_{i} = j, x_{i}] P[m_{i} = j | x_{i}]$$
where $P[m_{i} = j | x_{i}] = \frac{\alpha_{j} f(x_{i} | \theta_{j})}{\sum_{l=1}^{L} \alpha_{l} f(x_{i} | \theta_{l})}$ unlabeled examples can be used to help estimate this term



SSL: Why unlabeled data can be helpful? (con't)

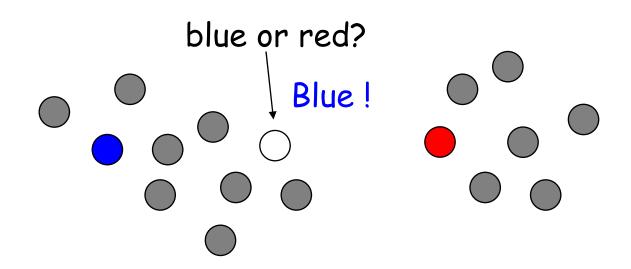
Intuitively,





SSL: Why unlabeled data can be helpful? (con't)

Intuitively,





✓ Generative methods

Using a generative model for the classifier and employing EM to model the label estimation or parameter estimation process [Miller & Uyar, NIPS'96; Nigam et al., MLJ00; Fujino et al., AAAI'05; etc.]

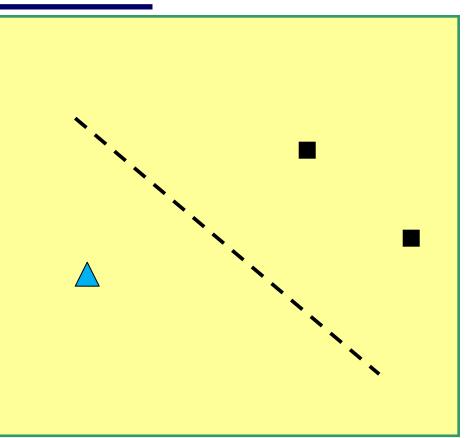
✓ S3VMs (Semi-Supervised SVMs)

Using unlabeled data to adjust the decision boundary such that it goes through the less dense region [Joachims, ICML'99; Chapelle & Zien, AISTATS'05; Collobert et al., ICML'06; etc.]

✓ Graph-based methods

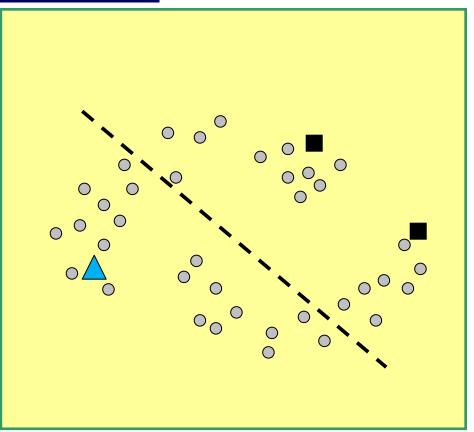


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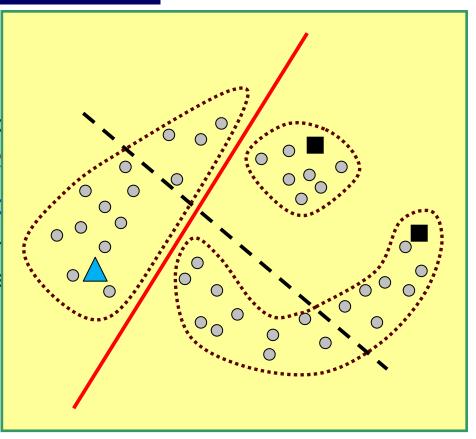


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✓ Graph-based methods

Using unlabeled data to regularize the learning process via graph regularization [Blum & Chawla, ICML'01; Belkin & Niyogi, MLJ04; Zhou et al., NIPS'04; etc.]



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Using a generative model for the classifier and employing EM to model the label estimation or parameter estimation process [Miller & Uyar, NIPS'96; Nigam et al., MLJ00; Fujino et al., AAAI'05; etc.]

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- Using unlabeled data to regularize t regularization [Blum & Chawla, ICML'01; Belkin & Niyogi, MLJ04; Zhou et al., NIPS'04; etc.]
- Disagreement-based methods



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- ✓ Generative methods
- ✓ S3VMs (Semi-Supervised SVMs)
- ✓ Graph-based methods
- ✓ Disagreement-based methods

 multiple learners are trained for the task and the disagreements among the learners are exploited during the SSL process [Blum & Mitchell, COLT'98; Goldman & Zhou, ICML'00; Zhou & Li, TKDE05; etc.]

SSL reviews:

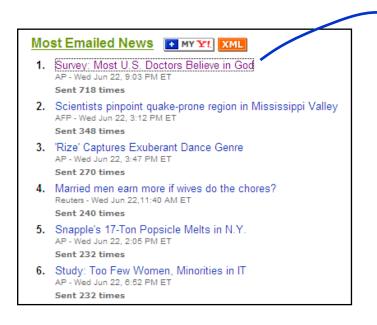
- Chapelle et al., eds. Semi-Supervised Learning, MIT Press, 2006
- Zhu, Semi-Supervise Learning Literature Survey, 2006
- Zhou & Li, Semi-supervised learning by disagreement, KAIS, 2009

Co-training



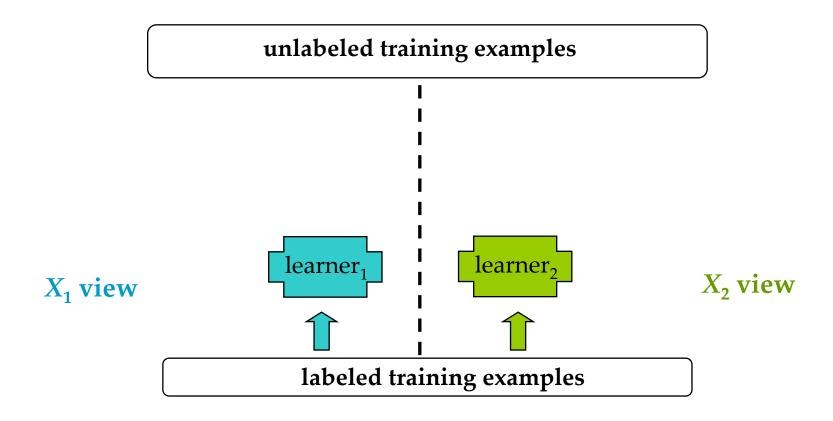
In some applications, there are two sufficient and redundant views, i.e. two attribute sets each of which is sufficient for learning and conditionally independent to the other given the class label

e.g. two views for web page classification: 1) the text appearing on the page itself, and 2) the anchor text attached to hyperlinks pointing to this page, from other pages

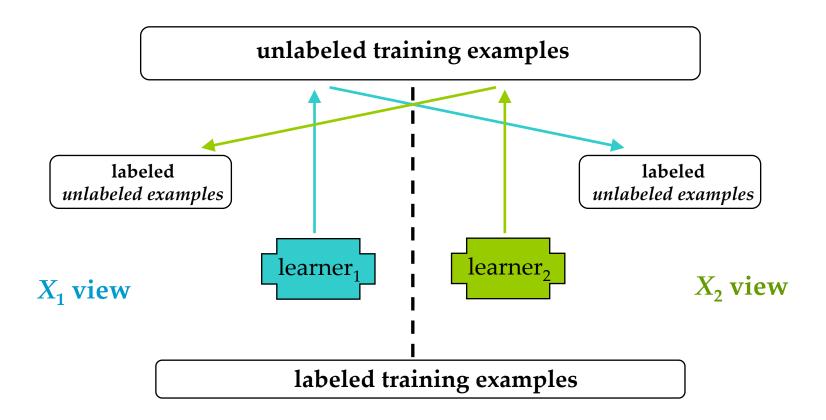




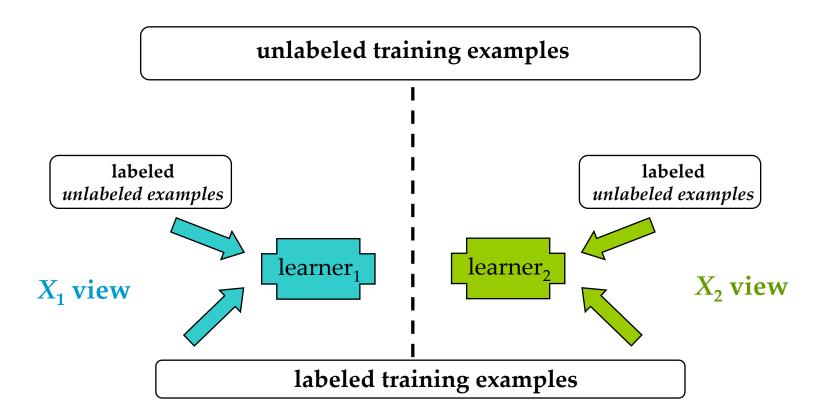




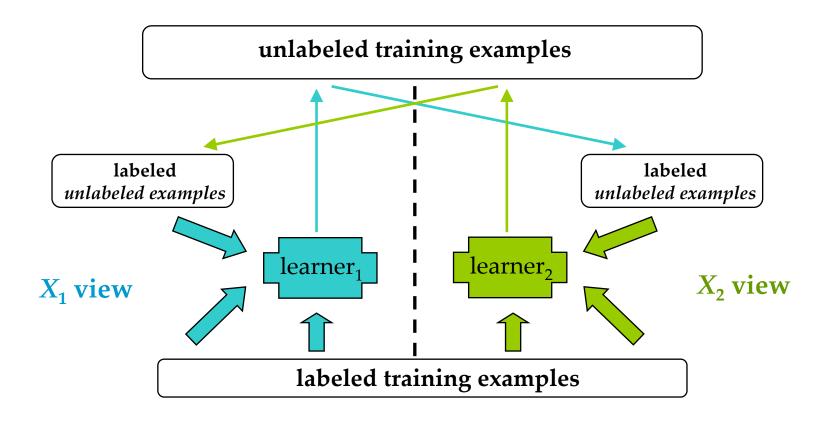












Theoretical results



- [A. Blum & T. Mitchell, COLT'98] Given a conditional independence assumption on the distribution D, if the target class is learnable from random classification noise in the standard PAC model, then any initial weak predictor can be boosted to arbitrarily high accuracy by co-training
- [5. Dasgupta et al., NIPS'01] When the requirement of sufficient and redundant views is met, the co-trained classifiers could make few generalization errors by maximizing their agreement over the unlabeled data
- [M.-F. Balcan et al., NIPS'04] Given appropriately strong PAClearners on each view, a weaker "expansion" assumption on the underlying data distribution is sufficient for iterative co-training to succeed

Applications



Although the requirement of sufficient and redundant views is quite difficult to meet, co-training has already been used in many domains, e.g.,

- Statistical parsing [A. Sarkar, NAACL01; M. Steedman et al., EACL03; R. Hwa et al., ICML03w]
- Noun phrase identification [D. Pierce & C. Cardie, EMNLP01]
- Image retrieval [Z.-H. Zhou et al., ECML'04, TOIS06]
- •

Single-view variant



[S. Goldman & Y. Zhou, ICML'00] used <u>two different supervised</u> <u>learning algorithms</u> whose hypothesis partitions the example space into a set of equivalent classes

e.g. for a decision tree each leaf defines an equivalent class

Actually they used the ID3 decision tree and HOODG decision tree

Two key issues:

- How to combine the two classifiers?
 - Using 10-fold CV to estimate the predictive confidence of the two classifiers and the involved equivalent classes
- How to choose unlabeled instance to label?
 Using 10-fold CV to estimate the labeling confidence

Weakness: Time-consuming 10-fold CV is used for many times in every round of the co-training process

Tri-training



The intuition:

If three classifiers are involved, maybe it is not necessary to measure the labeling confidence explicitly

- > if two classifiers agree, then label for the other classifier
- > the prediction can be made by voting these three classifiers

Additional benefit:

Ensemble learning can be utilized to improve the generalization





A problem:

"Majority teach minority" may be wrong in some cases

- If the prediction of h_2 and h_3 on x is correct, then h_1 will receive a valid new example for further training
- Otherwise, h_1 will get an example with noisy label

however, even in the worse case, the increase in the classification noise rate can be compensated if the amount of newly labeled examples is sufficient, under certain conditions



Tri-training (con't)

According to [D. Angluin & P. Laird, MLJ88], if a sequence σ of m samples is drawn, where the sample size m satisfies

$$m \ge \frac{2}{\epsilon^2 \left(1 - 2\eta\right)^2} \ln\left(\frac{2N}{\delta}\right)$$

 ε : the hypothesis worst-case classification error rate

 η (< 0.5): an upper bound on the classification noise rate

N: the number of hypothesis

 δ : the confidence

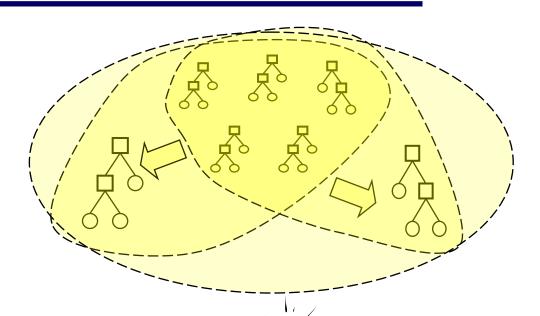
then a hypothesis H_i that minimizes disagreement with σ will have the PAC property: $\Pr\left[d(H_i, H^*) \geq \epsilon\right] \leq \delta$

From this we derived the tri-training criterion:

$$0 < \frac{\check{e}_1^t}{\check{e}_1^{t-1}} < \frac{|L^{t-1}|}{|L^t|} < 1$$

Co-Forest





Error of base classifier:



Diversity among base classifier:

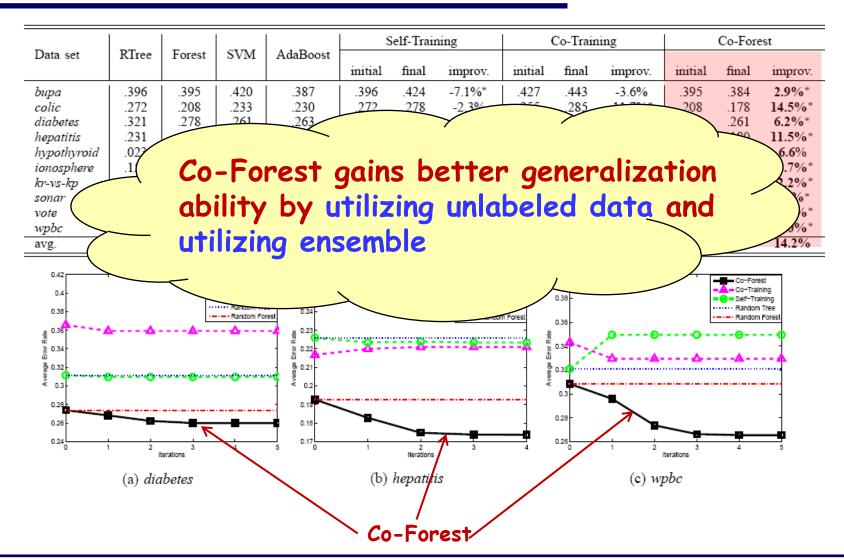




- Injecting Randomness (RF)
- Selecting unlabeled from an unlabeled example pool



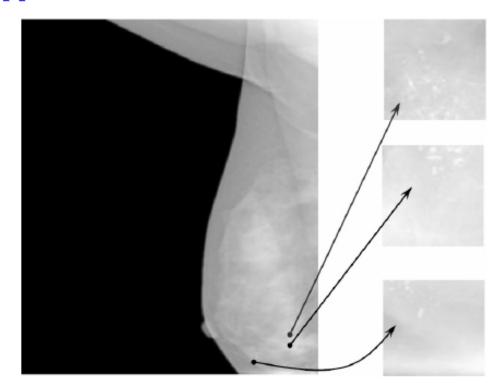
Co-Forest (con't)



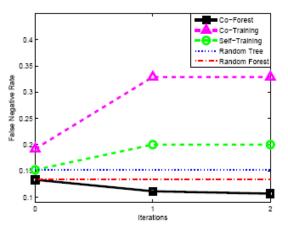




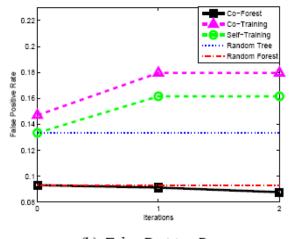
Application to Microcalcification Detection



Co-Forest can help to reduce the false-negative rate while maintaining the false-positive rate by utilizing undiagnosed samples



(a) False Negative Rate



(b) False Positive Rate





Semi-supervised Boosting methods:

- ✓ SS MarginBoost [F. d'Alché-Buc et al., NIPS'01]
- ✓ ASSEMBLE.AdaBoost [K. Bennett et al., KDD'02]
 Winner of the NIPS'01 Unlabeled Data Competition
- ✓ SemiBoost [P.K. Mallapragada et al., TPAMI in press]
- ✓ Multi-class SSBoost [H. Valizadegan et al., ECML'08]

Comparing with the huge amount of literatures on semi-supervised learning and ensemble learning, the literatures on SSL ensemble methods are too few

Problem



"Despite the theoretical and practical relevance of semi-supervised classification, the proposed approaches so far dealt with only single classifiers, and, in particular, no work was clearly devoted to this topic within the MCS literature"

Fabio Roli, MCS'05 Keynote

- □ SSL: Using unlabeled data is sufficient, why bother multiple learners?
- Ensemble: Using MCS is sufficient, why need unlabeled data?

Outline



- > Ensemble Learning
- > Semi-Supervised Learning
- > Classifier Combination vs. Unlabeled Data
 - ✓ Is classifier combination helpful to SSL?
 - ✓ Are unlabeled data helpful to ensemble?
- > Conclusion





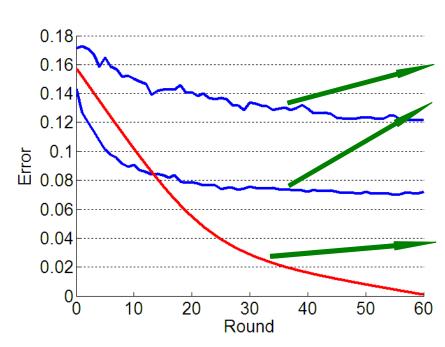
In many SSL studies, it was shown that very strong classifiers can be attained by using unlabeled data

e.g., [A. Blum & T. Mitchell, COLT'98] - Given a conditional independence assumption on the distribution D, if the target class is learnable from random classification noise in the standard PAC model, then any initial weak predictor can be boosted to arbitrarily high accuracy by co-training

So, a single classifier seems enough

However, in empirical studies ...





Performance of Co-training

Performances of the learners observed in experiments: the performances could not be improved further after a number of rounds

why?

Previous theoretical studies indicated that the performances could always be improved



Condition for co-training to work

Lemma 1. Given the initial labeled data set \mathcal{L} which is clean, and assuming that the size of \mathcal{L} is sufficient to learn two classifiers h_1^0 and h_2^0 whose upper bound of the generalization error is $a_0 < 0.5$ and $b_0 < 0.5$ with high probability (more than $1 - \delta$) in the PAC model, respectively, i.e., $l \ge \max[\frac{1}{a_0} \ln \frac{|\mathcal{H}|}{\delta}, \frac{1}{b_0} \ln \frac{|\mathcal{H}|}{\delta}]$. Then h_1^0 selects u number of unlabeled instances from \mathcal{U} to label and puts them into σ_2 which contains all the examples in \mathcal{L} , and then h_2^1 is trained from σ_2 by minimizing the empirical risk. If $lb_0 \le e \sqrt[M]{M!} - M$, then

$$\Pr[d(h_2^1, h^*) \ge b_1] \le \delta , \qquad (1)$$

where $M = ua_0$ and $b_1 = \max[\frac{lb_0 + ua_0 - ud(h_1^0, h_2^1)}{l}, 0]$.

Roughly speaking, the key requirement of co-training is that the initial learners should have large difference; it is not important that whether the difference is achieved by exploiting two views or not



Is the theoretical/empirical gap occasional?

Theorem In the Co-Training Process, if $u \gg l$, then for any $0 < \epsilon < 1$,

$$Pr[d(h_1^0, h_2^1) \ge \epsilon] \le \delta,$$

and

$$Pr[|d(h_1^0, h^*) - d(h_2^1, h^*)| \ge \epsilon] \le \delta.$$

Roughly speaking, as the co-training process continues, the learners will become more and more similar, and therefore it is a "must"-phenomenon that co-training could not improve the performance further after a number of iterations



Will classifier combination help?

"Later Stop"



Theorem 1. When
$$d(h_1^0, h_2^0) > a_0 > b_0$$
 and $\gamma \ge \frac{1}{2} + \frac{u(a_0 + b_0 - d(h_1^0, h_2^0))}{2ld(h_1^0, h_2^0)}$, even when $Pr[h_j^1(x) \ne h^*(x)] \ge Pr[h_j^0(x) \ne h^*(x)]$ $(j = 1, 2)$, $Pr[h_{com}^1(x) \ne h^*(x)]$ is still less than $Pr[h_{com}^0(x) \ne h^*(x)]$.

Roughly speaking, even when the individual learners could not improve the performance any more, classifier combination is still possible to improve generalization further by using more unlabeled data

"Earlier Success"



Theorem 2. Suppose
$$a_0 > b_0$$
, when $\gamma < \frac{d(h_1^0, h_2^0) + b_0 - a_0}{2d(h_1^0, h_2^0)}$, $Pr[h_{com}^0(x) \neq h^*(x)] < \min[a_0, b_0]$.

Roughly speaking, the classifier combination is possible to reach a good performance earlier than the individual classifiers

Outline



- > Ensemble Learning
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First reason



When there are very few labeled training examples, ensemble could not work

SSL may be able to enable ensemble learning in such situation

At least how many labeled examples are needed for SSL?



OLTV (One Labeled example and Two Views)

We show that when there are two sufficient views, SSL with a <u>single labeled example</u> is possible

 $\mathcal X$ and $\mathcal Y$ – two views

 $(\langle \boldsymbol{x}, \boldsymbol{y} \rangle, c)$ - a labeled example

where $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ are the two portions of the example, $c \in \{0,1\}$ is the label

Assuming there exist functions $f_{\mathcal{X}}$ over \mathcal{X} and $f_{\mathcal{Y}}$ over \mathcal{Y} , satisfying $f_{\mathcal{X}}(x)=f_{\mathcal{Y}}(y)=c$

which means that both are sufficient views

The Task:

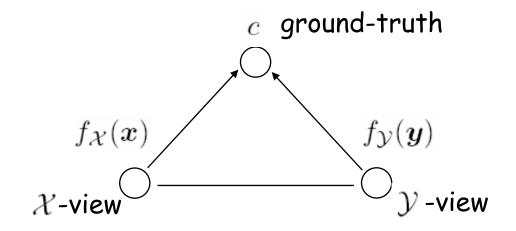
Given $(\langle x_0, y_0 \rangle, 1)$ and unlabeled examples $\mathcal{U} = \{(\langle x_i, y_i \rangle, c_i)\}$ $(i = 1, 2, ..., l-1; c_i \text{ is unknown})$, to train a classifier

OLTV (con't)



For a sufficient view there should exist at least one projection which is correlated strongly with the ground-truth

If two sufficient views are conditionally independent given the class label, the most strongly correlated pair of projections should be in accordance with the ground-truth



CCA (canonical correlation analysis) [Hotelling, Biometrika1936] can be used

OLTV (con't)



A number of correlated pairs of projections will be identified. The strength of the correlation can be measured by λ

m - the number of pairs of correlated projections that have been identified $sim_{i,j}$ - the similarity between $\langle x_i, y_i \rangle$ and $\langle x_0, y_0 \rangle$ in the j-th projection $sim_{i,j}$ can be defined in many ways, such as:

$$sim_{i,j} = \exp(-d^2(P_j(x_i), P_j(x_0))) + \exp(-d^2(P_j(y_i), P_j(y_0)))$$

Then, the confidence of $\langle x_i, y_i \rangle$ being a positive instance can be estimated:

$$\rho_i = \sum_{j=1}^{m} \lambda_j sim_{i,j}$$

Thus, several unlabeled instances with the highest and lowest ρ values can be picked out respectively to be used as extra positive and negative instances

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OLTV (con't)

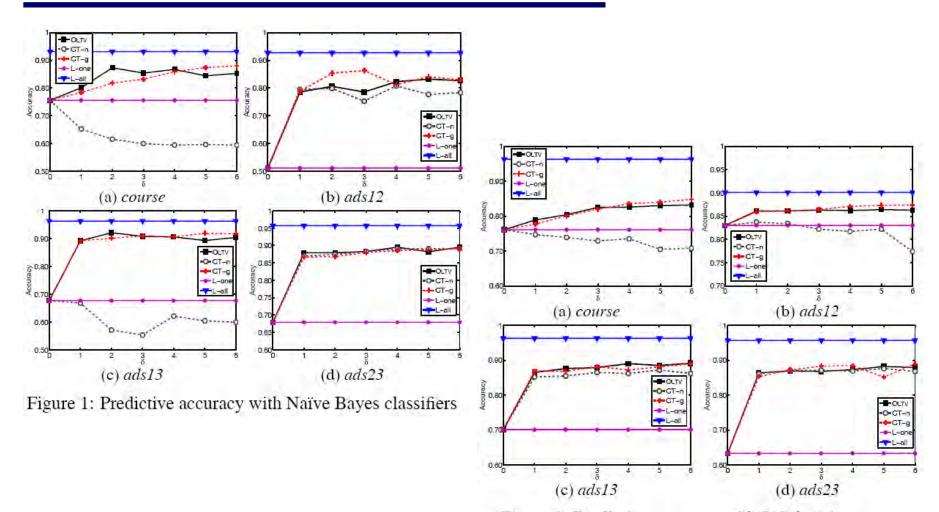


Figure 2: Predictive accuracy with J48 decision trees



Second reason (possibly more important)

Diversity among the base learners is (possibly) the key of ensembles

Unlabeled data can be exploited for diversityaugment





Basic idea:

In addition to maximize accuracy and diversity on labeled data, maximizing diversity on unlabeled data

Labeled training set: $\mathcal{L} = \{(x_1, y_1), \cdots, (x_l, y_l)\}$

Unlabeled training set : $\mathcal{U} = \{u_1, \cdots, u_n\}$

Unlabeled data set derived from $\mathcal{L}:~ ilde{\mathcal{L}}=\{x_1,\cdots,x_l\}$

Assume the ensemble \mathcal{E} consists of m linear classifiers

 $\{oldsymbol{w}_1\cdots,oldsymbol{w}_m\}$ where $oldsymbol{w}_k$ is weight vector of the k-th classifier

 $oldsymbol{W} = [oldsymbol{w}_1, \cdots, oldsymbol{w}_m]$ is the matrix formed by concatenating $oldsymbol{w}_k$'s



A preliminary method (con't)

Generate the ensemble by minimizing the loss function:

$$V(\mathcal{L},\mathcal{U},\boldsymbol{W}) = \frac{1}{2} \sum_{k=1}^{m} ||\boldsymbol{w}_k||_2^2 + C_1 \cdot \boxed{V_{acc}(\mathcal{L},\boldsymbol{W}) + C_2 \cdot V_{div}(\mathcal{D},\boldsymbol{W})}$$
 loss on accuracy

$$V_{acc}(\mathcal{L}, \mathbf{W}) = \sum_{k=1}^{m} \sum_{i=1}^{l} loss(\mathbf{w}_k, \mathbf{x}_i, y_i)$$

$$loss(\mathbf{w}_k, \mathbf{x}_i, y_i) = \begin{cases} 0 & \text{if } y_i \langle \mathbf{w}_k, \mathbf{x}_i \rangle \ge 1\\ (1 - y_i \langle \mathbf{w}_k, \mathbf{x}_i \rangle)^2 & \text{if } y_i \langle \mathbf{w}_k, \mathbf{x}_i \rangle < 1 \end{cases}$$



A preliminary method (con't)

Generate the ensemble by minimizing the loss function:

$$\begin{split} V(\mathcal{L},\mathcal{U},\boldsymbol{W}) &= \frac{1}{2} \sum_{k=1}^{m} ||\boldsymbol{w}_{k}||_{2}^{2} + C_{1} \cdot V_{acc}(\mathcal{L},\boldsymbol{W}) + C_{2} \cdot \boxed{V_{div}(\mathcal{D},\boldsymbol{W})} \\ V_{div}(\mathcal{D},\boldsymbol{W}) &= \sum_{p=1}^{m-1} \sum_{q=p+1}^{m} d(\boldsymbol{w}_{p},\boldsymbol{w}_{q},\mathcal{D}) \\ d(\boldsymbol{w}_{p},\boldsymbol{w}_{q},\mathcal{D}) &= \begin{cases} 0 & \text{if } \mathcal{D} = \emptyset \\ \frac{\sum_{\boldsymbol{x} \in \mathcal{D}} \operatorname{sign}(\langle \boldsymbol{w}_{p},\boldsymbol{x} \rangle) \cdot \operatorname{sign}(\langle \boldsymbol{w}_{q},\boldsymbol{x} \rangle)}{|\mathcal{D}|} & \text{if } \mathcal{D} \neq \emptyset \end{cases} \end{split}$$

We study two cases:
$$L_{CD}$$
 ($\mathcal{D} = \tilde{\mathcal{L}}$) and $L_{CD}U_D$ ($\mathcal{D} = \tilde{\mathcal{L}} \bigcup \mathcal{U}$)



Preliminary results

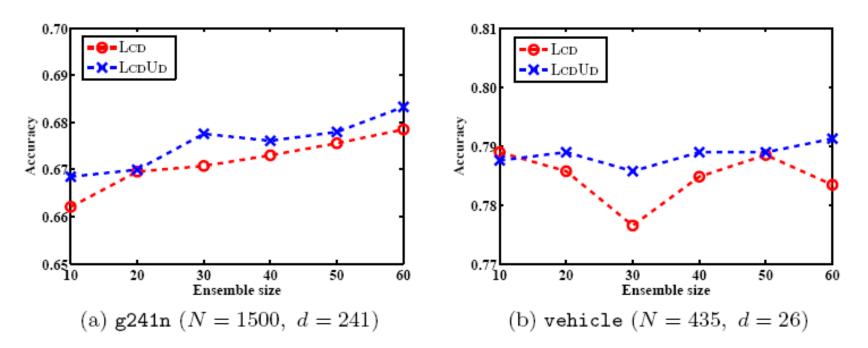


Fig. 1. Comparing the performance of LCD and LCDUD. N is the number of instances; d is the dimensionality.

Conclusion



Ensemble learning and Semi-supervised learning are mutually beneficial

- □ Classifier Combination is helpful to SSL:
 - Later Stop
 - Earlier Success
- Unlabeled Data is helpful to Ensemble:
 - Enable ensemble with very few labeled data
 - Diversity augment

Promising Future



Ensemble -> Strong Classifier

SSL -> Strong Classifier

Ensemble and SSL -> Strong² Classifier

Thanks!