

10601  
Machine Learning

Semi supervised learning

# Can Unlabeled Data improve supervised learning?

Important question! In many cases, unlabeled data is plentiful, labeled data expensive

- Medical outcomes ( $x = \langle \text{patient}, \text{treatment} \rangle$ ,  $y = \text{outcome}$ )
- Text classification ( $x = \text{document}$ ,  $y = \text{relevance}$ )
- Customer modeling ( $x = \text{user actions}$ ,  $y = \text{user intent}$ )
- ...

# When can Unlabeled Data help supervised learning?

Consider setting:

- Set  $X$  of instances drawn from unknown distribution  $P(X)$
- Wish to learn target function  $f: X \rightarrow Y$  (or,  $P(Y|X)$ )
- Given a set  $H$  of possible hypotheses for  $f$

Given:

- iid labeled examples  $L = \{\langle x_1, y_1 \rangle \dots \langle x_m, y_m \rangle\}$
- iid unlabeled examples  $U = \{x_{m+1}, \dots, x_{m+n}\}$

Determine:

$$\hat{f} \leftarrow \arg \min_{h \in H} \Pr_{x \in P(X)} [h(x) \neq f(x)]$$

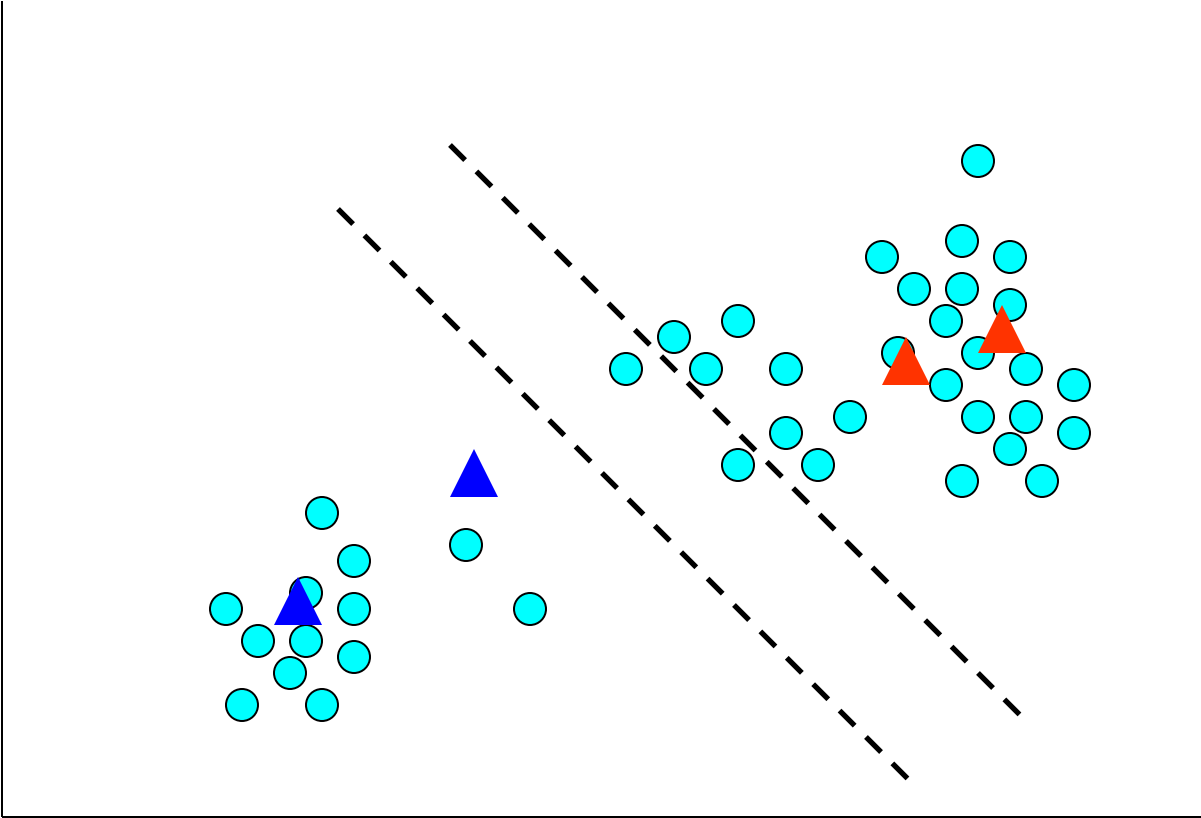
# Four Ways to Use Unlabeled Data for Supervised Learning

1. Use to re-weight labeled examples
2. Use to help EM learn class-specific generative models
3. If problem has redundantly sufficient features, use CoTraining.
4. Use to detect/preempt overfitting

# 1. Use unlabeled data to reweight labeled examples

- Most machine learning algorithms (neural nets, decision trees, SVMs) attempt to *minimize errors over labeled examples*
- But our ultimate goal is to *minimize error over future examples* drawn from the same underlying distribution
- If we know the underlying distribution, we should weight each training example by its probability according to this distribution
- Unlabeled data allows us to estimate this distribution more accurately, and to reweight our labeled examples accordingly

# Example



# 1. reweight labeled examples

Can use  $U \rightarrow \hat{P}(X)$  to alter optimization problem

- Wish to find

$$\hat{f} \leftarrow \operatorname{argmin}_{h \in H} \sum_{x \in X} \delta(h(x) \neq f(x)) P(x)$$

- Often approximate as

$$\hat{f} \leftarrow \operatorname{argmin}_{h \in H} \frac{1}{|L|} \sum_{\langle x, y \rangle \in L} \delta(h(x) \neq y)$$

1 if hypothesis  $h$  disagrees with true function  $f$ , else 0

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# of times we have  $x$  in the labeled set

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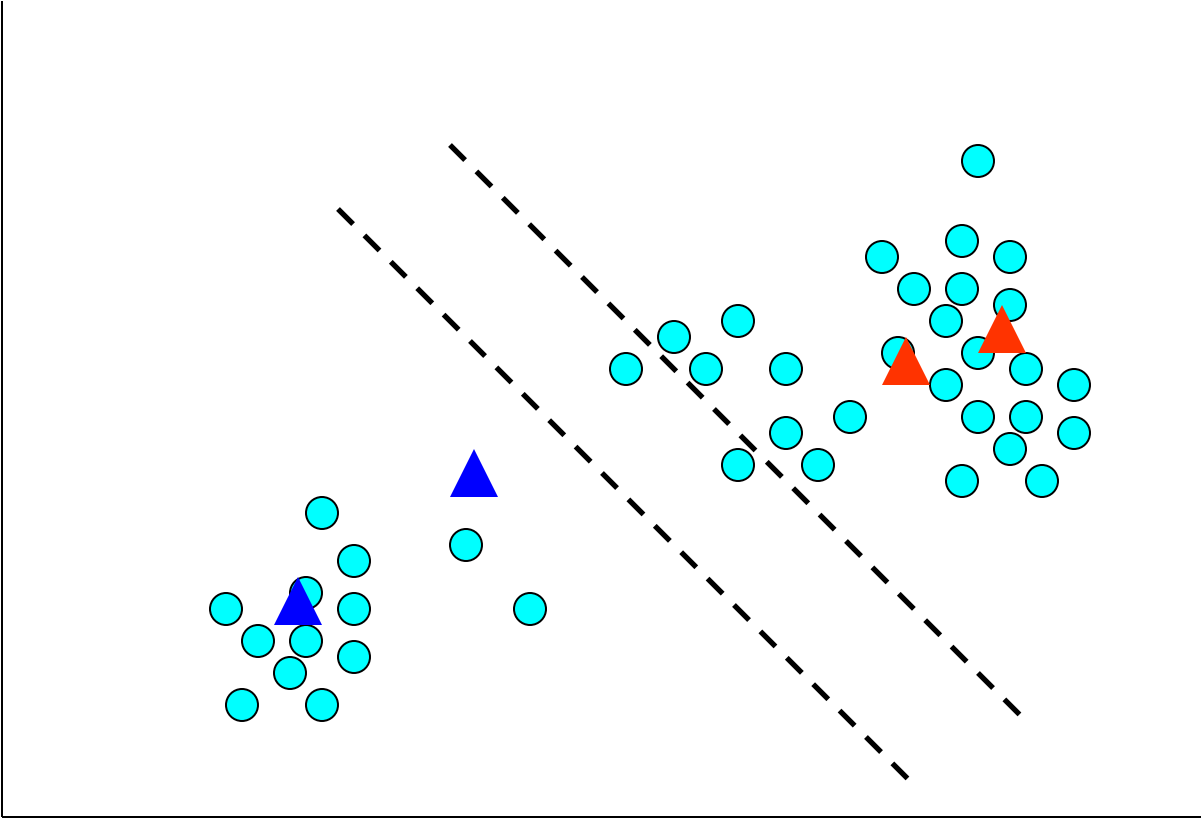
$$\hat{f} \leftarrow \operatorname{argmin}_{h \in H} \sum_{x \in X} \delta(h(x) \neq f(x)) \frac{n(x, L)}{|L|}$$

- Can use  $U$  for improved approximation:

$$\hat{f} \leftarrow \operatorname{argmin}_{h \in H} \sum_{x \in X} \delta(h(x) \neq f(x)) \frac{n(x, L) + n(x, U)}{|L| + |U|}$$

# of times we have  $x$  in the unlabeled set

# Example



## 2. Improve EM clustering algorithms

- Consider completely unsupervised clustering, where we assume data  $X$  is generated by a mixture of probability distributions, one for each cluster
  - For example, Gaussian mixtures
- Some classifier learning algorithms such as Gaussian Bayes classifiers also assumes the data  $X$  is generated by a mixture of distributions, one for each class  $Y$
- Supervised learning: estimate  $P(X|Y)$  from labeled data
- Opportunity: estimate  $P(X|Y)$  from labeled and unlabeled data, using EM as in clustering

# Bag of Words Text Classification



the world of  
**TOTAL**

**▶ All About The Company**  
Global Activities  
Corporate Structure  
TOTAL's Story  
Upstream Strategy  
Downstream Strategy  
Chemicals Strategy  
TOTAL Foundation  
Homepage

**all about the company**

Our energy exploration, production, and distribution operations span the globe, with activities in more than 100 countries.

At TOTAL, we draw our greatest strength from our fast-growing oil and gas reserves. Our strategic emphasis on natural gas provides a strong position in a rapidly expanding market.

Our expanding refining and marketing operations in Asia and the Mediterranean Rim complement already solid positions in Europe, Africa, and the U.S.

Our growing specialty chemicals sector adds balance and profit to the core energy business.



aardvark	0
about	2
all	2
Africa	1
apple	0
anxious	0
...	
gas	1
...	
oil	1
...	
Zaire	0

# Baseline: Naïve Bayes Learner

## ***Train:***

For each class  $c_j$  of documents

1. Estimate  $P(c_j)$
2. For each word  $w_i$  estimate  $P(w_i / c_j)$

## ***Classify (doc):***

Assign *doc* to most probable class

$$\arg \max_j P(c_j) \prod_{w_i \in doc} P(w_i | c_j)$$

Naïve Bayes assumption: words are conditionally independent, given class

### Faculty

associate	0.00417
chair	0.00303
member	0.00288
ph	0.00287
director	0.00282
fax	0.00279
journal	0.00271
recent	0.00260
received	0.00258
award	0.00250

### Students

resume	0.00516
advisor	0.00456
student	0.00387
working	0.00361
stuff	0.00359
links	0.00355
homepage	0.00345
interests	0.00332
personal	0.00332
favorite	0.00310

### Courses

homework	0.00413
syllabus	0.00399
assignments	0.00388
exam	0.00385
grading	0.00381
midterm	0.00374
pm	0.00371
instructor	0.00370
due	0.00364
final	0.00355

### Departments

departmental	0.01246
colloquia	0.01076
epartment	0.01045
seminars	0.00997
schedules	0.00879
webmaster	0.00879
events	0.00826
facilities	0.00807
eople	0.00772
postgraduate	0.00764

### Research Projects

investigators	0.00256
group	0.00250
members	0.00242
researchers	0.00241
laboratory	0.00238
develop	0.00201
related	0.00200
arpa	0.00187
affiliated	0.00184
project	0.00183

### Others

type	0.00164
jan	0.00148
enter	0.00145
random	0.00142
program	0.00136
net	0.00128
time	0.00128
format	0.00124
access	0.00117
begin	0.00116

# Expectation Maximization (EM) Algorithm

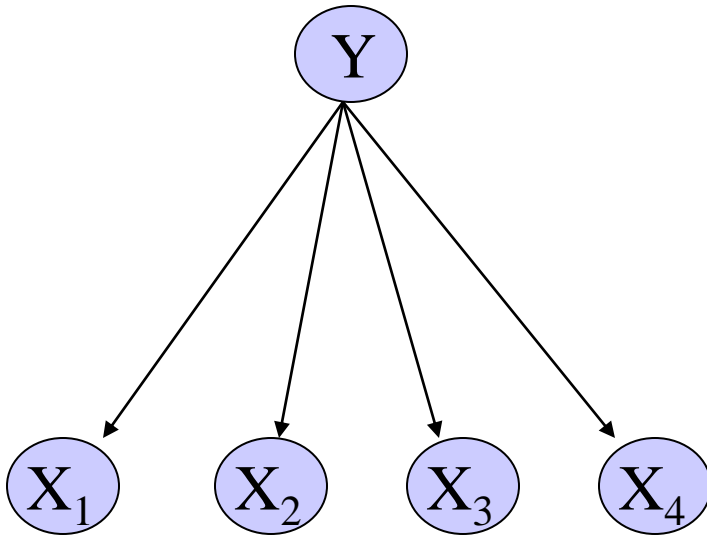
- Use labeled data  $L$  to learn initial classifier  $h$

Loop:

- E Step:
  - Assign probabilistic labels to  $U$ , based on  $h$
- M Step:
  - Retrain classifier  $h$  using both  $L$  (with fixed membership) and assigned labels to  $U$  (soft membership)
- Under certain conditions, guaranteed to converge to locally maximum likelihood  $h$

## 2. Generative Bayes model

Learn  $P(Y|X)$



Y	X1	X2	X3	X4
1	0	0	1	1
0	0	1	0	0
0	0	0	1	0
?	0	1	1	0
?	0	1	0	1




E Step:

$$\begin{aligned} P(y_i = c_j | d_i; \hat{\theta}) &= \frac{P(c_j | \hat{\theta}) P(d_i | c_j; \hat{\theta})}{P(d_i | \hat{\theta})} \\ &= \frac{P(c_j | \hat{\theta}) \prod_{k=1}^{|d_i|} P(w_{d_{i,k}} | c_j; \hat{\theta})}{\sum_{r=1}^{|\mathcal{C}|} P(c_r | \hat{\theta}) \prod_{k=1}^{|d_i|} P(w_{d_{i,k}} | c_r; \hat{\theta})}. \end{aligned}$$

M Step:

$w_t$  is t-th word in vocabulary


$$\hat{\theta}_{w_t | c_j} \equiv P(w_t | c_j; \hat{\theta}) = \frac{1 + \sum_{i=1}^{|\mathcal{D}|} N(w_t, d_i) P(y_i = c_j | d_i)}{|V| + \sum_{s=1}^{|\mathcal{V}|} \sum_{i=1}^{|\mathcal{D}|} N(w_s, d_i) P(y_i = c_j | d_i)},$$

$$\hat{\theta}_{c_j} \equiv P(c_j | \hat{\theta}) = \frac{1 + \sum_{i=1}^{|\mathcal{D}|} P(y_i = c_j | d_i)}{|\mathcal{C}| + |\mathcal{D}|}.$$

Table 3. Lists of the words most predictive of the **course** class in the WebKB data set, as they change over iterations of EM for a specific trial. By the second iteration of EM, many common **course**-related words appear. The symbol  $D$  indicates an arbitrary digit.

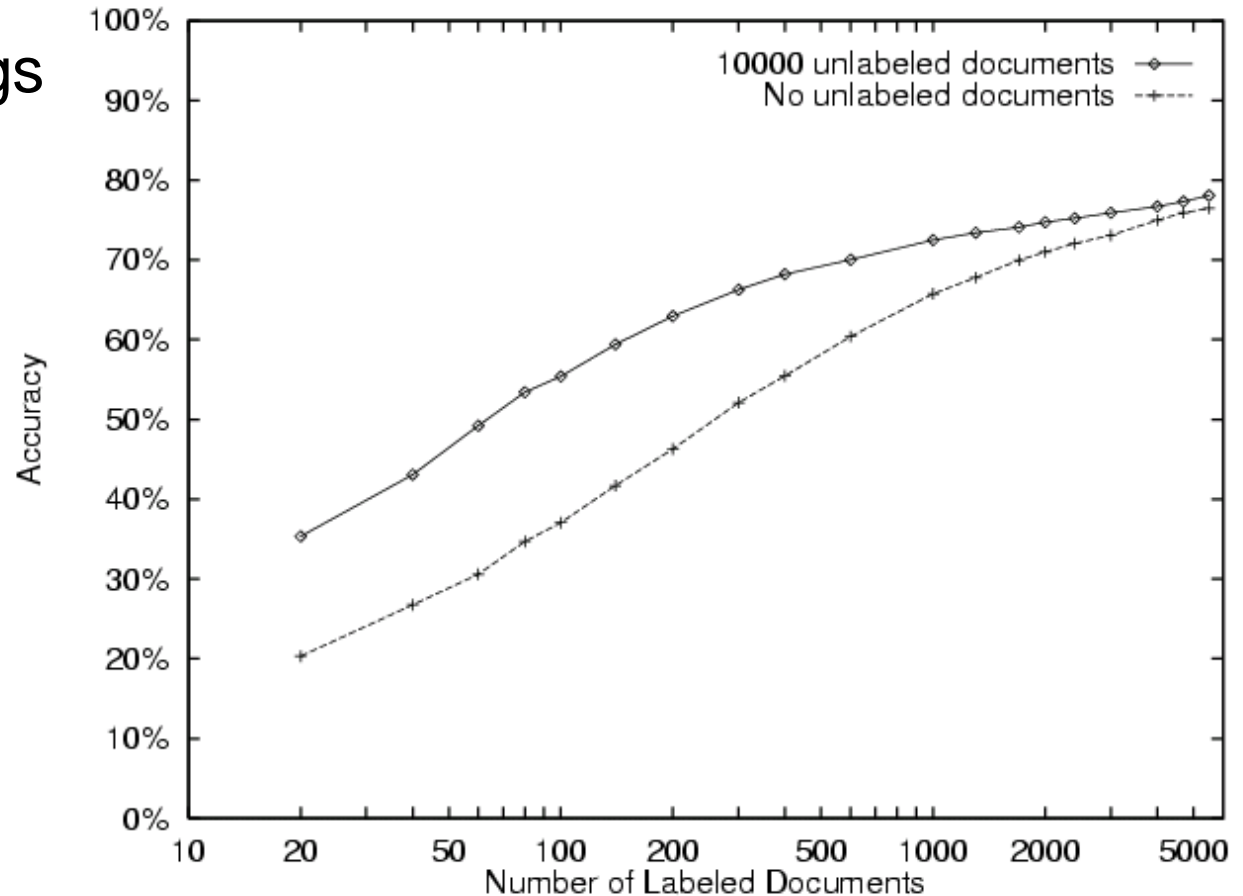
Iteration 0	Iteration 1	Iteration 2
intelligence	$DD$	$D$
$DD$	$D$	$DD$
artificial	lecture	lecture
understanding	cc	cc
$DDw$	$D^*$	$DD:DD$
dist	$DD:DD$	due
identical	handout	$D^*$
rus	due	homework
arrange	problem	assignment
games	set	handout
dartmouth	tay	set
natural	$DDam$	hw
cognitive	yurttas	exam
logic	homework	problem
proving	kfoury	$DDam$
prolog	sec	postscript
knowledge	postscript	solution
human	exam	quiz
representation	solution	chapter
field	assaf	ascii

Using one  
labeled  
example per  
class

# Experimental Evaluation

## Newsgroup postings

- 20 newsgroups,  
1000/group



# 3. If Problem Setting Provides Redundantly Sufficient Features, use CoTraining

- In some settings, available data features are so redundant that we can train two classifiers using different features
- In this case, the two classifiers should agree on the classification for each unlabeled example
- Therefore, we can use the unlabeled data to constrain training of both classifiers, forcing them to agree

### 3. CoTraining

*learn*  $f : X \rightarrow Y$

*where*  $X = X_1 \times X_2$

*where*  $x$  drawn from unknown distribution

*and*  $\exists g_1, g_2 \quad (\forall x) g_1(x_1) = g_2(x_2) = f(x)$

# Redundantly Sufficient Features

Professor Faloutsos

my advisor



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## Christos Faloutsos

**Current Position:** Assoc. Professor of [Computer Science](#). (97-98: [on leave at CMU](#))

**Join Appointment:** [Institute for Systems Research](#) (ISR).

**Academic Degrees:** Ph.D. and M.Sc. ([University of Toronto](#)); B.Sc. ([Nat. Tech. U. Ath](#))

## Research Interests:

- Query by content in multimedia databases;
- Fractals for clustering and spatial access methods;
- Data mining;

# CoTraining Algorithm

[Blum&Mitchell, 1998]

Given: labeled data  $L$ ,

unlabeled data  $U$

Loop:

Train  $g_1$  (hyperlink classifier) using  $L$

Train  $g_2$  (page classifier) using  $L$

Allow  $g_1$  to label  $p$  positive,  $n$  negative examps from  $U$

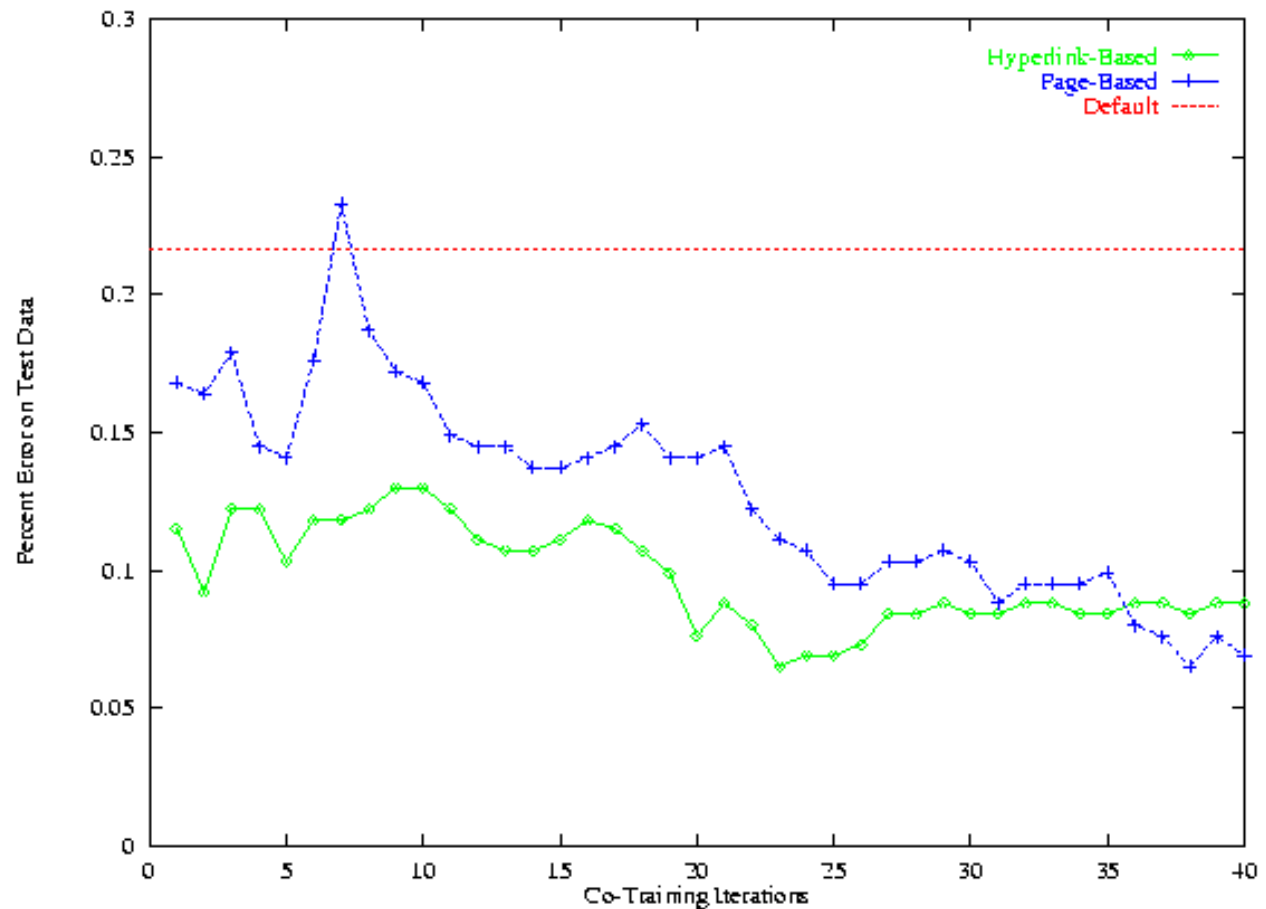
Allow  $g_2$  to label  $p$  positive,  $n$  negative examps from  $U$

Add the intersection of the self-labeled examples to  $L$

# CoTraining: Experimental Results

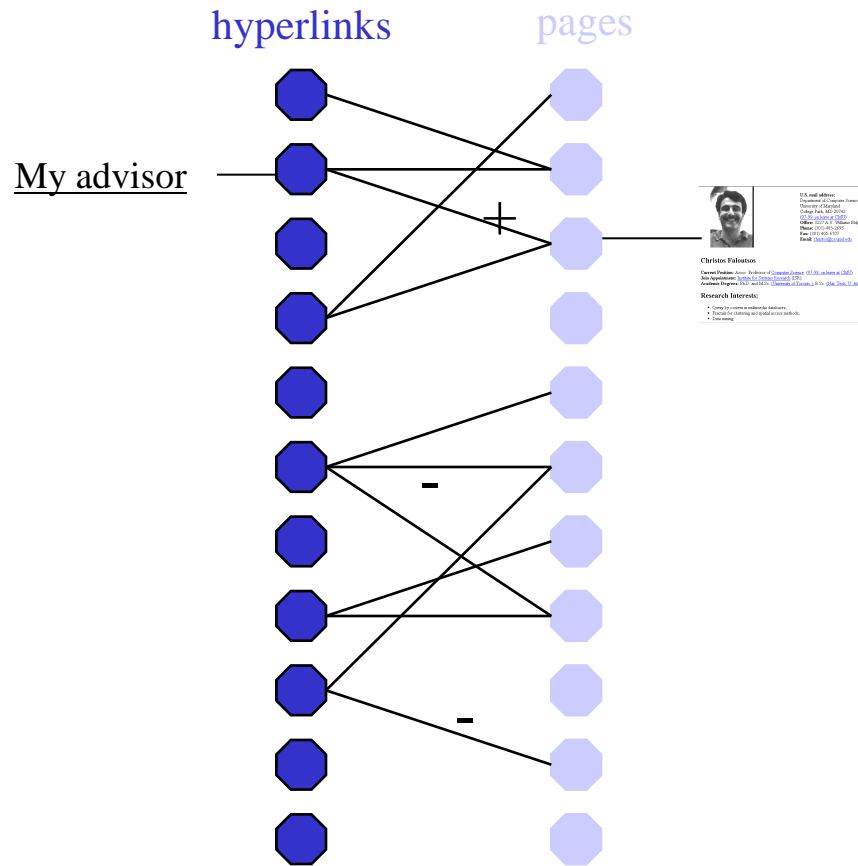
- begin with 12 labeled web pages (academic course)
- provide 1,000 additional unlabeled web pages
- average error: learning from labeled data 11.1%;
- average error: cotraining 5.0% (when both agree)

Typical run:





# Co-Training Rote Learner



# Classifying Jobs for FlipDog

FlipDog.com • Employers • Support

Home Find Jobs Your Account Research Employers

Search Results | Modify Search | New Search

zen systems Mid-Sr. Sun HW Engineer Pleasanton, CA

nd Crazy College Grad w/ Ambition & Personality? Join our IT Recruiting Team.

MentalShock Why work for one startup when you can work for many?

Sort results by:  Search these jobs for:  [Search tips](#)

26 - 50 of 159 jobs shown below Previous More Results

<a href="#">C++/Java Consultants</a> at <a href="#">Elite Placement Services</a>	November 01, 2000 Houston, TX Computing/MIS Software Development
<a href="#">Chief Software Architect</a> at <a href="#">Elite Placement Services</a>	November 01, 2000 Houston, TX Computing/MIS Software Development
<a href="#">Web Application Developers</a> at <a href="#">MI Systems, Inc.</a>	November 01, 2000 Houston, TX Computing/MIS Internet Development
<a href="#">Sales Consulting Engineer</a> at <a href="#">Visual Numerics, Inc.</a>	November 01, 2000 Houston, TX Computing/MIS Technical Support/Help Des
<a href="#">Peoplesoft Software Analyst (Systems Analyst III)</a> at <a href="#">I.T. Staffing, Inc.</a>	October 27, 2000 Houston, TX Computing/MIS Software Development
<a href="#">Peoplesoft Software Analyst (Systems Analyst III)</a> at <a href="#">I.T. Staffing, Inc.</a>	October 27, 2000 Houston, TX Computing/MIS Software Development

X1: job title

X2: job description

# 4. Use $U$ to Detect/Preempt Overfitting

- Overfitting is a problem for many learning algorithms (e.g., decision trees, neural networks)
- The symptom of overfitting: complex hypothesis  $h_2$  performs better on training data than simpler hypothesis  $h_1$ , but worse on test data
- Unlabeled data can help detect overfitting, by comparing predictions of  $h_1$  and  $h_2$  over the unlabeled examples
  - The rate at which  $h_1$  and  $h_2$  disagree on  $U$  should be the same as the rate on  $L$ , unless overfitting is occurring

# Defining a distance metric

- Definition of distance metric
  - Non-negative  $d(f,g) \geq 0$ ;
  - symmetric  $d(f,g) = d(g,f)$ ;
  - triangle inequality  $d(f,g) \leq d(f,h) + d(h,g)$

- Classification with zero-one loss:

$$d(h_1, h_2) \equiv \int \delta(h_1(x) \neq h_2(x)) p(x) dx$$

- Regression with squared loss:

$$d(h_1, h_2) \equiv \sqrt{\int (h_1(x) - h_2(x))^2 p(x) dx}$$

# Using the distance metric

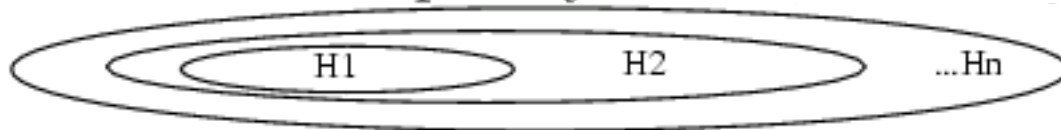
Define *metric* over  $H \cup \{f\}$

$$d(h_1, h_2) \equiv \int \delta(h_1(x) \neq h_2(x))p(x)dx$$

$$\hat{d}(h_1, f) = \frac{1}{|L|} \sum_{x_i \in L} \delta(h_1(x_i) \neq y_i)$$

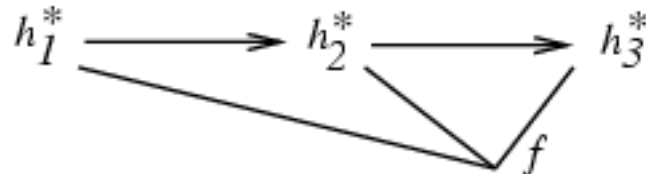
$$\hat{d}(h_1, h_2) = \frac{1}{|U|} \sum_{x \in U} \delta(h_1(x) \neq h_2(x))$$

Organize  $H$  into complexity classes



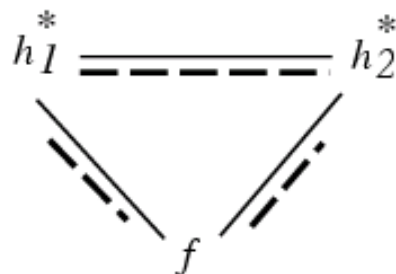
Let  $h_i^*$  be hypothesis with lowest  $\hat{d}(h, f)$  in  $H_i$

Prefer  $h_1^*$ ,  $h_2^*$ , or  $h_3^*$ ?



## Idea: Use $U$ to Avoid Overfitting

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Note:

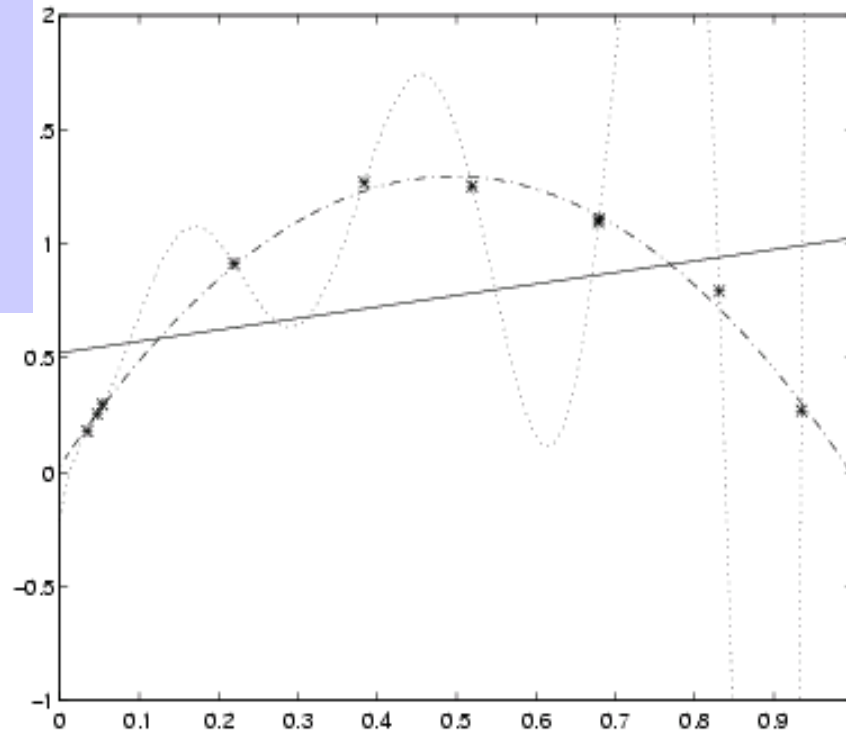
- $\hat{d}(h_i^*, f)$  optimistically biased (too short)
- $\hat{d}(h_i^*, h_j^*)$  unbiased
- Distances must obey triangle inequality!

$$d(h_1, h_2) \leq d(h_1, f) + d(f, h_2)$$

→ Heuristic:

- Continue training until  $\hat{d}(h_i, h_{i+1})$  fails to satisfy triangle inequality

Generated  $y$   
values contain  
zero mean  
Gaussian noise  $\varepsilon$   
 $Y=f(x)+\varepsilon$



An example of minimum squared error polynomials of degrees 1, 2, and 9 for a set of 10 training points. The large degree polynomial demonstrates erratic behavior off the training set.

# Experimental Evaluation of TRI

[Schuermans & Southey, MLJ 2002]

- Use it to select degree of polynomial for regression
- Compare to alternatives such as cross validation, structural risk minimization, ...

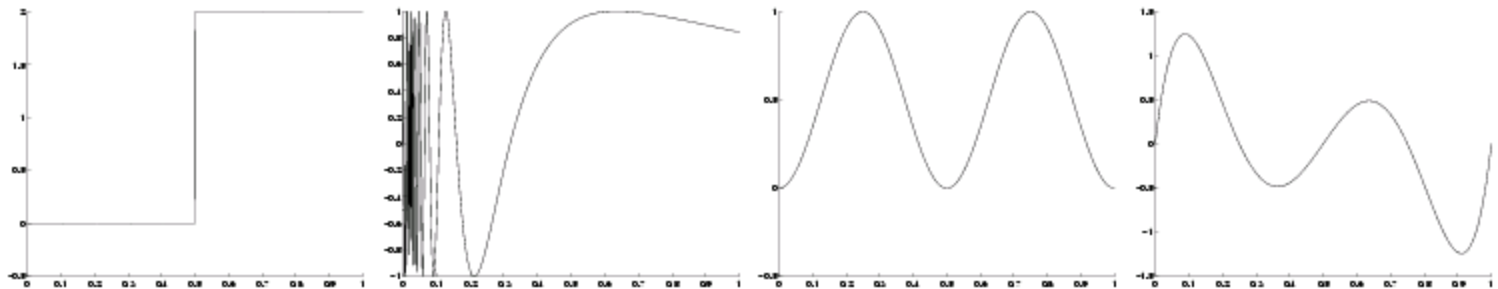


Figure 5: Target functions used in the polynomial curve fitting experiments (in order):  $\text{step}(x \geq 0.5)$ ,  $\sin(1/x)$ ,  $\sin^2(2\pi x)$ , and a fifth degree polynomial.



Approximation ratio:

true error of selected hypothesis

true error of best hypothesis considered

Results using 200 unlabeled,  $t$  labeled

Cross validation (Ten-fold)

Structural risk minimization

performance  
in top .50 of  
trials

$t = 20$	TRI	CVT	SRM	RIC	GCV	BIC	AIC	FPE	ADJ
25	1.00	1.06	1.14	7.54	5.47	15.2	22.2	25.8	1.02
50	1.06	1.17	1.39	224	118	394	585	590	1.12
75	1.17	1.42	3.62	5.8e3	3.9e3	9.8e3	1.2e4	1.2e4	1.24
95	1.44	6.75	56.1	6.1e5	3.7e5	7.8e5	9.2e5	8.2e5	1.54
100	2.41	1.1e4	2.2e4	1.5e8	6.5e7	1.5e8	1.5e8	8.2e7	3.02

$t = 30$	TRI	CVT	SRM	RIC	GCV	BIC	AIC	FPE	ADJ
25	1.00	1.08	1.17	4.69	1.51	5.41	5.45	2.72	1.06
50	1.08	1.17	1.54	34.8	9.19	39.6	40.8	19.1	1.14
75	1.19	1.37	9.68	258	91.3	266	266	159	1.25
95	1.45	6.11	419	4.7e3	2.7e3	4.8e3	5.1e3	4.0e3	1.51
100	2.18	643	1.6e7	1.6e7	1.6e7	1.6e7	1.6e7	1.6e7	2.10

Table 1: Fitting  $f(x) = \text{step}(x \geq 0.5)$  with  $P_x = U(0, 1)$  and  $\sigma = 0.05$ . Tables give distribution of approximation ratios achieved at training sample size  $t = 20$  and  $t = 30$ , showing percentiles of approximation ratios achieved in 1000 repeated trials.

# Summary

Several ways to use unlabeled data in supervised learning

1. Use to reweight labeled examples
2. Use to help EM learn class-specific generative models
3. If problem has redundantly sufficient features, use CoTraining
4. Use to detect/preempt overfitting

Ongoing research area

# Further Reading

- EM approach: K.Nigam, et al., 2000. "Text Classification from Labeled and Unlabeled Documents using EM", *Machine Learning*, 39, pp.103—134.
- CoTraining: A. Blum and T. Mitchell, 1998. "Combining Labeled and Unlabeled Data with Co-Training," *Proceedings of the 11th Annual Conference on Computational Learning Theory (COLT-98)*.
- S. Dasgupta, et al., "PAC Generalization Bounds for Co-training", *NIPS 2001*
- Model selection: D. Schuurmans and F. Southey, 2002. "Metric-Based methods for Adaptive Model Selection and Regularization," *Machine Learning*, 48, 51—84.

# Acknowledgment

Some of these slides are based in on slides from Tom Mitchell.