Semi-Supervised Learning

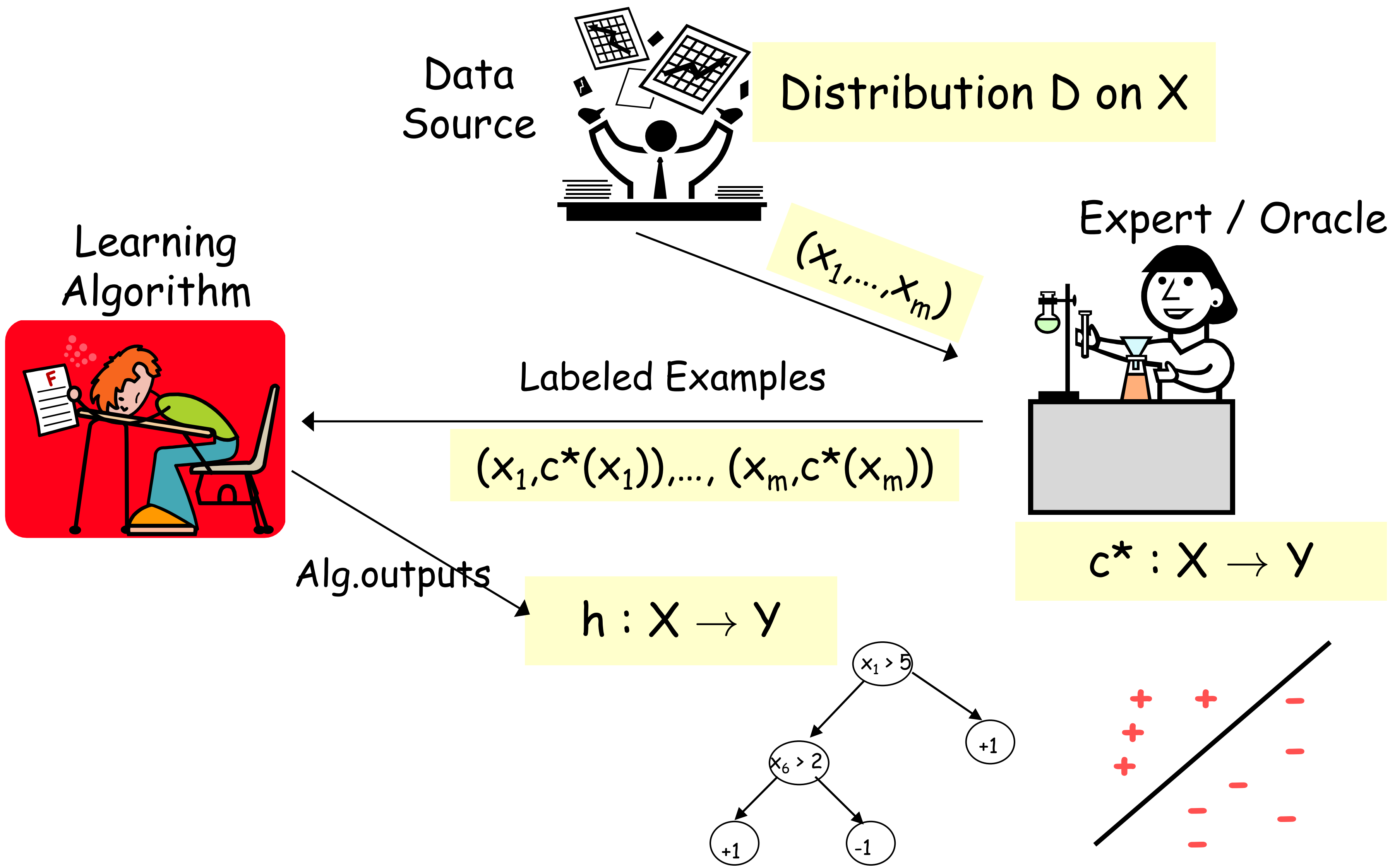
Maria-Florina Balcan

03/30/2015

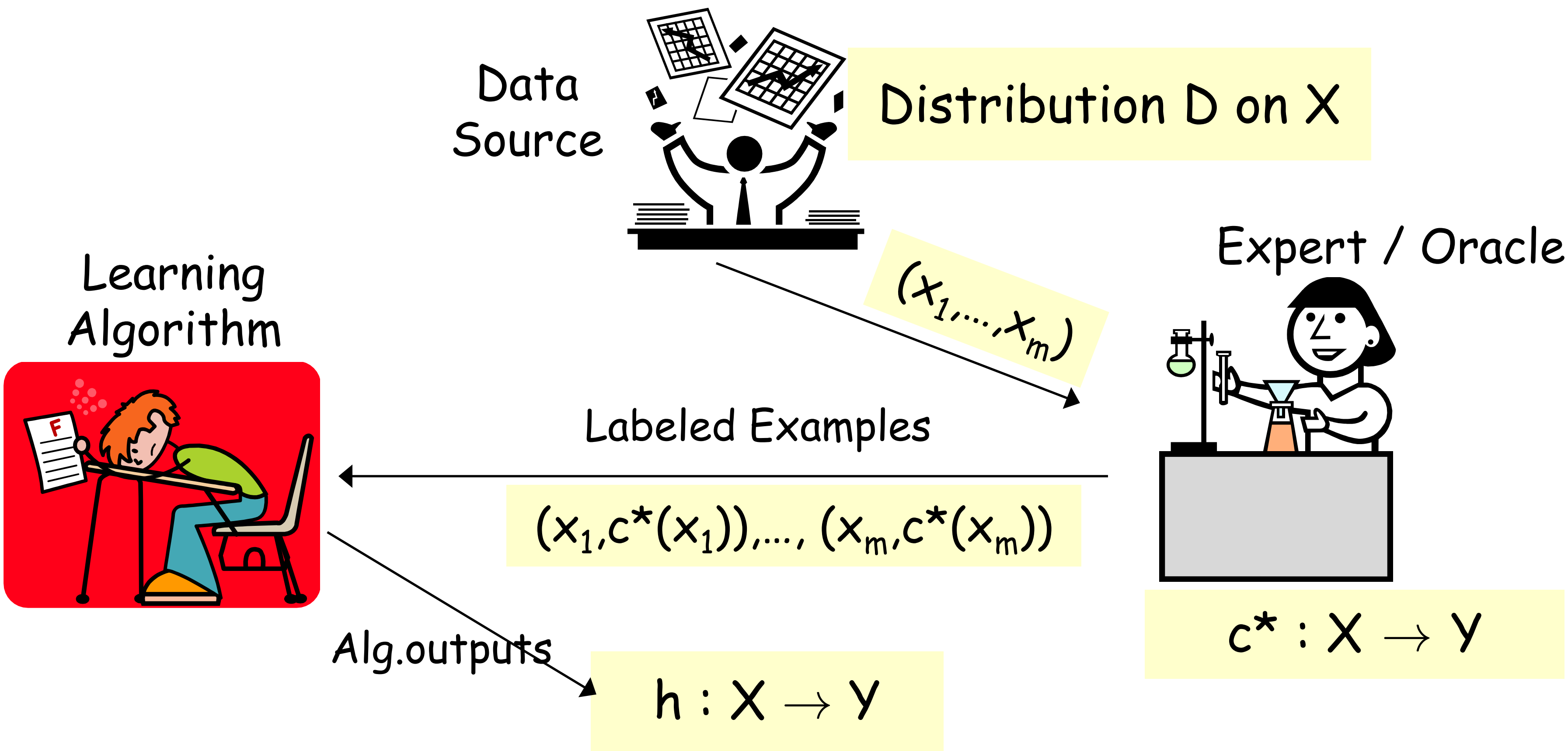
Readings:

- Semi-Supervised Learning. Encyclopedia of Machine Learning. Jerry Zhu, 2010
- Combining Labeled and Unlabeled Data with Co-Training. Avrim Blum, Tom Mitchell. COLT 1998.

Fully Supervised Learning



Fully Supervised Learning



S_l={(x_1, y_1), …,(x_{m_l}, y_{m_l})}

x_i drawn i.i.d from D, $y_i = c^*(x_i)$

Goal: h has small error over D.

$$\mathrm{err}_D(h) = \Pr_{x\sim D}(h(x) \neq c^*(x))$$

Two Core Aspects of Supervised Learning

Algorithm Design. How to optimize?

Computation

Automatically generate rules that do well on observed data.

- E.g.: Naïve Bayes, logistic regression, SVM, Adaboost, etc.

Confidence Bounds, Generalization

(Labeled) Data

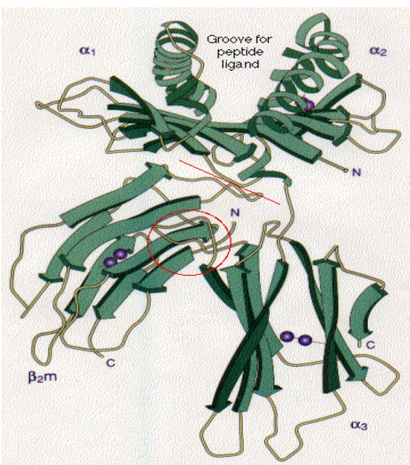
Confidence for rule effectiveness on future data.

- VC-dimension, Rademacher complexity, margin based bounds, etc.

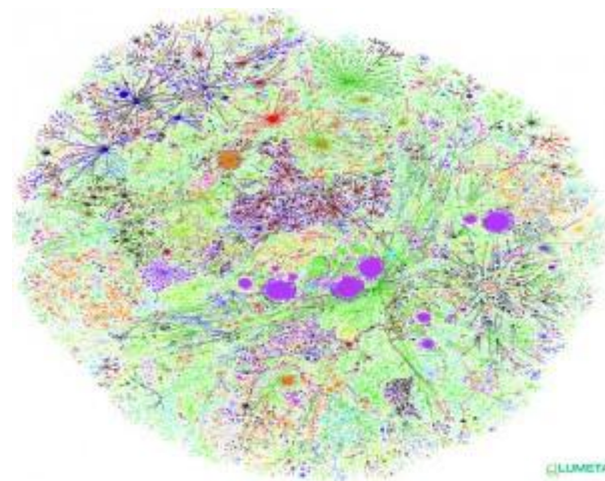
Classic Paradigm Insufficient Nowadays

Modern applications: massive amounts of raw data.

Only a tiny fraction can be annotated by human experts.



Protein sequences



Billions of webpages

Images

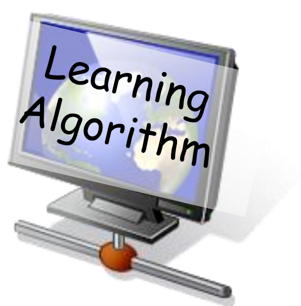
Modern ML: New Learning Approaches

Modern applications: massive amounts of raw data.

Techniques that best utilize data, minimizing need for expert/human intervention.

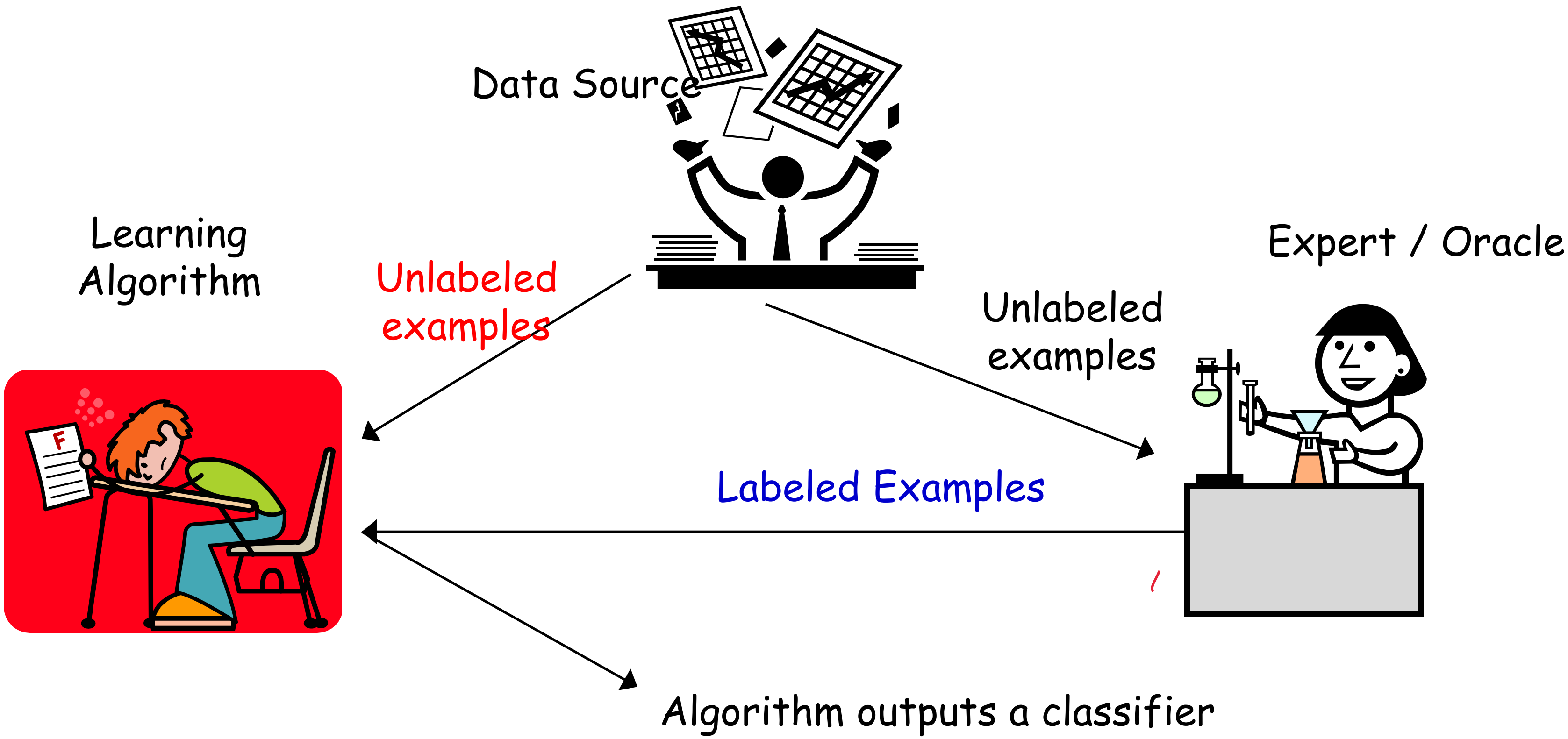
Paradigms where there has been great progress.

- Semi-supervised Learning, (Inter)active Learning.



Quiz

Semi-Supervised Learning



$S_l=\{(x_1,y_1),\ldots,(x_{m_l},y_{m_l})\}$

x_i drawn i.i.d from D, $y_i = c^*(x_i)$

$S_u=\{x_1,\ldots,x_{m_u}\}$ drawn i.i.d from D

Inductive: **Goal:** h has small error over D.

$\min_h \; err_D(h) = \Pr_{x\sim D}(h(x) \neq c^*(x))$

Transductive: $\min_h \; err_{S_u}(h) = \Pr_{x\sim S_u}(h(x) \neq c^*(x))$

Semi-supervised Learning

- Major topic of research in ML.
- Several methods have been developed to try to use unlabeled data to improve performance, e.g.:
  - Transductive SVM [Joachims '99]
  - Co-training [Blum & Mitchell '98]
  - Graph-based methods [B&C01], [ZGL03]

Test of time awards at ICML!

Workshops [ICML '03, ICML' 05, ...]

Books:
- Semi-Supervised Learning, MIT 2006
  O. Chapelle, B. Scholkopf and A. Zien (eds)
- Introduction to Semi-Supervised Learning, Morgan & Claypool, 2009 Zhu & Goldberg

Semi-supervised Learning

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Test of time awards at ICML!

Both wide spread applications and solid foundational understanding!!!

Semi-supervised Learning

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  - Co-training [Blum & Mitchell '98]
  - Graph-based methods [B&C01], [ZGL03]

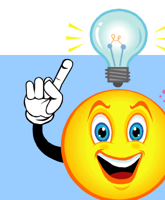
Test of time awards at ICML!

Today: discuss these methods.

Very interesting, they all exploit unlabeled data in different, very interesting and creative ways.

Semi-supervised learning: no querying. Just have lots of additional unlabeled data.

A bit puzzling; unclear what unlabeled data can do for us…. It is missing the most important info. How can it help us in substantial ways?



Key Insight

Unlabeled data useful if we have beliefs not only about the form of the target, but also about its relationship with the underlying distribution.

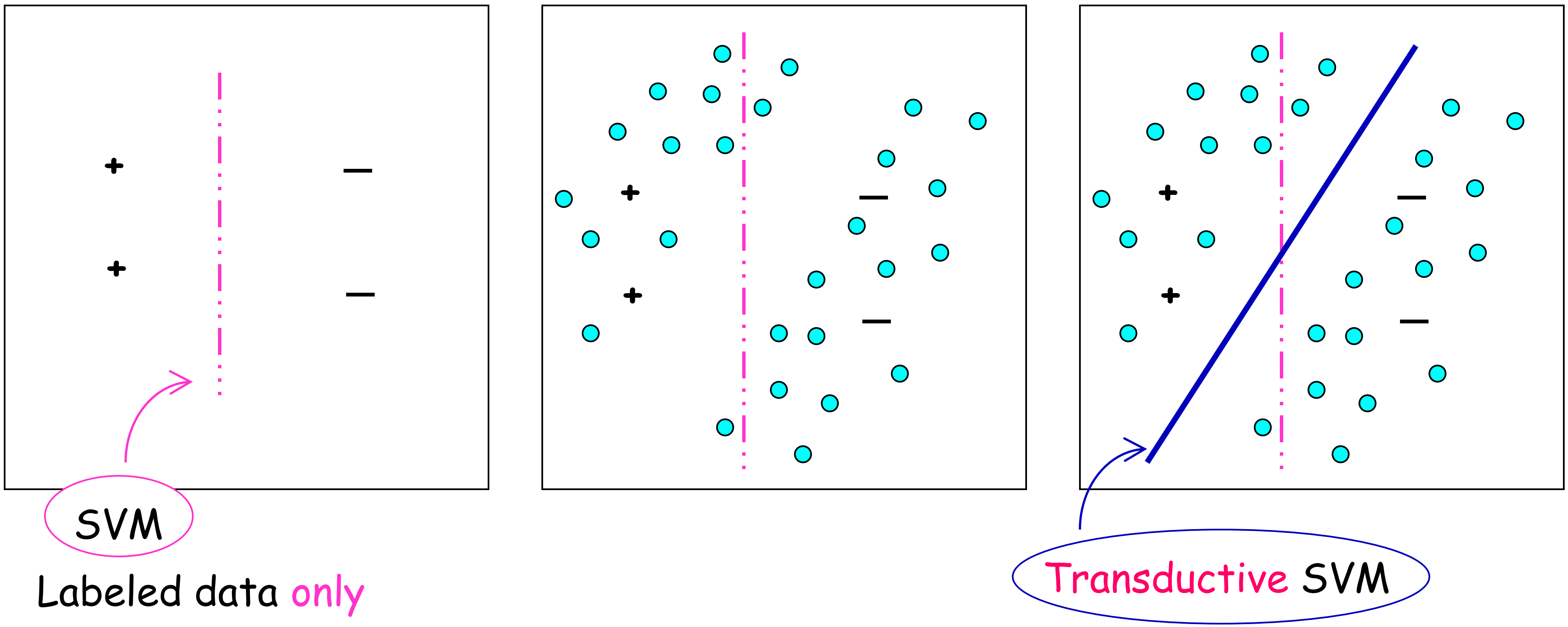
Semi-supervised SVM

[Joachims '99]

Margins based regularity

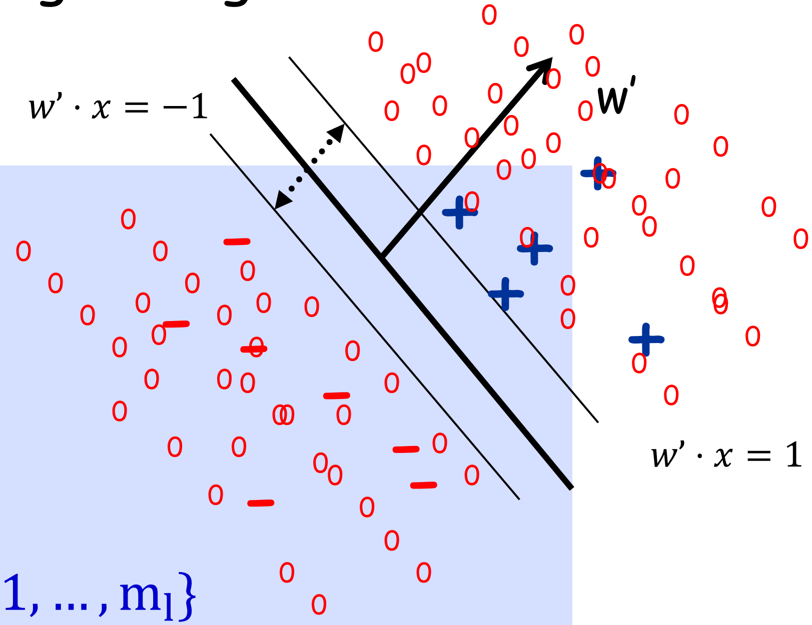
Target goes through low density regions (large margin).

- assume we are looking for linear separator
- belief: should exist one with large separation



Transductive Support Vector Machines

Optimize for the separator with large margin wrt labeled and unlabeled data. [Joachims '99]



Input: $S_l=\{(x_1,y_1), \ldots,(x_{m_l},y_{m_l})\}$

$S_u=\{x_1, \ldots,x_{m_u}\}$

$\operatorname{argmin}_{\cancel{w}} ||w||^2$ s.t.:

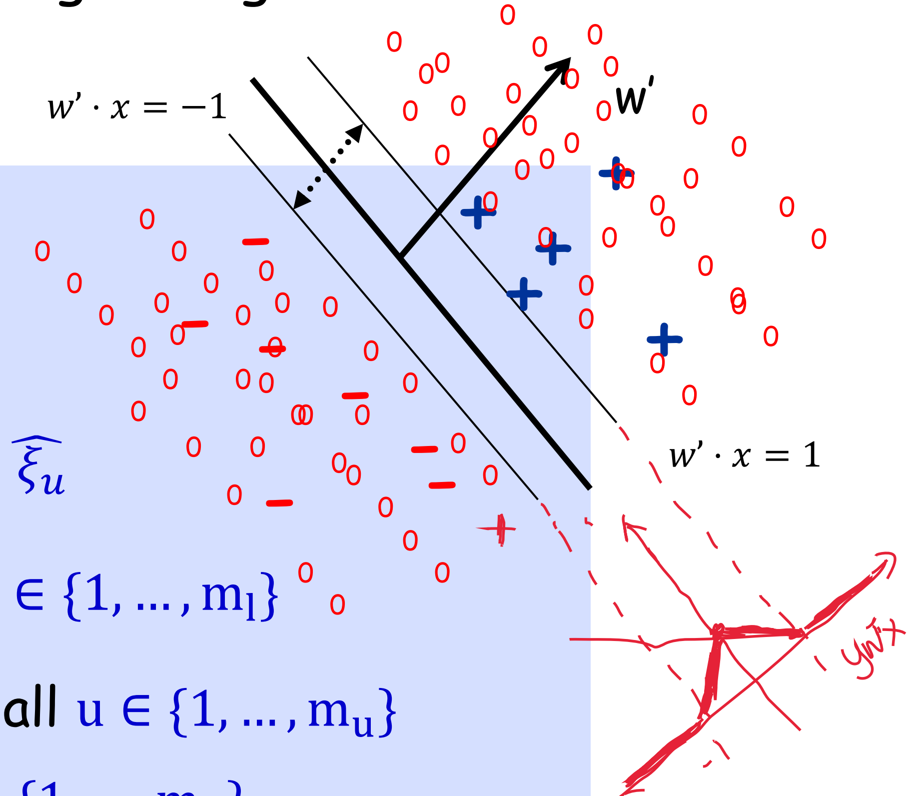
$w, \hat{y}_u$

- $y_i\, w \cdot x_i \geq 1$, for all $i \in \{1, \ldots, m_l\}$
- $\widehat{y_u} w \cdot x_u \geq 1$, for all $u \in \{1, \ldots, m_u\}$
- $\widehat{y_u} \in \{-1, 1\}$ for all $u \in \{1, \ldots, m_u\}$

Find a labeling of the unlabeled sample and w s.t. w separates both labeled and unlabeled data with maximum margin.

Transductive Support Vector Machines

Optimize for the separator with large margin wrt labeled and unlabeled data. [Joachims '99]



Input: $S_l = \{(x_1, y_1), \dots, (x_{m_l}, y_{m_l})\}$

$S_u = \{x_1, \dots, x_{m_u}\}$

$w, \xi_l, \xi_u, \hat{y}_u$

$$\mathrm{argmin}_w \, ||w||^2 + C \sum_i \xi_i + C \sum_u \hat{\xi}_u$$

$\xi_i = (1 - y_i w^T x_i)_+$: Hinge-loss

- $y_i \, w \cdot x_i \geq 1 - \xi_i$, for all $i \in \{1, \dots, m_l\}$

$\xi_m = (1 - |w^T x_i|)_+$: Hat-loss (Sym-hinge)

- $\hat{y}_u w \cdot x_u \geq 1 - \hat{\xi}_u$, for all $u \in \{1, \dots, m_u\}$
- $\hat{y}_u \in \{-1, 1\}$ for all $u \in \{1, \dots, m_u\}$

Find a labeling of the unlabeled sample and w s.t. w separates both labeled and unlabeled data with maximum margin.

Transductive Support Vector Machines

Optimize for the separator with large margin wrt labeled and unlabeled data.

$$\min_w \underline{\|w\|^2} + \underline{C_l \sum_{i=1}^{n} (1 - y_i w^T x_i)_+} + \underline{C_u \sum_{i=1}^{n} (1 - |w^T x_i|)_+}$$

(non-convex)

Input: $S_l = \{(x_1, y_1), \ldots, (x_{m_l}, y_{m_l})\}$

$S_u = \{x_1, \ldots, x_{m_u}\}$

$$\text{argmin}_w \, \|w\|^2 + C_l \textstyle\sum_i \xi_i + C_u \sum_u \widehat{\xi_u}$$

- $y_i \, w \cdot x_i \geq 1 - \xi_i$, for all $i \in \{1, \ldots, m_l\}$
- $\widehat{y_u} w \cdot x_u \geq 1 - \widehat{\xi_u}$, for all $u \in \{1, \ldots, m_u\}$
- $\widehat{y_u} \in \{-1, 1\}$ for all $u \in \{1, \ldots, m_u\}$

NP-hard..... Convex only after you guessed the labels... too many possible guesses...

Transductive Support Vector Machines

Optimize for the separator with large margin wrt labeled and unlabeled data.

Heuristic (Joachims) high level idea:

- First maximize margin over the labeled points S_l
- Use this to give initial labels to unlabeled points S_u based on this separator.
- Try flipping labels of unlabeled points to see if doing so can increase margin

Keep going until no more improvements. Finds a locally-optimal solution.

Experiments [Joachims99]

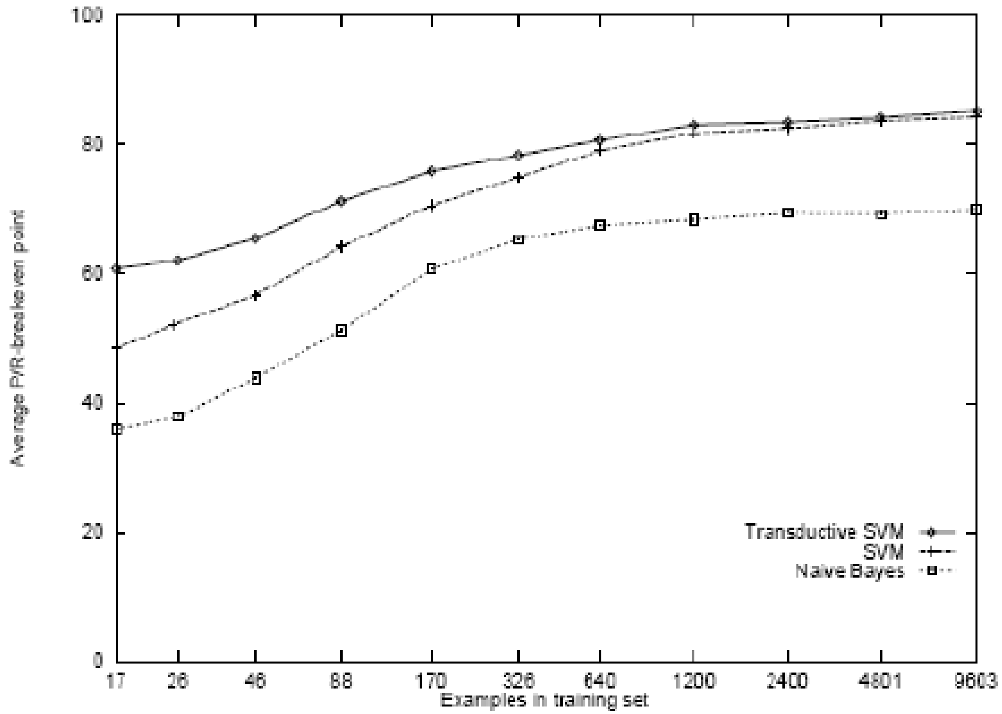


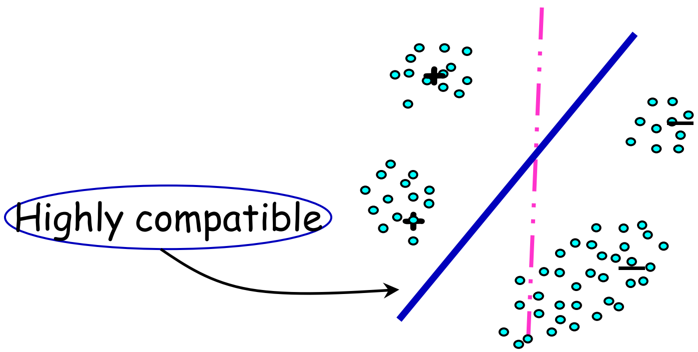
Figure 6: Average P/R-breakeven point on the Reuters dataset for different training set sizes and a test set size of 3,299.

S_t

$|S_u|$

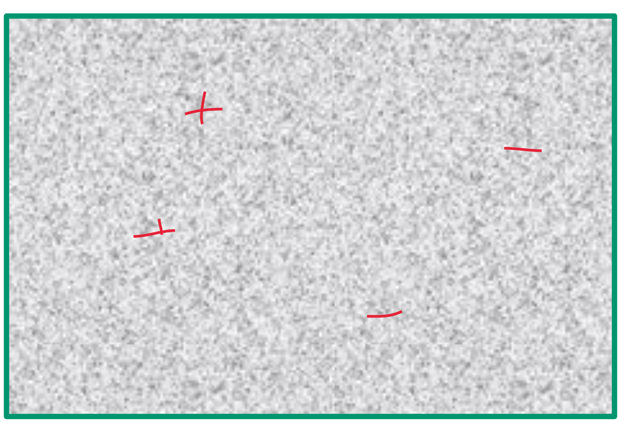
Transductive Support Vector Machines

Helpful distribution



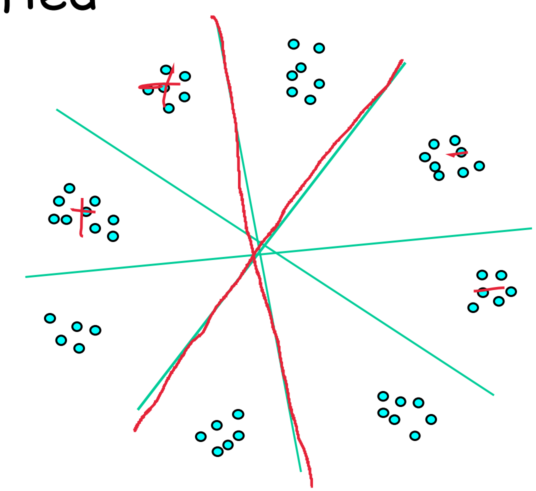
Non-helpful distributions

Margin not satisfied



Margin satisfied

$1/\gamma^2$ clusters, all partitions separable by large margin



Co-training

[Blum & Mitchell '98]

Different type of underlying regularity assumption:

Consistency or Agreement Between Parts

Co-training: Self-consistency

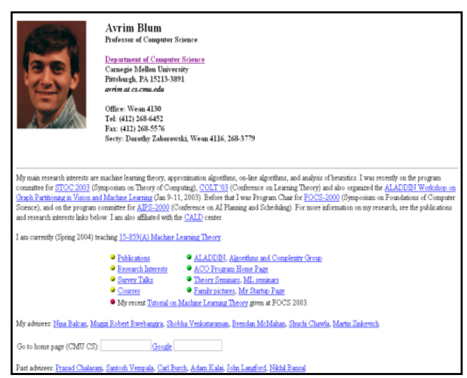
Agreement between two parts : co-training [Blum-Mitchell98].

- examples contain two sufficient sets of features, $x = \langle x_1, x_2 \rangle$
- belief: the parts are consistent, i.e. $\exists\, c_1, c_2$ s.t. $c_1(x_1)=c_2(x_2)=c^*(x)$

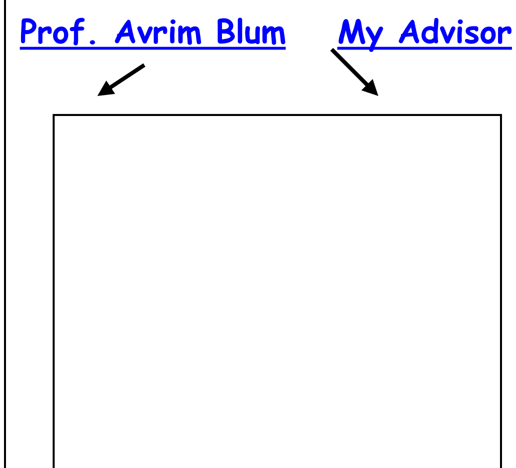
For example, if we want to classify web pages: $x = \langle x_1, x_2 \rangle$

as faculty member homepage or not

x - Link info & Text info



x_1- Text info



x_2- Link info

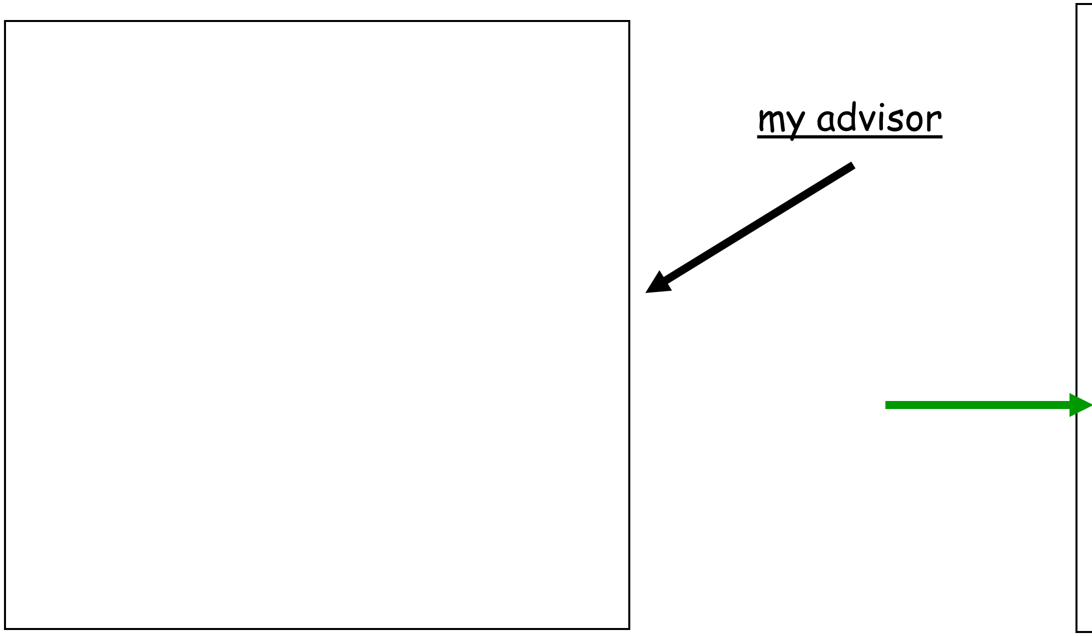
Iterative Co-Training

Idea: Use small labeled sample to learn initial rules.

link
- E.g., "my advisor" pointing to a page is a good indicator it is a faculty home page.

text
- E.g., "I am teaching" on a page is a good indicator it is a faculty home page.

Idea: Use unlabeled data to propagate learned information.



Avrim Blum's home page — Page 1 of 1

Avrim Blum
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Check out our new faculty members Ryan O'Donnell and Luis von Ahn.

My main research interests are machine learning theory, approximation algorithms, on-line algorithms, and algorithmic game theory. I was/am on the Program Committees for FOCS 2008 (Symp. Foundations of Computer Science), ACM-EC 2008 (Electronic Commerce), and COLT 2007 (Conference on Learning Theory), and was recently local organizer for COLT 2006 and FOCS 2005. I also co-organized the 2005 Foundations of Computational Mathematics Workshop on Algorithmic Game Theory and Metric Embeddings. A while back I served as Program Chair for FOCS 2000 and I've done some work in AI Planning. For more information on my research, see the publications and research interests links below. I am also affiliated with the Machine Learning department.

I am currently (Spring 2008) teaching 15-859(B) Machine Learning Theory.

- Publications
- Research Interests
- Survey Talks
- Courses
- ALADDIN, Algorithms and Complexity Group
- ACO Program Home Page
- Theory Seminars, Theory lunch ML lunch
- Family pictures, Other pictures, My Startup Page
- My Tutorial on Machine Learning Theory given at FOCS 2003 and a short essay.

My advisees: Aaron Roth, Katrina Ligett, Nina Balcan, Mugizi Robert Rwebangira, Shobha Venkataraman.

Past advisees: Prasad Chalasani, Santosh Vempala, Carl Burch, Adam Kalai, John Langford, Nikhil Bansal, Martin Zinkevich, Shuchi Chawla, Brendan McMahan.

Google

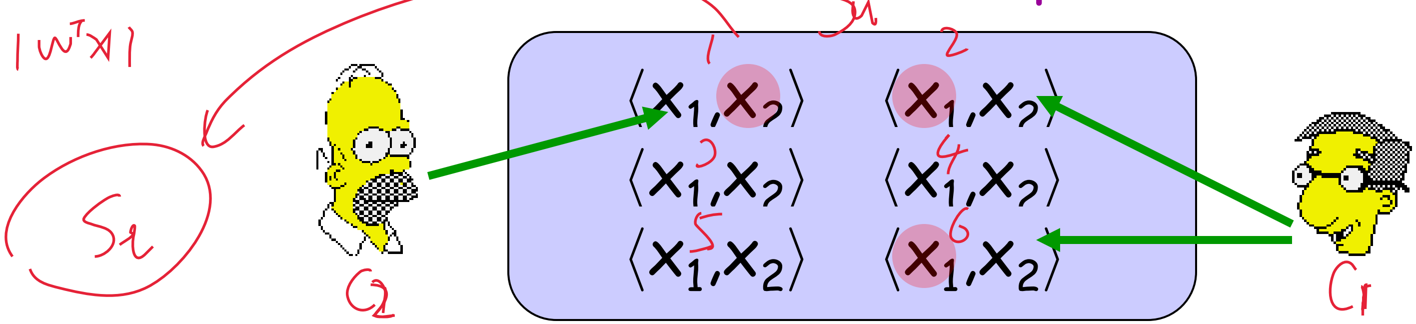
Iterative Co-Training

Idea: Use small labeled sample to learn initial rules.

- E.g., "my advisor" pointing to a page is a good indicator it is a faculty home page.
- E.g., "I am teaching" on a page is a good indicator it is a faculty home page.

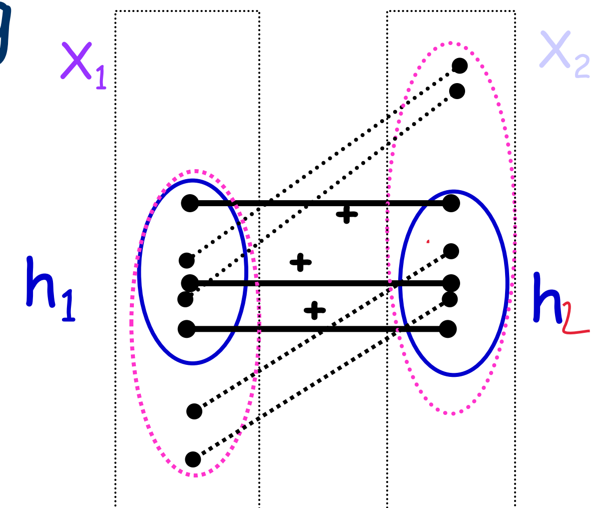
Idea: Use unlabeled data to propagate learned information.

Look for unlabeled examples where one rule is confident and the other is not. Have it label the example for the other.



Training 2 classifiers, one on each type of info. Using each to help train the other.

Iterative Co-Training



Works by using unlabeled data to propagate learned information.

- Have learning algos A_1, A_2 on each of the two views.
- Use labeled data to learn two initial hyp. h_1, h_2.

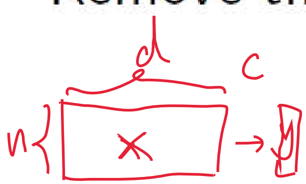
Repeat

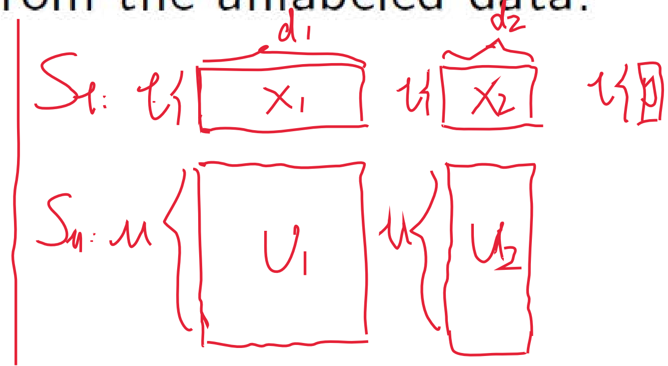
- Look through unlabeled data to find examples where one of h_i is confident but other is not.
- Have the confident h_i label it for algorithm A_{3-i}.

Co-Training Algorithm

Input: labeled data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$
each instance has two views $\mathbf{x}_i = [\mathbf{x}_i^{(1)}, \mathbf{x}_i^{(2)}]$,
and a learning speed k.

1. let $L_1 = L_2 = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_l, y_l)\}$.
2. Repeat until unlabeled data is used up:
3. Train view-1 $f^{(1)}$ from L_1, view-2 $f^{(2)}$ from L_2.
4. Classify unlabeled data with $f^{(1)}$ and $f^{(2)}$ separately.
5. Add $f^{(1)}$'s top k most-confident predictions $(\mathbf{x}, f^{(1)}(\mathbf{x}))$ to L_2.
   Add $f^{(2)}$'s top k most-confident predictions $(\mathbf{x}, f^{(2)}(\mathbf{x}))$ to L_1.
   Remove these from the unlabeled data.



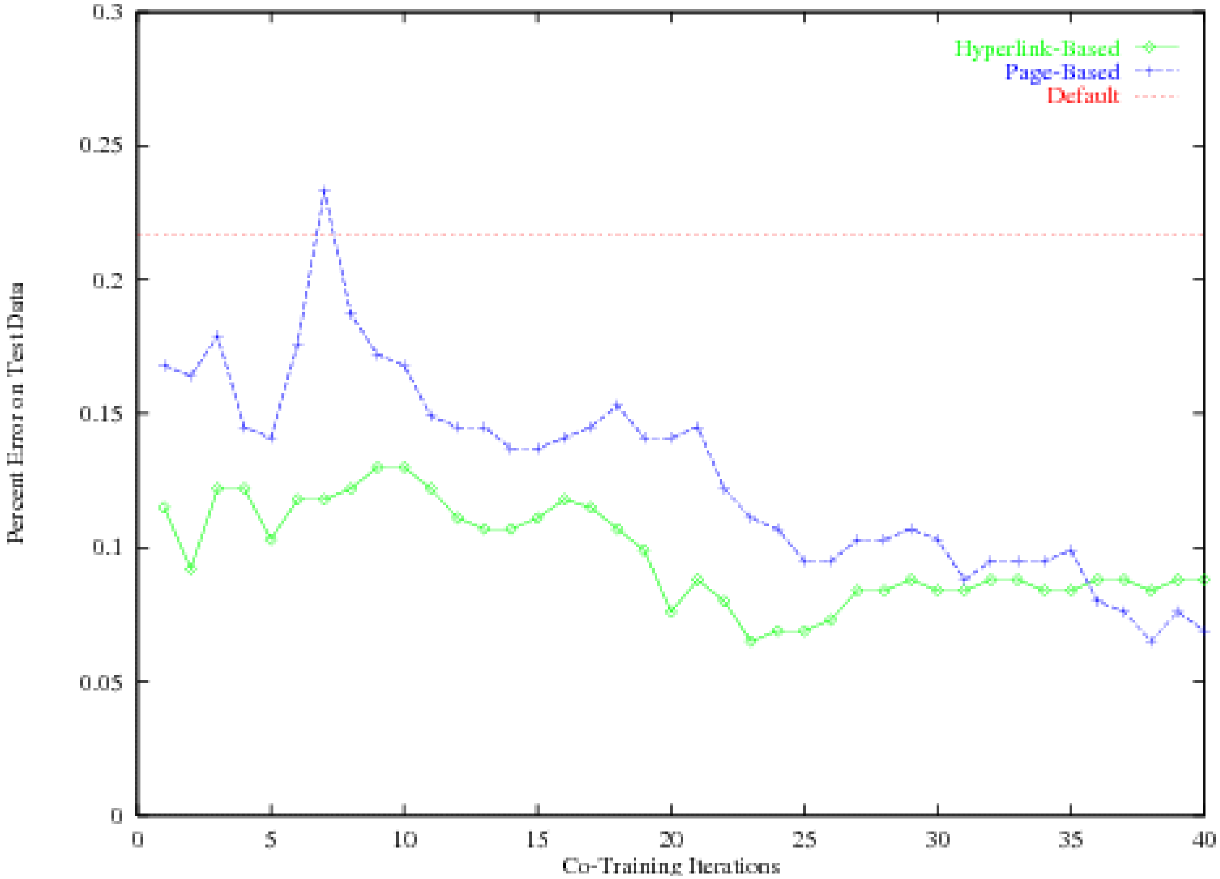


Original Application: Webpage classification

12 labeled examples, 1000 unlabeled

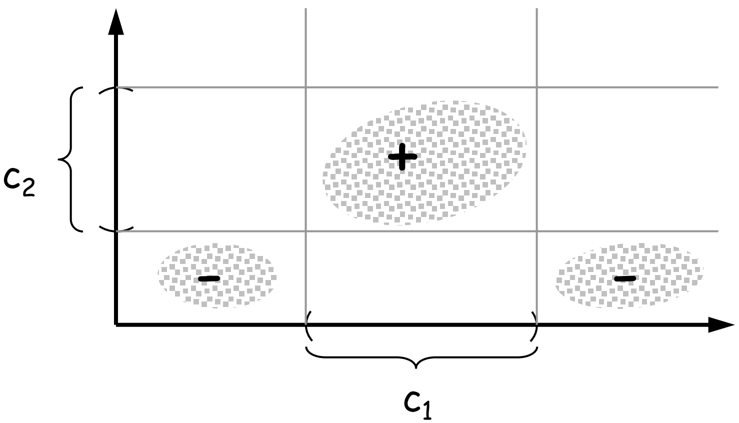
	Page-based	Hyperlink-based	Combined
Std. Supervised	12.9	12.4	11.1
Co-training	6.2	11.6	5.0
Just say neg	22	22	22

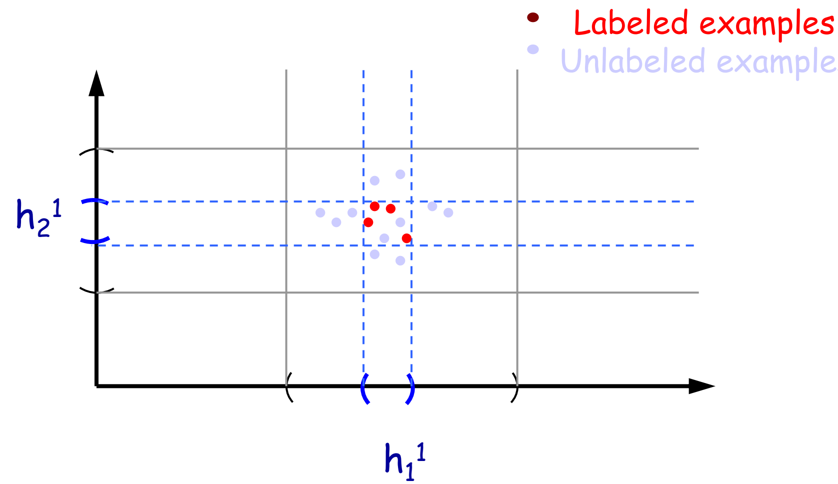
(sample run)



Iterative Co-Training

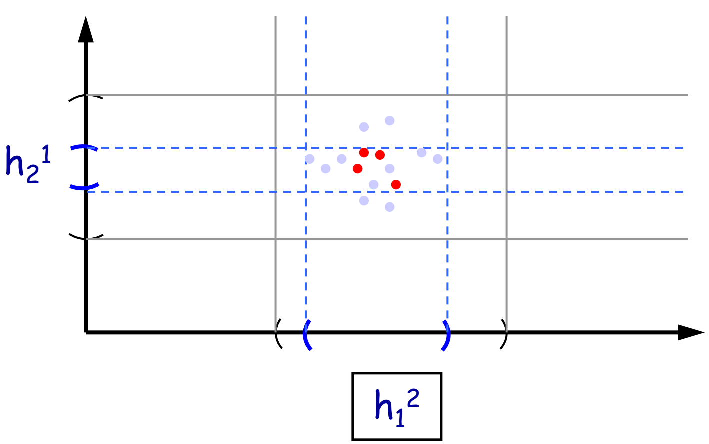
A Simple Example: Learning Intervals

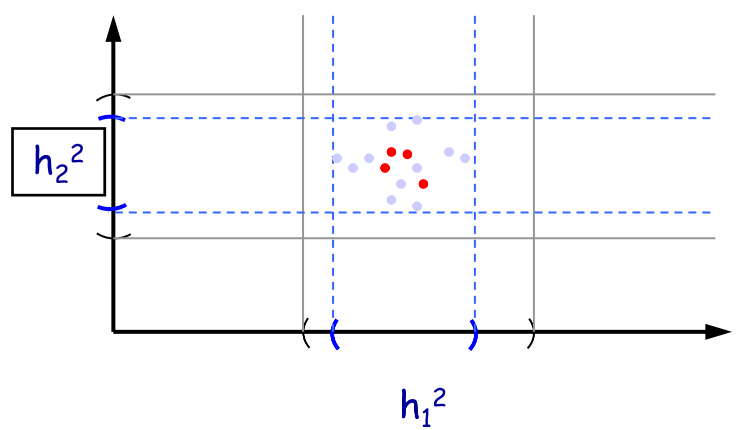




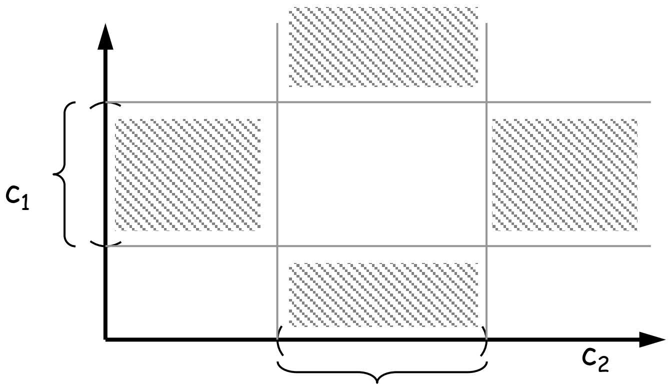
Use labeled data to learn h_1^1 and h_2^1

Use unlabeled data to bootstrap



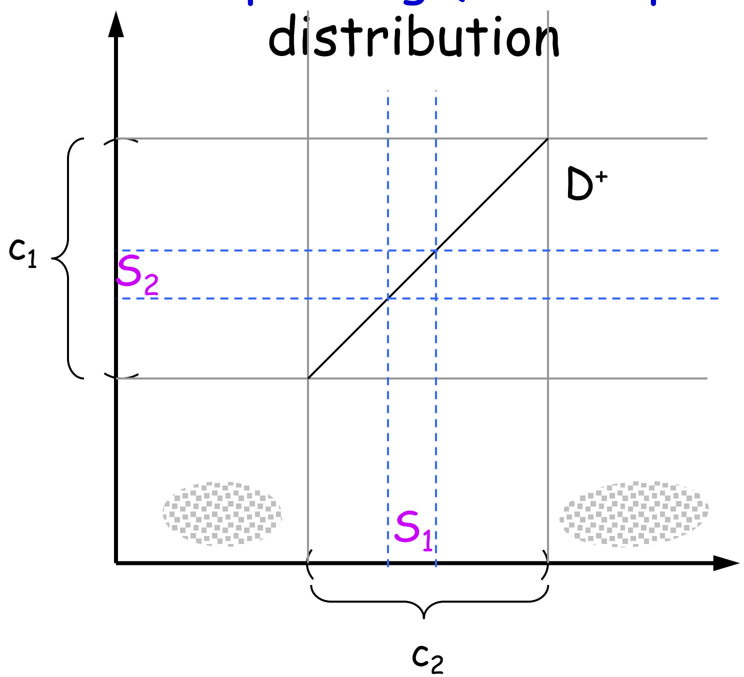


Expansion, Examples: Learning Intervals

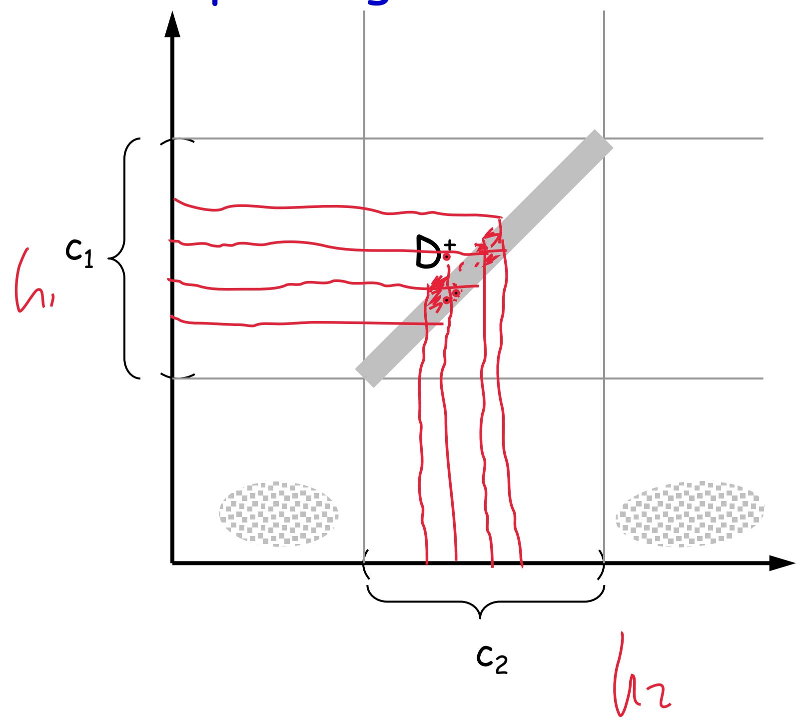


Consistency: zero probability mass in the regions

Non-expanding (non-helpful) distribution



Expanding distribution



Co-training [BM'98]

Say that h_1 is a weakly-useful predictor if

$$\Pr[h_1(x) = 1 | c_1(x) = 1] > \Pr[h_1(x) = 1 | c_1(x) = 0] + \gamma.$$

Has higher probability of saying positive on a true positive than it does on a true negative, by at least some gap γ

Say we have enough labeled data to produce such a starting point.

Theorem: if C is learnable from random classification noise, we can use a weakly-useful h_1 plus unlabeled data to create a strong learner under independence given the label.

Co-training/Multi-view SSL: Direct Optimization of Agreement

Input: $S_l=\{(x_1,y_1), \ldots,(x_{m_l},y_{m_l})\}$
$S_u=\{x_1, \ldots,x_{m_u}\}$

$$\sum_{v \neq v'} \sum_{i=1}^{m_u} \| h_v(x_i) - h_{v'}(x_i) \|_2^2$$

$$\| h_1(x_i) - h_2(x_i) \|_2^2 \qquad + C_2 \sum_{l=1}^{2} \Omega(h_l).$$

$$\operatorname{argmin}_{h_1,h_2} \sum_{l=1}^{2} \sum_{i=1}^{m_l} l(h_l(x_i),y_i) + C \sum_{i=1}^{m_u} \text{agreement}(h_1(x_i),h_2(x_i))$$

Co-regularization.

Each of them has small labeled error

Regularizer to encourage agreement over unlabeled dat

E.g.,

P. Bartlett, D. Rosenberg, AISTATS 2007; K. Sridharan, S. Kakade, COLT 2008

Co-training/Multi-view SSL: Direct Optimization of Agreement

Input: $S_l=\{(x_1,y_1), \ldots, (x_{m_l}, y_{m_l})\}$
$S_u=\{x_1, \ldots, x_{m_u}\}$

$$\mathrm{argmin}_{h_1,h_2} \sum_{l=1}^{2}\sum_{i=1}^{m_l} l(h_l(x_i), y_i) + C\sum_{i=1}^{m_u} \mathrm{agreement}(h_1(x_i), h_2(x_i))$$

- $l(h(x_i), y_i)$ loss function
  - E.g., square loss $l(h(x_i), y_i) = (y_i - h(x_l))^2$
  - E.g., 0/1 loss $l(h(x_i), y_i) = 1_{y_i \neq h(x_i)}$

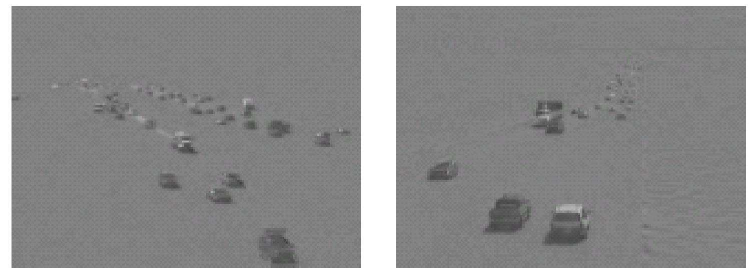
E.g.,

P. Bartlett, D. Rosenberg, AISTATS 2007; K. Sridharan, S. Kakade, COLT 2008

Many Other Applications

E.g., [Levin-Viola-Freund03] identifying objects in images.
Two different kinds of preprocessing.

Original images



Foreground images

Goal: car detection
#labeled images: 50
#unlabeled images: 22,000

Graph

Similarity Based Regularity

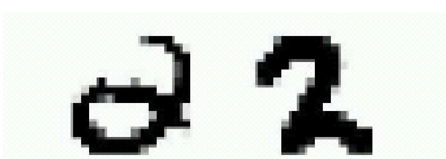
[Blum&Chwala01], [ZhuGhahramaniLafferty03]

(Tranductive)

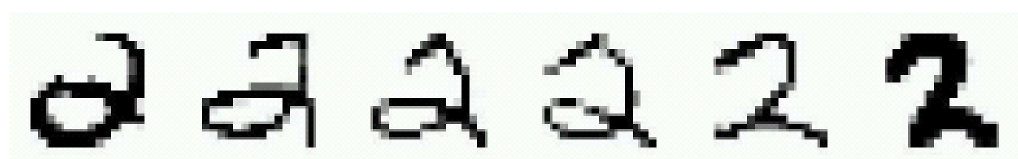
Graph-based Methods

- Assume we are given a pairwise similarity fnc and that very similar examples probably have the same label.
- If we have a lot of labeled data, this suggests a Nearest-Neighbor type of algorithm.
- If you have a lot of unlabeled data, perhaps can use them as "stepping stones".

E.g., handwritten digits [Zhu07]:



not similar

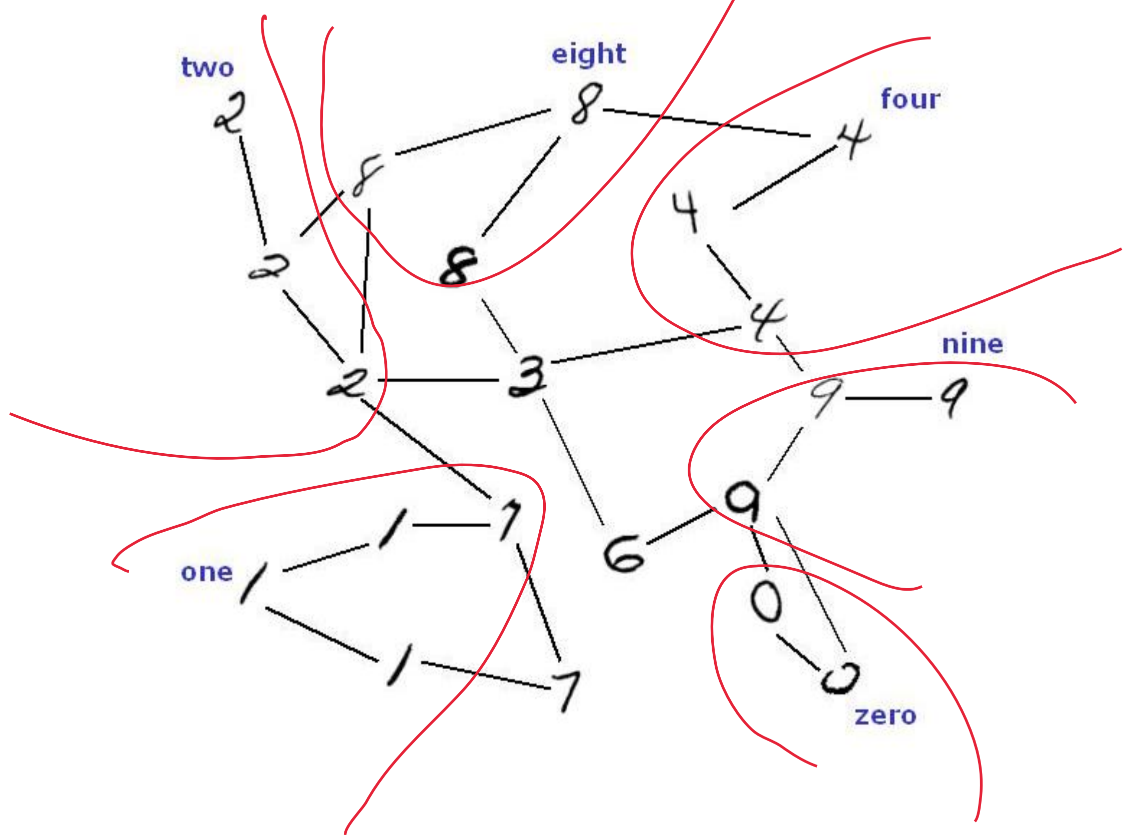


'indirectly' similar
with stepping stones

Graph-based Methods

Idea: construct a graph with edges between very similar examples.

Unlabeled data can help "glue" the objects of the same class together.

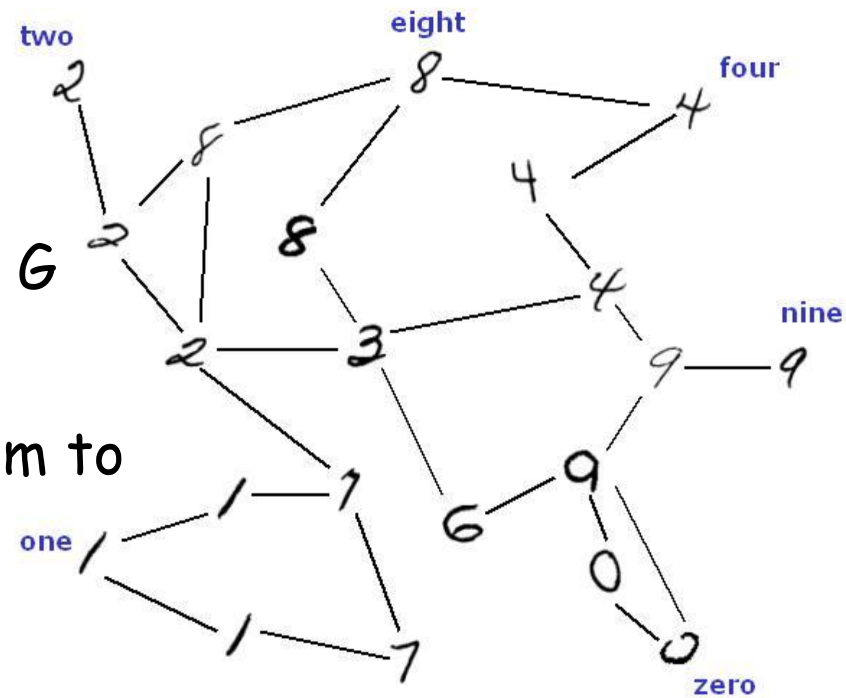


Graph-based Methods

Often, transductive approach. (Given L + U, output predictions on U). Are alllowed to output any labeling of $L \cup U$.

Main Idea:

- Construct graph G with edges between very similar examples.
- Might have also glued together in G examples of different classes.
- Run a graph partitioning algorithm to separate the graph into pieces.



Several methods:

- Minimum/Multiway cut [Blum&Chawla01]
- Minimum "soft-cut" [ZhuGhahramaniLafferty'03]
- Spectral partitioning
- …

How to Create the Graph

- Empirically, the following works well:

1. Compute distance between i, j
2. For each i, connect to its kNN. k very small but still connects the graph
3. Optionally put weights on (only) those edges

$$\exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

4. Tune σ

How to Create the Graph

G : Graph

$G = \langle V, E \rangle$

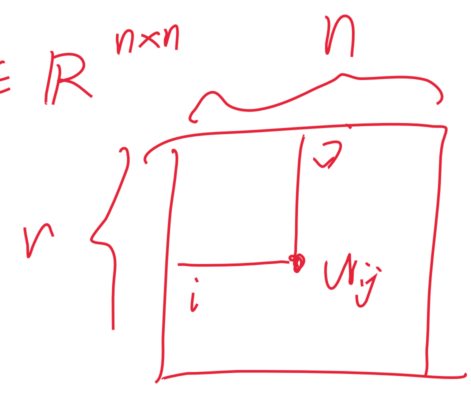
V (Vertex/Node) : sample ($S_l \cup S_u$)

E (Edge) : pairwise-similarity .

① Adjacency graph : k-NN / ε-NN ← $A \in \{0, 1\}^{n \times n}$

0-1/binary matrix

② Graph weighting ← 0-1 / Gaussian kernel . ← $W \in R^{n \times n}$

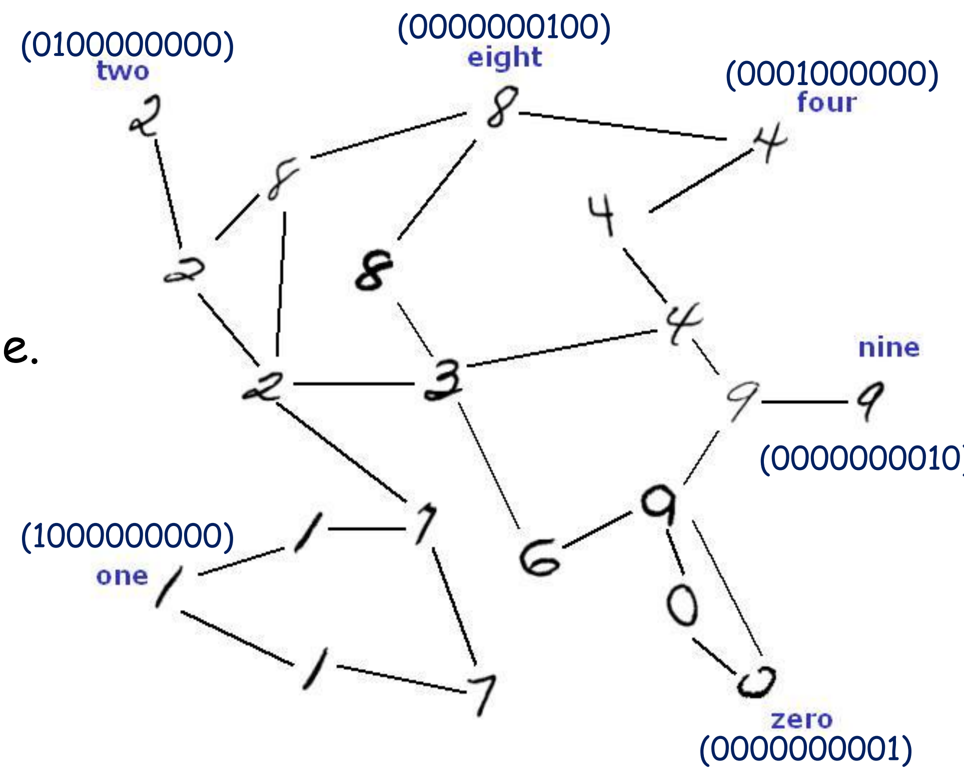


Minimum "soft cut"

[ZhuGhahramaniLafferty'03]

Objective Solve for probability vector over labels f_i on each unlabeled point i.

(labeled points get coordinate vectors in direction of their known label)



- Minimize $\sum_{e=(i,j)} w_e \left\| f_i - f_j \right\|^2$

  where $\|f_i - f_j\|$ is Euclidean distance.

- Can be done efficiently by solving a set of linear equations.

Minimum "soft cut"

① Initial label assignment

$$f \in \{-1, 0, 1\}$$

$$f_i = \begin{cases} \pm 1, & x_i \in S_l \\ 0, & x_i \in S_u \end{cases}$$

② Predict label assignment.

$$\min_f \underline{\sum_{i,j} w_{ij} (f_i - f_j)^2}$$

$$= \sum_{i,j} w_{ij} (f_i^2 - 2 f_i f_j + f_j^2)$$

$$= \underbrace{2 \sum_{i,j} w_{ij} f_i^2}_{f^T D f} - \underbrace{2 \sum_{i,j} w_{ij} f_i f_j}_{f^T W f}$$

$$f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix} \in R^{n \times 1}$$

Diagonal $(D)_{ii} = \sum_{j=1}^{n} w_{ij}$

$$= 2 f^T \underline{(D - W)} f$$

L : Laplacian matrix

$$\min_f f^T L f$$

s.t. $f_i = y_i, \ \forall x_i \in S_l$

$$f \begin{cases} \{-1, 1\} : & \text{hard.} \\ \mathbb{R} : & \text{soft} \end{cases}$$

$\underline{\mathrm{sgn}(f)} \rightarrow$ soft

$$\min_w \sum_{i=1}^{n_l} (1 - y_i w^T x_i)_+ + \lambda_1 \|w\|_2^2 + \lambda_2 \underline{(w^T U^T) L (U w)}$$

$$U = \overbrace{\begin{bmatrix} \end{bmatrix}}^{d} \Big\} n_u$$

$f = Uw$, $\quad f^T L f$

What You Should Know

- Unlabeled data useful if we have beliefs not only about the form of the target, but also about its relationship with the underlying distribution.
- Different types of algorithms (based on different beliefs).
  - Transductive SVM [Joachims '99]
  - Co-training [Blum & Mitchell '98]
  - Graph-based methods [B&C01], [ZGL03]

Supplementary Materials

1. Self-Training
2. Generative Models

Self-Training

Maybe a simple way of using unlabeled data

- Initialize $L = \{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$ and $U = \{\mathbf{x}_j\}_{j=l+1}^{n}$
- Repeat
  1. Train f from L using supervised learning
  2. Apply f to the unlabeled instances in U
  3. Remove a subset S from U ; add $\{(\mathbf{x}, f(\mathbf{x}))|\mathbf{x} \in S\}$ to L
- Until $U = \phi$

Self-Training

- A wrapper method
- The choice of learner for f is open
- Good for many real world tasks, e.g., natural language processing
- But mistake in choosing the f can reinforce itself

Generative Model

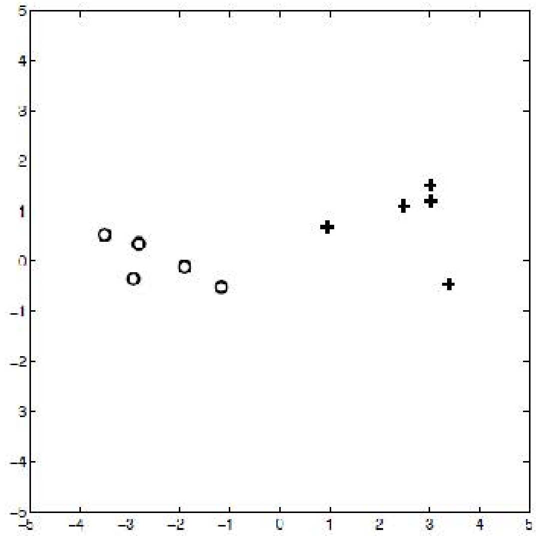
Gaussian mixture model (GMM)

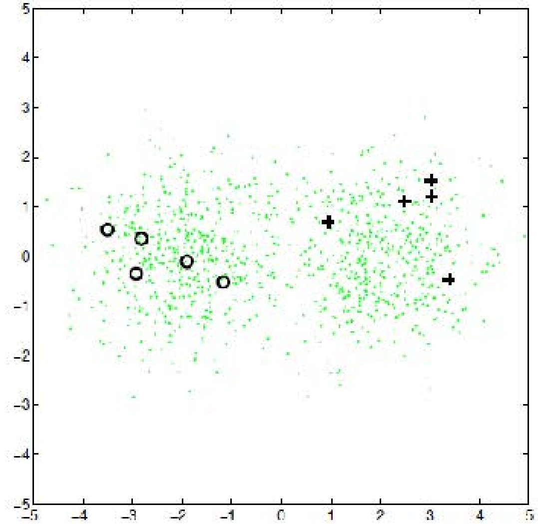
- Model parameters: $\theta = \{\pi_i, \mu_i, \Sigma_i\}_{i=1}^{K}$, π_i: class priors, μ_i:Gaussian means, Σ_i:covariance matrices
- Joint distribution

$$
\begin{aligned}
p(\mathbf{x}, \mathbf{y}|\theta) &= p(\mathbf{y}|\theta)p(\mathbf{x}|\mathbf{y}, \theta) \\
&= \sum_{i=1}^{K} \pi_i \mathcal{N}(\mathbf{x}; \mu_i, \Sigma_i)
\end{aligned}
$$

- Classification:

$$
p(\mathbf{y}|\mathbf{x}, \theta) = \frac{p(x, y|\theta)}{\sum_{i=1}^{K} p(\mathbf{x}, y_i|\theta)}
$$

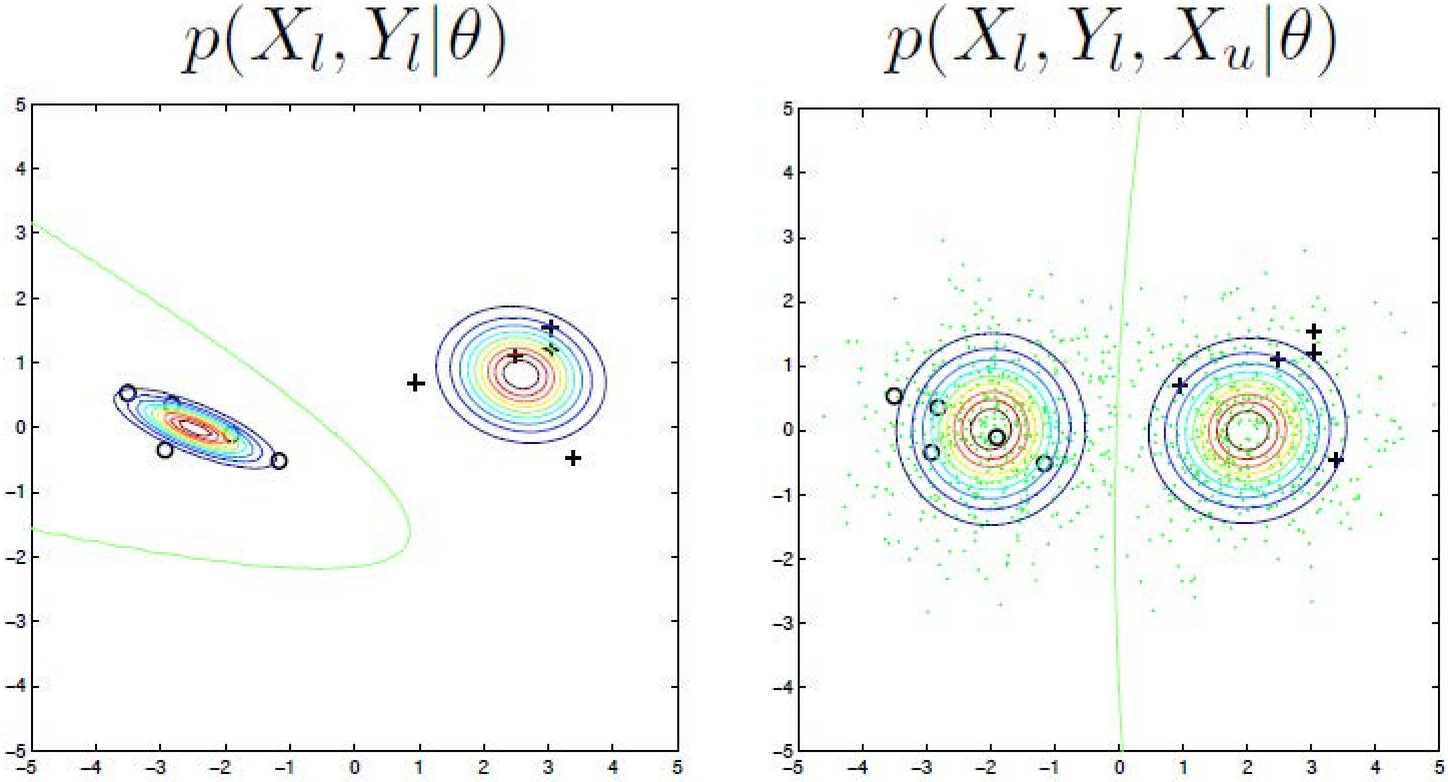




Generative Model

Effect of unlabeled data in GMM

The difference comes from maximizing different quantities



Generative Model

Assumption

knowledge of the model form $p(X, Y|\theta)$.

- joint and marginal likelihood

$$p(X_l, Y_l, X_u|\theta) = \sum_{Y_u} p(X_l, Y_l, X_u, Y_u|\theta)$$

- find the maximum likelihood estimate (MLE) of θ, the maximum a posteriori (MAP) estimate, or be Bayesian
- common mixture models used in semi-supervised learning:
  - Mixture of Gaussian distributions (GMM) – image classification
  - Mixture of multinomial distributions (Naïve Bayes) – text categorization
  - Hidden Markov Models (HMM) – speech recognition
- Learning via the Expectation-Maximization (EM) algorithm

Generative Model

Binary classification with GMM using MLE

- with only labeled data
  - $\log p(X_l, Y_l|\theta) = \sum_{i=1}^{l} \log p(y_i|\theta)p(x_i|y_i, \theta)$
  - MLE for θ trivial (sample mean and covariance)
- with both labeled and unlabeled data

$$\log p(X_l, Y_l, X_u|\theta) = \sum_{i=1}^{l} \log p(y_i|\theta)p(x_i|y_i, \theta) + \sum_{i=l+1}^{l+u} \log \left(\sum_{y=1}^{2} p(y|\theta)p(x_i|y, \theta) \right)$$

  - MLE harder (hidden variables): EM

Generative Model

The EM algorithm for GMM

1. Start from MLE $\theta = \{w, \mu, \Sigma\}_{1:2}$ on (X_l, Y_l),
   - w_c=proportion of class c
   - μ_c=sample mean of class c
   - Σ_c=sample cov of class c

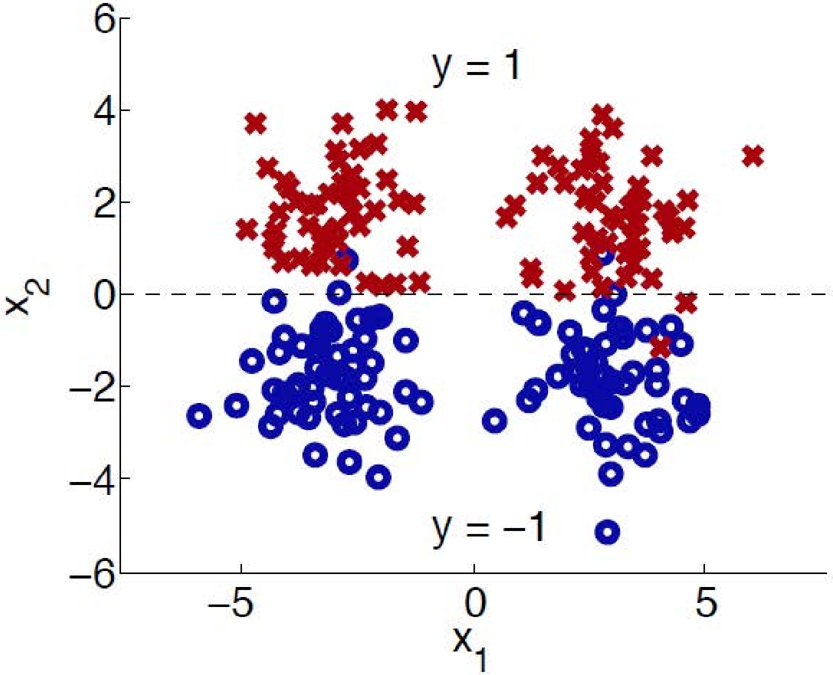
   repeat:
2. The E-step: compute the expected label $p(y|x,\theta) = \frac{p(x,y|\theta)}{\sum_{y'} p(x,y'|\theta)}$ for all $x \in X_u$
   - label $p(y=1|x,\theta)$-fraction of x with class 1
   - label $p(y=2|x,\theta)$-fraction of x with class 2
3. The M-step: update MLE θ with (now labeled) X_u

Can be viewed as a special form of self-training.

Generative Model

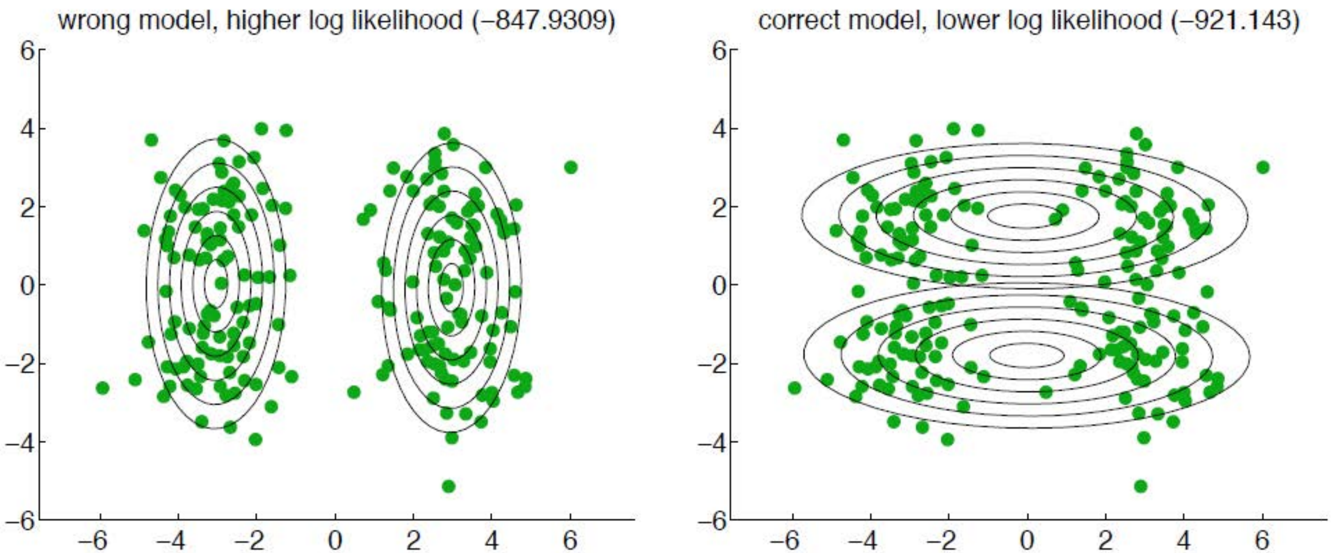
The assumption of GMM

- **Assumption**: the data actually comes from the mixture model, where the number of components, prior $p(y)$, and conditional $p(\mathbf{x}|y)$ are all correct.
- When the assumption is wrong:



Generative Model

The assumption of GMM



Heuristics to lessen the danger

- Carefully construct the generative model, e.g., multiple Gaussian distributions per class
- Down-weight the unlabeled data ($\lambda < 1$)

$$\log p(X_l, Y_l, X_u|\theta) = \sum_{i=1}^{l} \log p(y_i|\theta)p(x_i|y_i,\theta) + \lambda \sum_{i=l+1}^{l+u} \log \left(\sum_{y=1}^{2} p(y|\theta)p(x_i|y,\theta) \right)$$