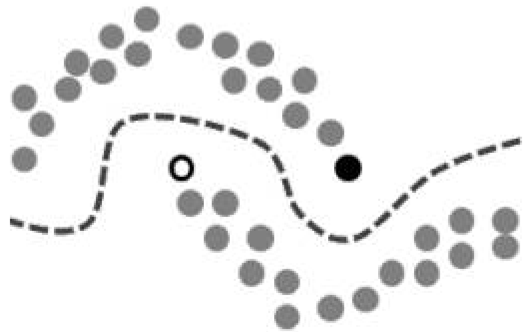
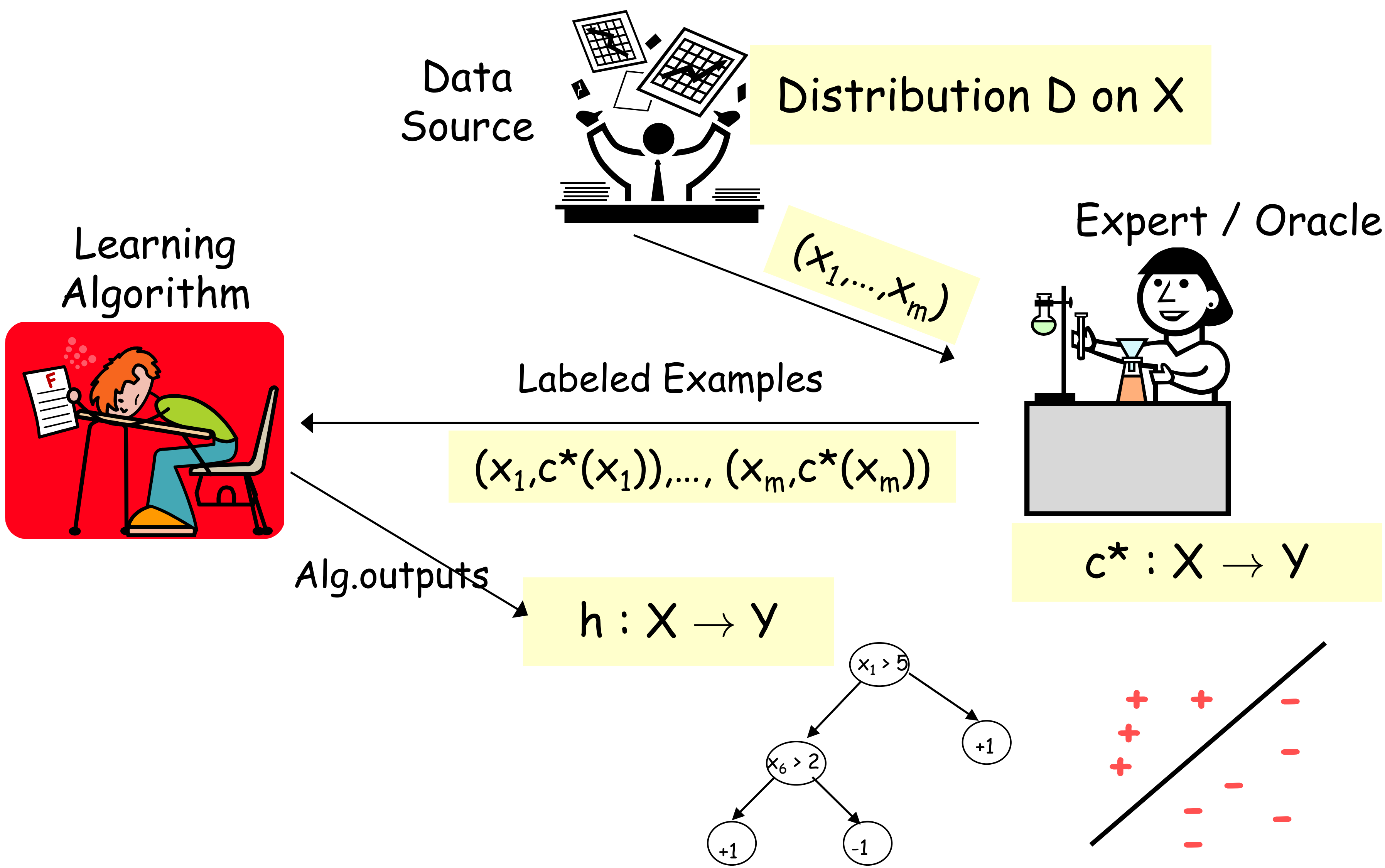
Semi-Supervised Learning



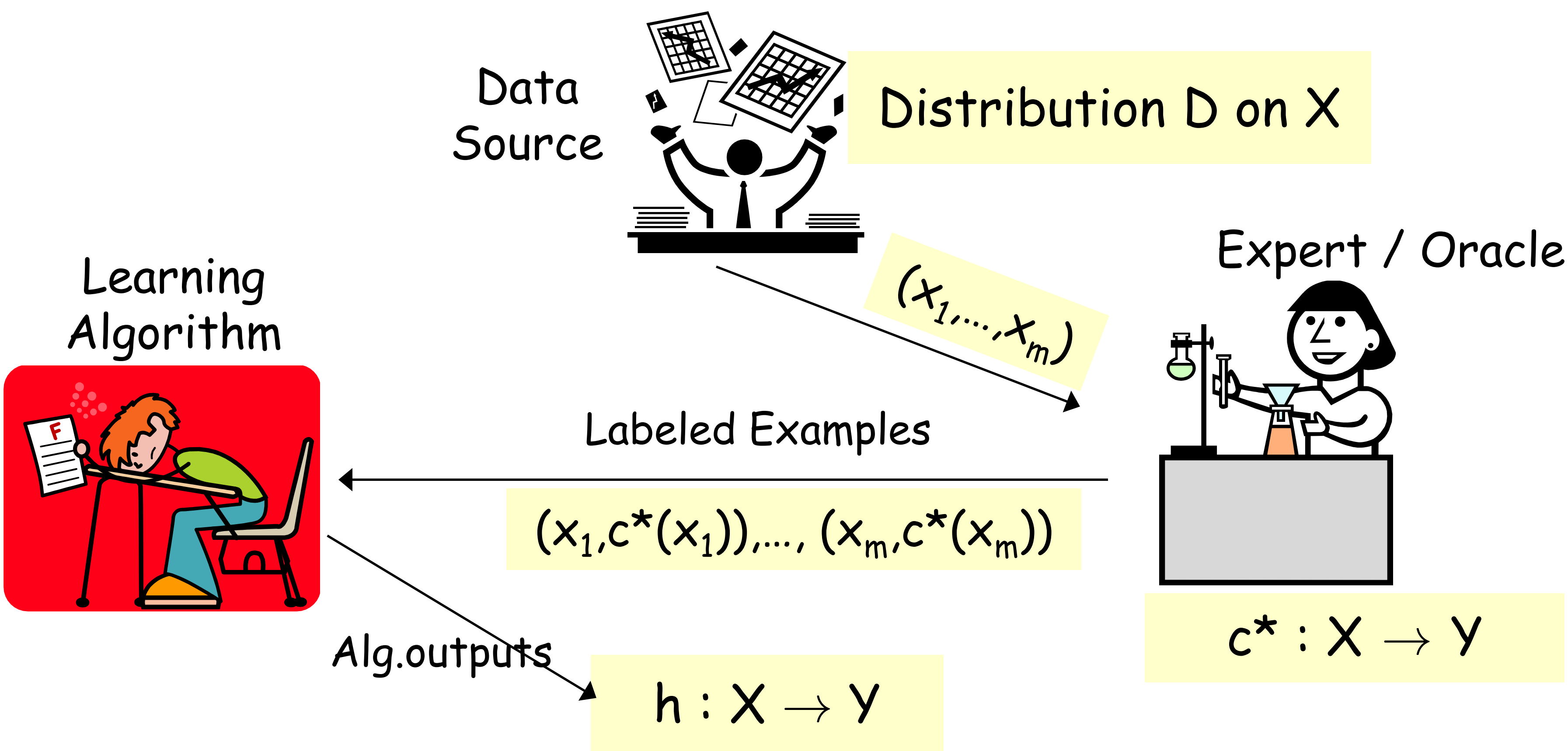
Readings:

- 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



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

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

Goal: h has small error over D.

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

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

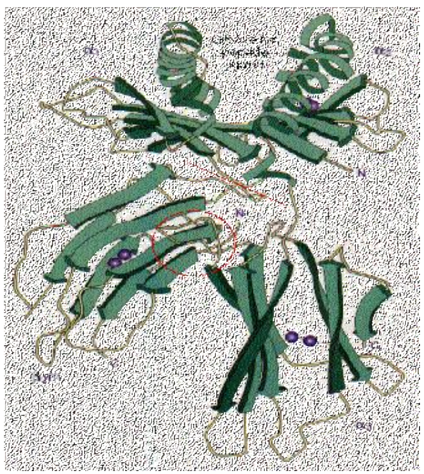
Confidence for rule effectiveness on future data.

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

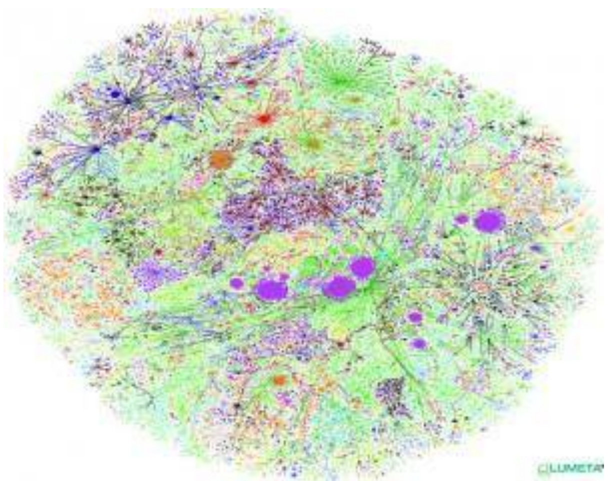
Classic Paradigm Insufficient Nowadays

Modern applications: massive amounts of raw data.

Only a tiny fraction can be annotated by human experts.



Protein sequences



Billions of webpages

Images

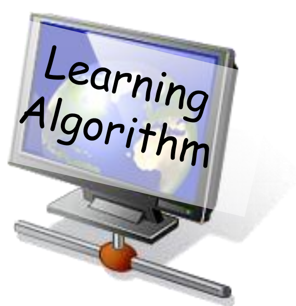
Modern ML: New Learning Approaches

Modern applications: massive amounts of raw data.

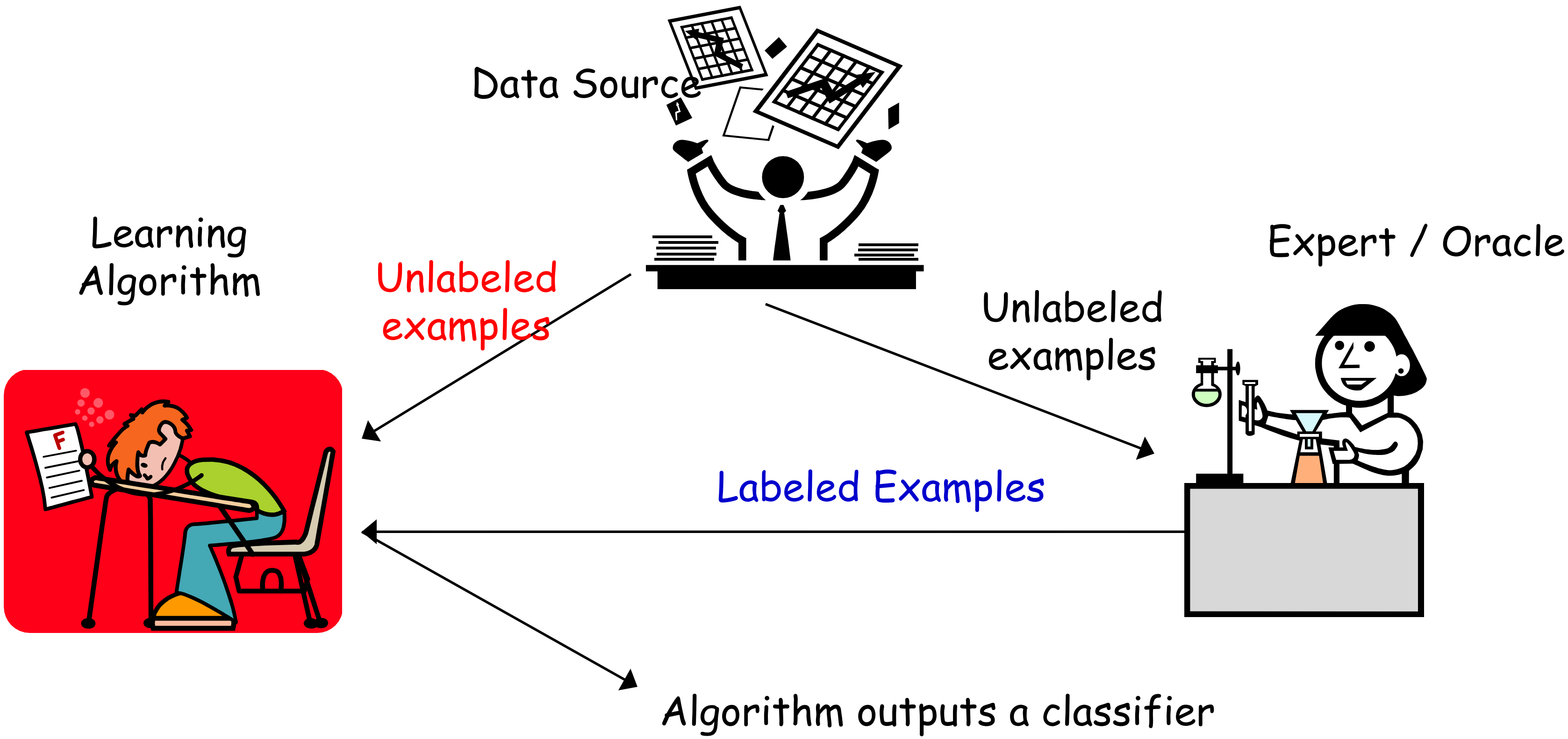
Techniques that best utilize data, minimizing need for expert/human intervention.

Paradigms where there has been great progress.

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



Semi-Supervised Learning



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

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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

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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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Test of time awards at ICML!

Today: discuss these methods.

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

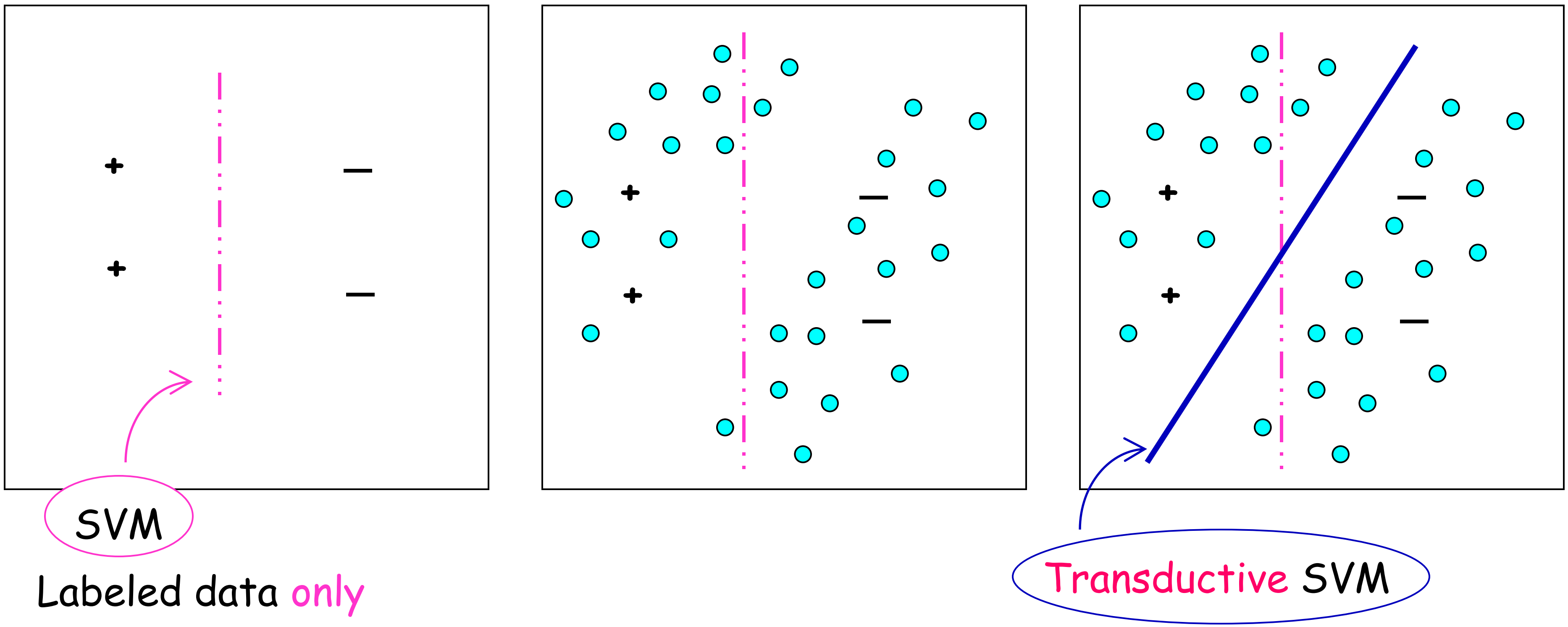
Semi-supervised SVM

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

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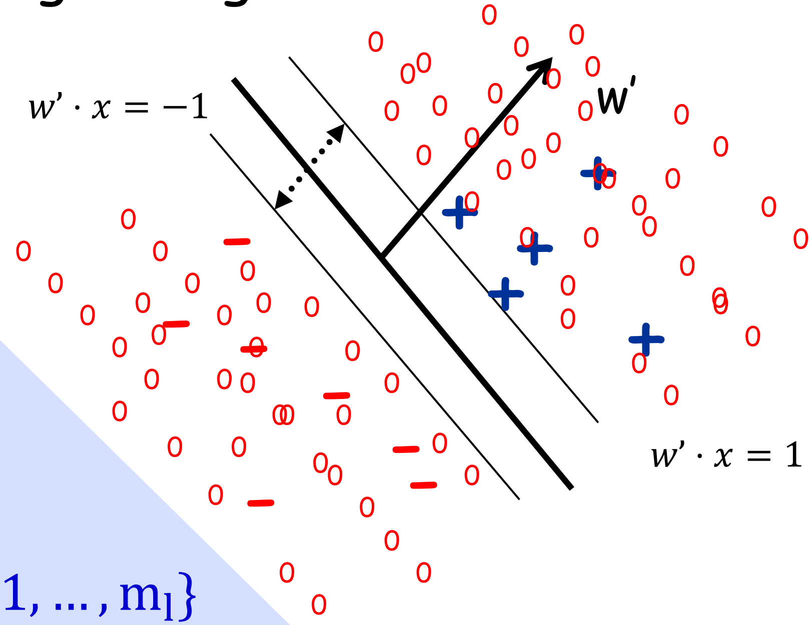

Input: $S_l = \{(x_1, y_1), \ldots, (x_{m_l}, y_{m_l})\}$

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

$\text{argmin}_w \; \|w\|^2$ s.t.:

- $y_i \, w \cdot x_i \geq 1$, 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 $u \in \{1, \ldots, m_u\}$

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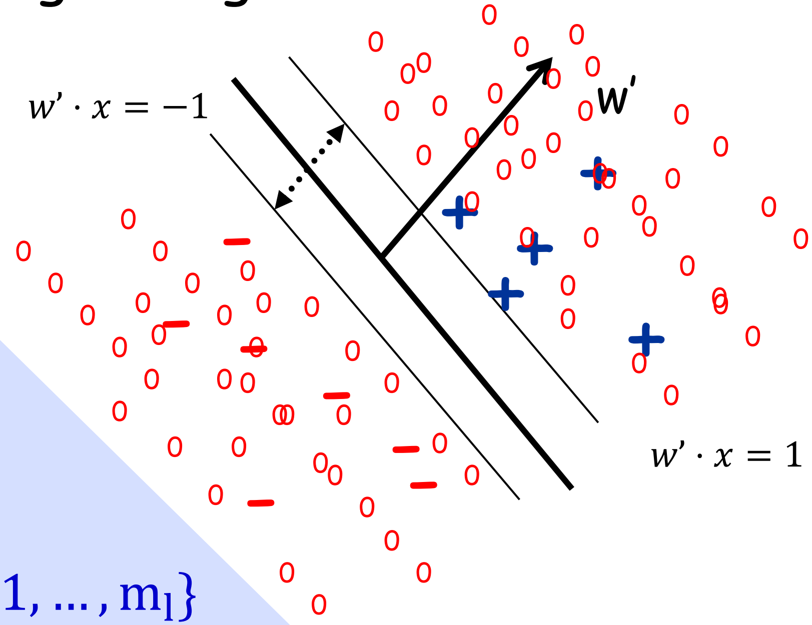

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Find a labeling of the unlabeled sample and w s.t. w separates both labeled and unlabeled data with maximum margin.

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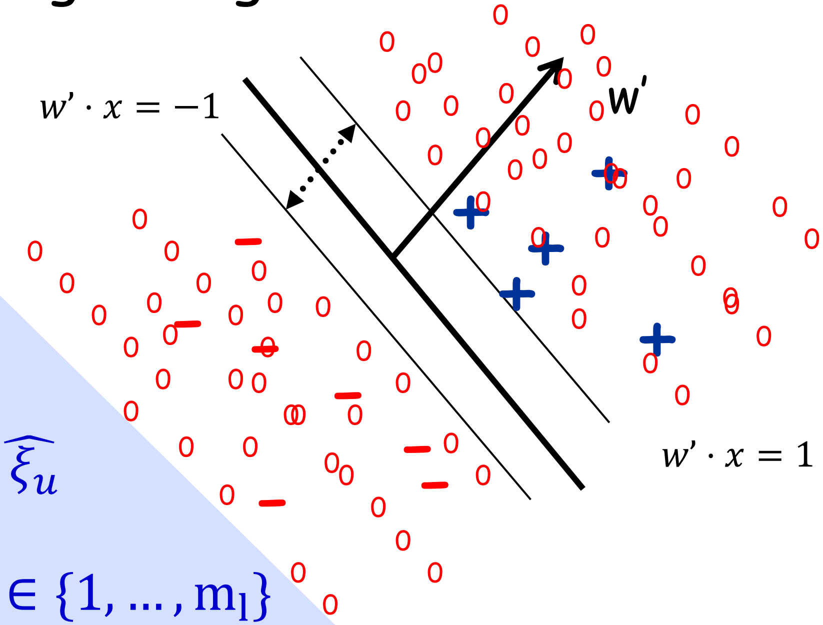

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$$\text{argmin}_w \; ||w||^2 + C \sum_i \xi_i + C \sum_u \widehat{\xi_u}$$

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

<u>Heuristic (Joachims) high level idea:</u>

- First maximize margin over the labeled points
- Use this to give initial labels to unlabeled points 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.

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

Prof. Avrim Blum   My Advisor

x - Link info & Text info

x_1- Text info

Prof. Avrim Blum   My Advisor

x_2- Link info

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.

my advisor

Avrim Blum's home page Page 1 of 1

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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

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Idea: Use unlabeled data to propagate learned information.

The co-training algorithm trains two predictors:

h(1) --> x(1) h(2) --> x(2)

If h(1) confidently predicts the label of an unlabeled instance x then the instance-label pair (x, h(1)(x)) is added to h(2)'s labeled data, and vice versa.

Note this promotes h(1) and h(2) to predict the same on x.

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

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

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

Each of them has small labeled error

Regularizer to encourage agreement over unlabeled dat

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

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

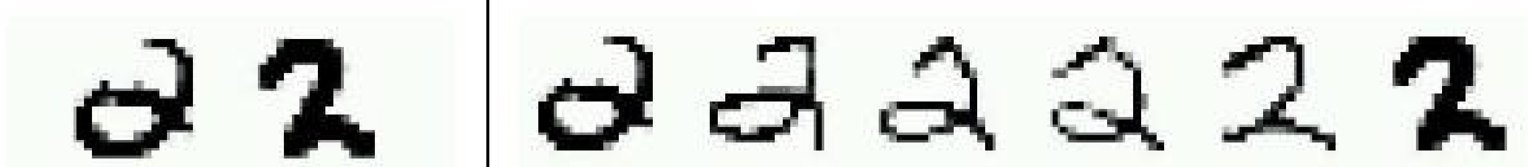
Similarity Based Regularity

[Blum&Chwala01], [ZhuGhahramaniLafferty03]

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]:



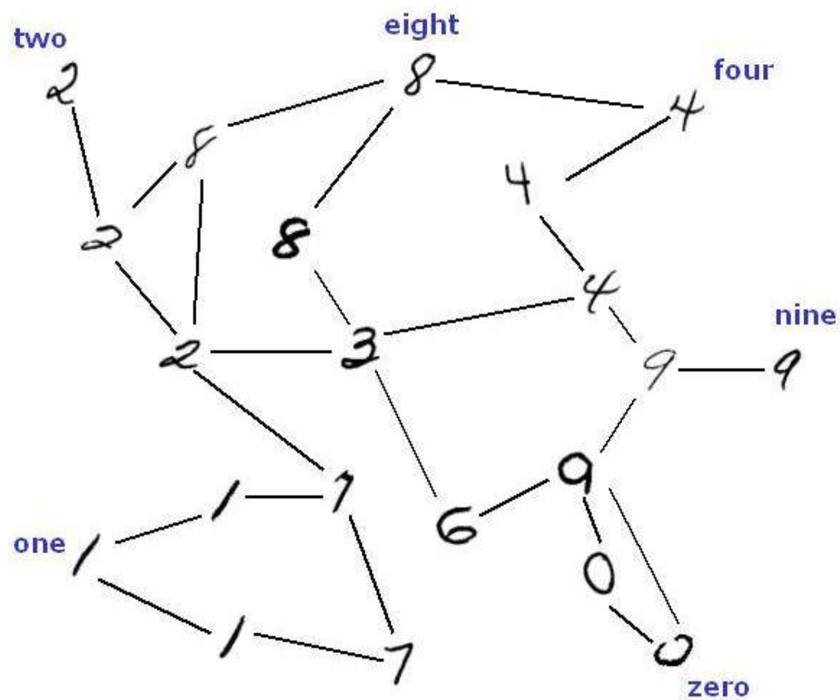
not similar

'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.

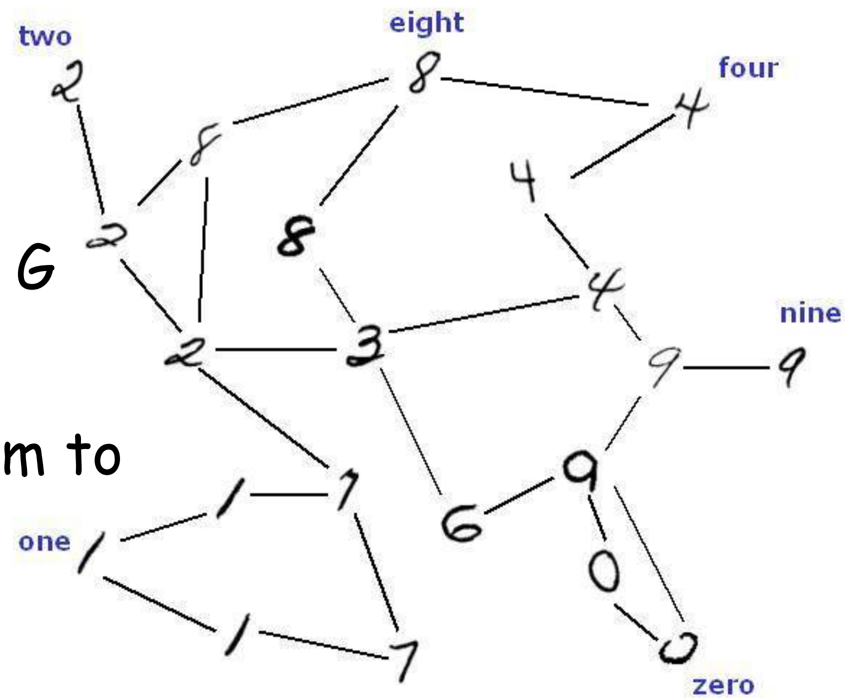


Graph-based Methods

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:

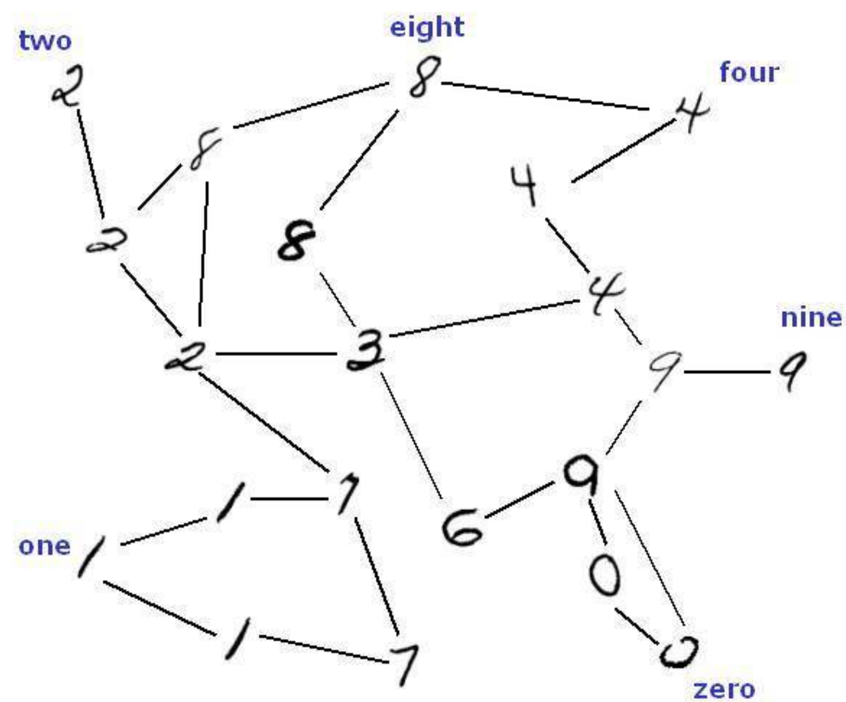
- Minimum/Multiway cut
- Minimum “soft-cut”
- Spectral partitioning
- …

Gaussian Fields and Harmonic Function
[ZhuGhahramaniLafferty'03]

graph G ={V, E, W}

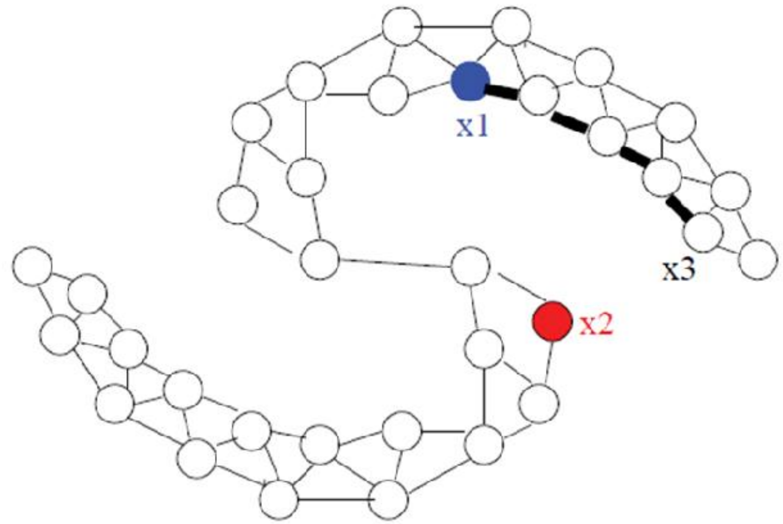
> vertices V are
the labeled and unlabeled instances

> The undirected edges E
connect instances i, j with weight wij



How to Create the Graph

- Empirically, the following works well:



1. Compute distance between i, j

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2$$

2. For each i, connect to its kNN. k very small but still connects the graph

3. Optionally put weights on (only) those edges

$$w_{ij} = \exp\left(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/\sigma^2\right)$$

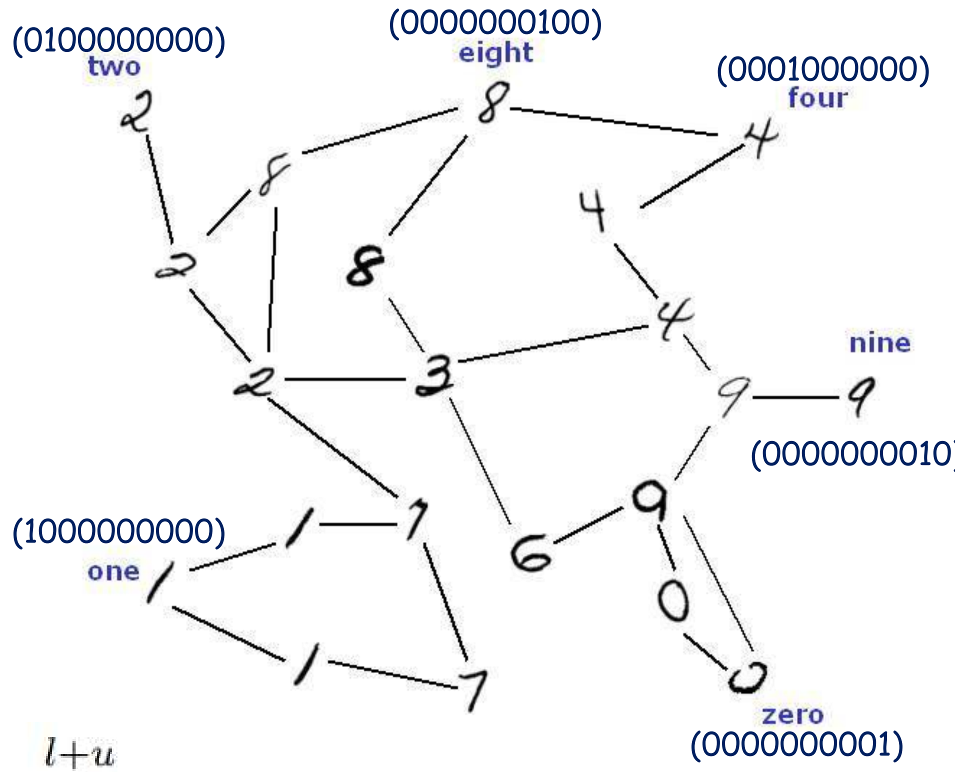
4. Tune σ

Gaussian Fields and Harmonic Function

[ZhuGhahramaniLafferty'03]

Large wij implies a preference for the predictions f(xi) and f(xj) to be the same.

$$\sum_{i,j=1}^{l+u} w_{ij} \left|\left| f(\mathbf{x}_i) - f(\mathbf{x}_j) \right|\right|^2$$



To find the f

$$\underset{f}{\operatorname{argmin}} \frac{1}{l} \sum_{i=1}^{l} c(f(\mathbf{x}_i), y_i) + \lambda_1 ||f||^2 + \lambda_2 \sum_{i,j=1}^{l+u} w_{ij} \left|\left| f(\mathbf{x}_i) - f(\mathbf{x}_j) \right|\right|^2$$

Label Propagation

[ZhuGhahramaniLafferty'05]

Nodes connected by edges of large similarity tend to have the same label through information propagated within the graph

Transition Matrix

$$P(i,j) = \frac{W(i,j)}{\sum_{k \in V} W(i,k)},$$

Label Matrix

Y(i,k) be 1 if instance i is labeled as class k,and 0 otherwise

$$Y_0 = \begin{array}{c}\left[\begin{array}{cc} 1 & 0 \\ 0 & 1 \\ \hline 0 & 0 \\ 0 & 0 \end{array}\right]_{n \times c}\end{array}\begin{array}{l}\text{Labeled} \\ \\ \text{Unlabeled}\end{array}$$

Label Propagation

[ZhuGhahramaniLafferty'05]

Algorithm

1. Construct a probabilistic transition matrix P by Eqn.(2).
2. Let $Y_0 = [Y_0^l; \mathbf{0}]$.
3. Performing the following steps for T steps:

   3.a $\qquad Y_{t+1} = P * Y_t,$

   3.b $\qquad Y_{t+1}^{(l)} = Y_0^l.$

4. Output Y_T