Tutorial on Semi-Supervised Learning

Xiaojin Zhu

Department of Computer Sciences
University of Wisconsin, Madison, USA

Theory and Practice of Computational Learning
Chicago, 2009

New book

Xiaojin Zhu and Andrew B. Goldberg. *Introduction to Semi-Supervised Learning*. Morgan & Claypool, 2009.

Outline

1. Part I
   - What is SSL?
   - Mixture Models
   - Co-training and Multiview Algorithms
   - Manifold Regularization and Graph-Based Algorithms
   - S3VMs and Entropy Regularization

2. Part II
   - Theory of SSL
   - Online SSL
   - Multimanifold SSL
   - Human SSL

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What is Semi-Supervised Learning?

Learning from both labeled and unlabeled data. Examples:

- Semi-supervised classification: training data l labeled instances $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$ and u unlabeled instances $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$, often $u \gg l$.
  Goal: better classifier f than from labeled data alone.

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We will mainly discuss semi-supervised classification.

Motivations

Machine learning

Promise: better performance for free...

- labeled data can be hard to get
  - labels may require human experts
  - labels may require special devices
- unlabeled data is often cheap in large quantity

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Cognitive science

Computational model of how humans learn from labeled and unlabeled data.

- concept learning in children: $\mathbf{x}$=animal, y=concept (e.g., dog)
- Daddy points to a brown animal and says "dog!"
- Children also observe animals by themselves

Example of hard-to-get labels

Task: speech analysis

- Switchboard dataset
- telephone conversation transcription
- 400 hours annotation time for each hour of speech

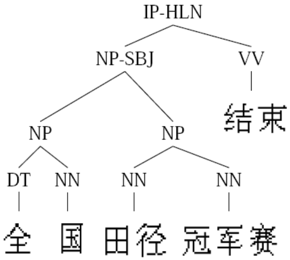
film ⇒ `f ih_n uh_gl_n m`

be all ⇒ `bcl b iy iy_tr ao_tr ao l_dl`

Another example of hard-to-get labels

Task: natural language parsing

- Penn Chinese Treebank
- 2 years for 4000 sentences



"The National Track and Field Championship has finished."

Notations

- instance $\mathbf{x}$, label y
- learner $f : \mathcal{X} \mapsto \mathcal{Y}$
- labeled data $(X_l, Y_l) = \{(x_{1:l}, y_{1:l})\}$
- unlabeled data $X_u = \{\mathbf{x}_{l+1:l+u}\}$, available during training. Usually $l \ll u$. Let $n = l + u$
- test data $\{(x_{n+1\ldots}, y_{n+1\ldots})\}$, not available during training

Semi-supervised vs. transductive learning

- Inductive semi-supervised learning: Given $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$, learn $f : \mathcal{X} \mapsto \mathcal{Y}$ so that f is expected to be a good predictor on future data, beyond $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$.

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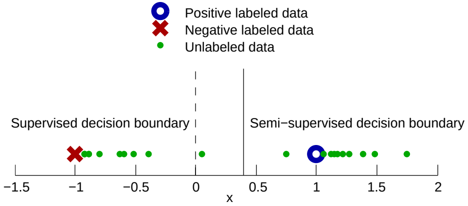
- Transductive learning: Given $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$, learn $f : \mathcal{X}^{l+u} \mapsto \mathcal{Y}^{l+u}$ so that f is expected to be a good predictor on the unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$. Note f is defined only on the given training sample, and is not required to make predictions outside them.

How can unlabeled data ever help?



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- with and without unlabeled data: decision boundary shift

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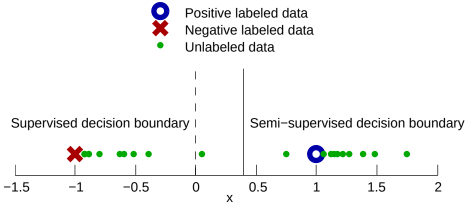

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This is only one of many ways to use unlabeled data.

Self-training algorithm

Our first SSL algorithm:

Input: labeled data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$.

1. Initially, let $L = \{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$ and $U = \{\mathbf{x}_j\}_{j=l+1}^{l+u}$.

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

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Self-training is a *wrapper* method

- the choice of learner for f in step 3 is left completely open
- good for many real world tasks like natural language processing
- but mistake by f can reinforce itself

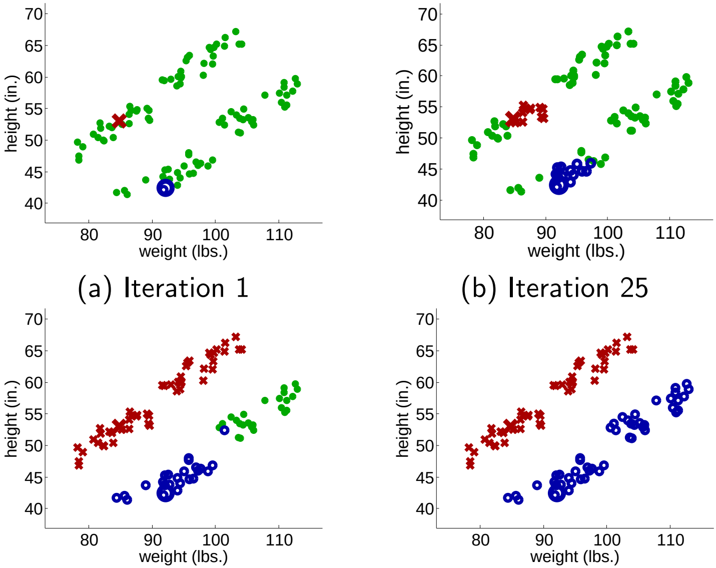
Self-training example: Propagating 1-Nearest-Neighbor

An instance of self-training.

Input: labeled data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$, unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$, distance function $d()$.

1. Initially, let $L = \{(\mathbf{x}_i, y_i)\}_{i=1}^{l}$ and $U = \{\mathbf{x}_j\}_{j=l+1}^{l+u}$.
2. Repeat until U is empty:
3. Select $\mathbf{x} = \mathrm{argmin}_{\mathbf{x} \in U} \min_{\mathbf{x}' \in L} d(\mathbf{x}, \mathbf{x}')$.
4. Set $f(\mathbf{x})$ to the label of $\mathbf{x}$'s nearest instance in L. Break ties randomly.
5. Remove $\mathbf{x}$ from U; add $(\mathbf{x}, f(\mathbf{x}))$ to L.

Propagating 1-Nearest-Neighbor: now it works



(a) Iteration 1

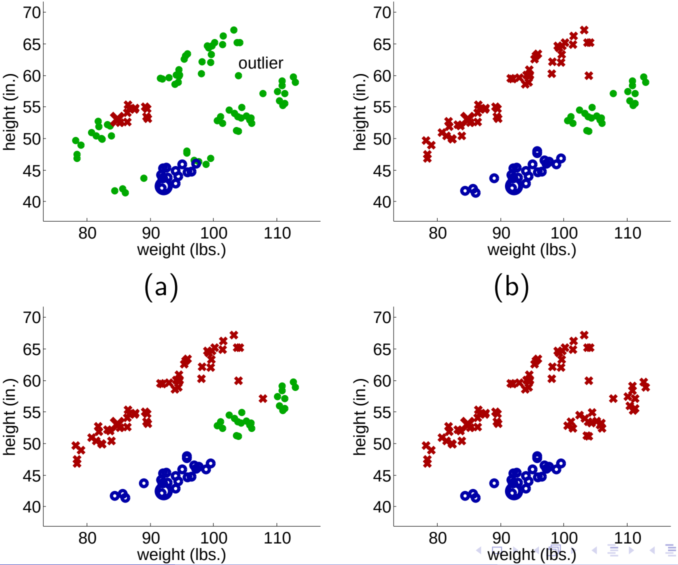
(b) Iteration 25

(c) Iteration 74

(d) Final labeling of all instances

Propagating 1-Nearest-Neighbor: now it doesn't

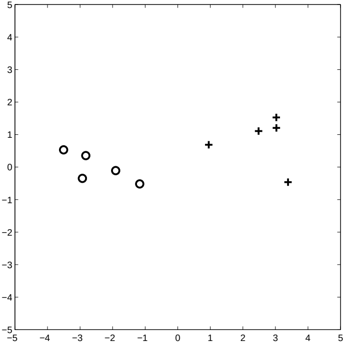
But with a single outlier...



Outline

A simple example of generative models

Labeled data (X_l, Y_l):



Assuming each class has a Gaussian distribution, what is the decision boundary?

A simple example of generative models

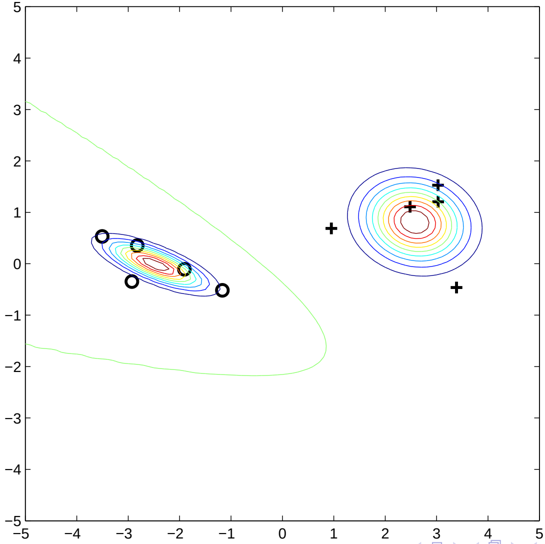
Model parameters: $\theta = \{w_1, w_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$
The GMM:

$$\begin{aligned} p(x, y|\theta) &= p(y|\theta)p(x|y, \theta) \\ &= w_y \mathcal{N}(x; \mu_y, \Sigma_y) \end{aligned}$$

Classification: $p(y|x, \theta) = \frac{p(x,y|\theta)}{\sum_{y'} p(x,y'|\theta)}$

A simple example of generative models

The most likely model, and its decision boundary:



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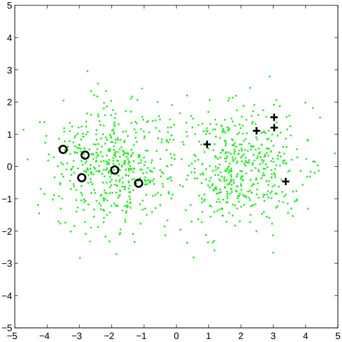
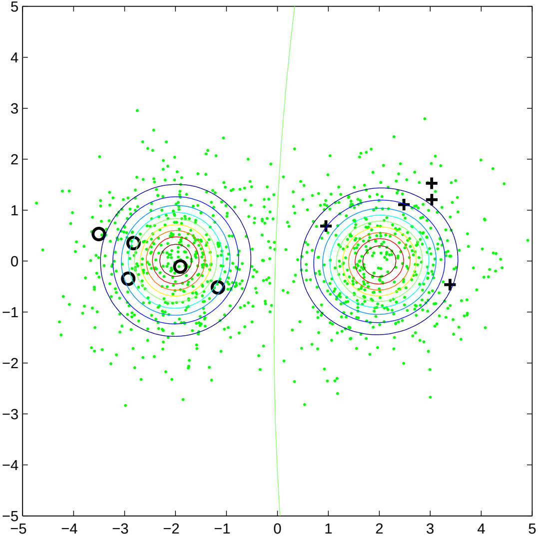
Adding unlabeled data:



A simple example of generative models

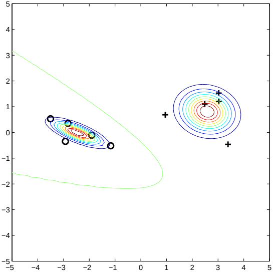
With unlabeled data, the most likely model and its decision boundary:



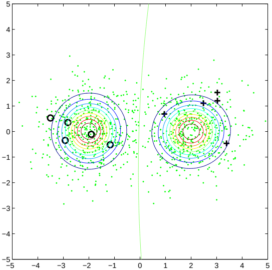
A simple example of generative models

They are different because they maximize different quantities.

$$p(X_l, Y_l|\theta)$$



$$p(X_l, Y_l, X_u|\theta)$$



Generative model for semi-supervised learning

Assumption

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

- joint and marginal likelihood

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

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- 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 (Baum-Welch)

Case study: GMM

Binary classification with GMM using MLE.

- with only labeled data
  - $\log p(X_l, Y_l|\theta) = \sum_{i=1}^{l} \log p(y_i|\theta)p(x_i|y_i, \theta)$
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- 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

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
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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 $x \in X_u$
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Can be viewed as a special form of self-training.

The assumption of mixture models

- **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.

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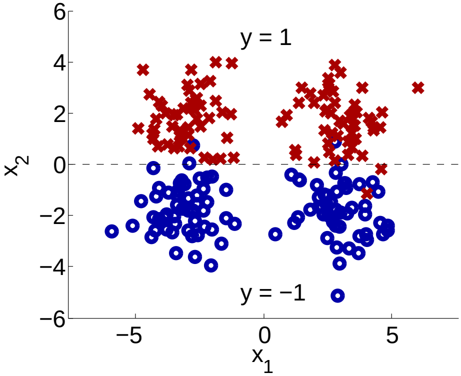
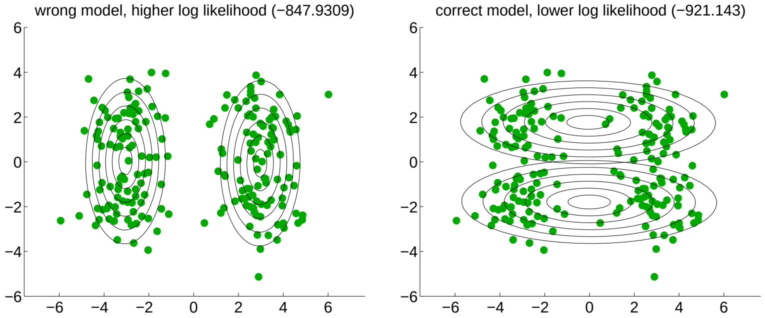
- When the assumption is wrong:



For example, classifying text by topic vs. by genre.

The assumption of mixture models



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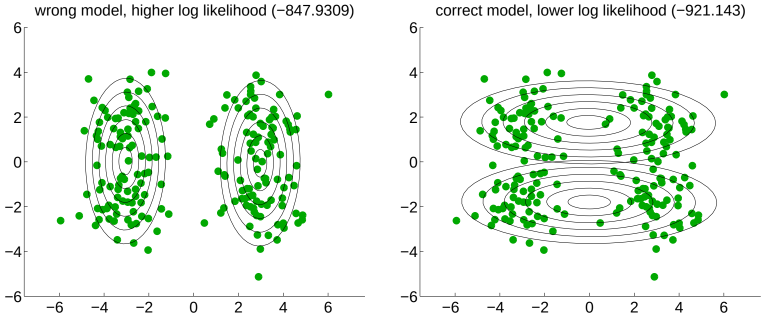

Heuristics to lessen the danger

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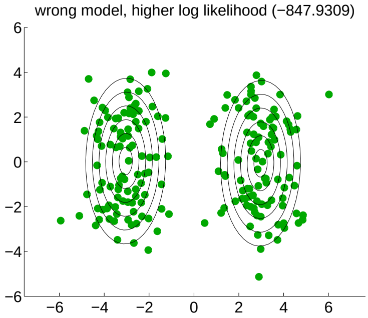

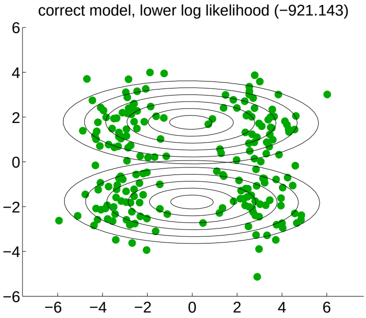

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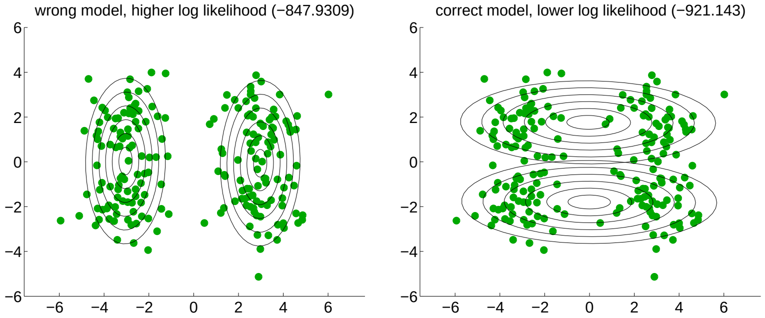

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Other dangers: identifiability, EM local optima

Related: cluster-and-label

Input: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_l, y_l)$, $\mathbf{x}_{l+1}, \ldots, \mathbf{x}_{l+u}$,
a clustering algorithm $\mathcal{A}$, a supervised learning algorithm $\mathcal{L}$

Related: cluster-and-label

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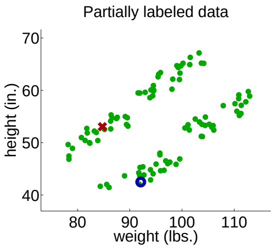
But again: **SSL sensitive to assumptions**—in this case, that the clusters coincide with decision boundaries. If this assumption is incorrect, the results can be poor.

Cluster-and-label: now it works, now it doesn't

Example: $\mathcal{A}$=Hierarchical Clustering, $\mathcal{L}$=majority vote.

single linkage



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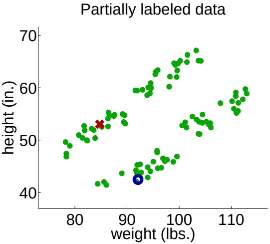

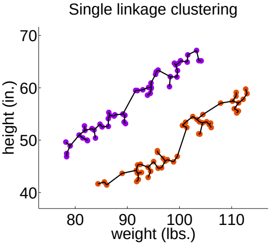

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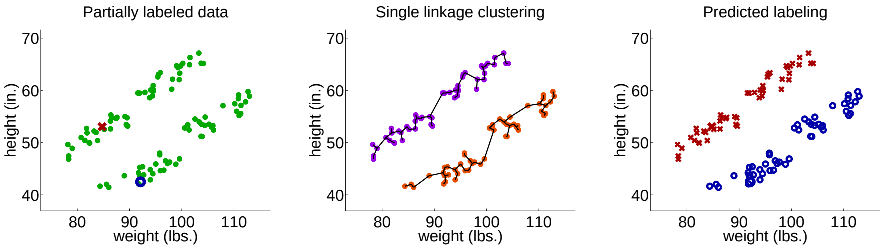

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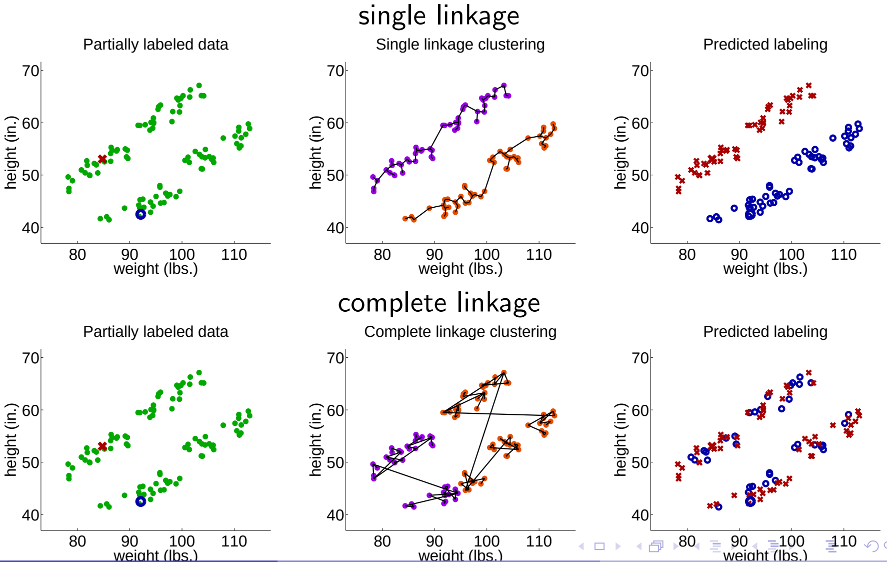

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Two Views of an Instance

Example: named entity classification `Person` (Mr. Washington) or `Location` (Washington State)

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instance 1: ... headquartered in (Washington State) ...
instance 2: ... (Mr. Washington), the vice president of ...

- a named entity has two views (subset of features) $\mathbf{x} = [\mathbf{x}^{(1)}, \mathbf{x}^{(2)}]$
- the words of the entity is $\mathbf{x}^{(1)}$
- the context is $\mathbf{x}^{(2)}$

Quiz

instance 1:	. . . headquartered in (Washington State)^L . . .
instance 2:	. . . (Mr. Washington)^P, the vice president of . . .
test:	. . . (Robert Jordan), a partner at . . .
test:	. . . flew to (China) . . .

Quiz

With more unlabeled data

instance 1:	. . . headquartered in (Washington State)^L . . .
instance 2:	. . . (Mr. Washington)^P, the vice president of . . .
instance 3:	. . . headquartered in (Kazakhstan) . . .
instance 4:	. . . flew to (Kazakhstan) . . .
instance 5:	. . . (Mr. Smith), a partner at Steptoe & Johnson . . .
test:	. . . (Robert Jordan), a partner at . . .
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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 $\mathbf{x}_i = [\mathbf{x}_i^{(1)}, \mathbf{x}_i^{(2)}]$,
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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.

Like self-training, but with two classifiers teaching each other.

Co-training assumptions

Assumptions

- feature split $x = [x^{(1)}; x^{(2)}]$ exists

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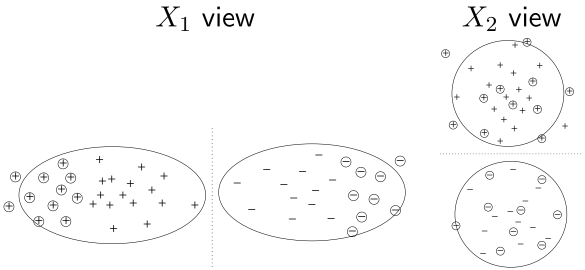
- $x^{(1)}$ or $x^{(2)}$ alone is sufficient to train a good classifier
- $x^{(1)}$ and $x^{(2)}$ are conditionally independent given the class



Multiview learning

Extends co-training.

- Loss Function: $c(\mathbf{x}, y, f(\mathbf{x})) \in [0, \infty)$. For example,
  - squared loss $c(\mathbf{x}, y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$
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- Regularized Risk Minimization $f^* = \mathrm{argmin}_{f \in \mathcal{F}} \hat{R}(f) + \lambda \Omega(f)$

Multiview learning

A special regularizer $\Omega(f)$ defined on unlabeled data, to encourage agreement among multiple learners:

$$\begin{aligned} \underset{f_1,\ldots,f_k}{\operatorname{argmin}} \quad & \sum_{v=1}^{k}\left(\sum_{i=1}^{l} c(\mathbf{x}_i, y_i, f_v(\mathbf{x}_i)) + \lambda_1 \Omega_{SL}(f_v)\right) \\ & +\lambda_2 \sum_{u,v=1}^{k} \sum_{i=l+1}^{l+u} c(\mathbf{x}_i, f_u(\mathbf{x}_i), f_v(\mathbf{x}_i)) \end{aligned}$$

Outline

Example: text classification

- Classify astronomy vs. travel articles
- Similarity measured by content word overlap

	d_1	d_3	d_4	d_2
asteroid	•	•		
bright	•	•		
comet		•		
year				
zodiac				
⋮				
airport				
bike				
camp			•	
yellowstone			•	•
zion				•

When labeled data alone fails

No overlapping words!

	d_1	d_3	d_4	d_2
asteroid	•			
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comet				
year				
zodiac		•		
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airport			•	
bike			•	
camp				
yellowstone				•
zion				•

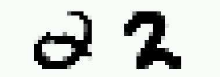
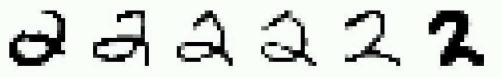
Unlabeled data as stepping stones

Labels "propagate" via similar unlabeled articles.

	d_1	d_5	d_6	d_7	d_3	d_4	d_8	d_9	d_2
asteroid	•								
bright	•	•							
comet		•	•						
year			•	•					
zodiac				•	•				
⋮									
airport						•			
bike						•	•		
camp							•	•	
yellowstone								•	•
zion									•

Another example

Handwritten digits recognition with pixel-wise Euclidean distance

	
not similar	'indirectly' similar with stepping stones

Graph-based semi-supervised learning

- Nodes: $X_l \cup X_u$
- Edges: similarity weights computed from features, e.g.,

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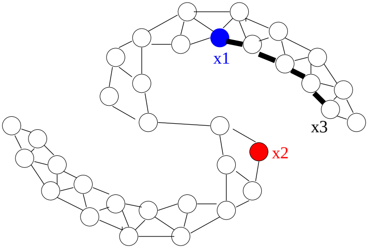
- Assumption Instances connected by heavy edge tend to have the same label.



The mincut algorithm

- Fix Y_l, find $Y_u \in \{0,1\}^{n-l}$ to minimize $\sum_{ij} w_{ij}|y_i - y_j|$.

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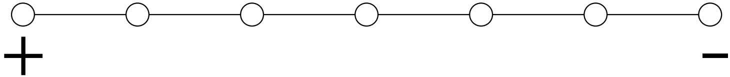
- Combinatorial problem, but has polynomial time solution.
- Mincut computes the modes of a discrete Markov random field, but there might be multiple modes



The harmonic function

Relaxing discrete labels to continuous values in $\mathbb{R}$, the harmonic function f satisfies

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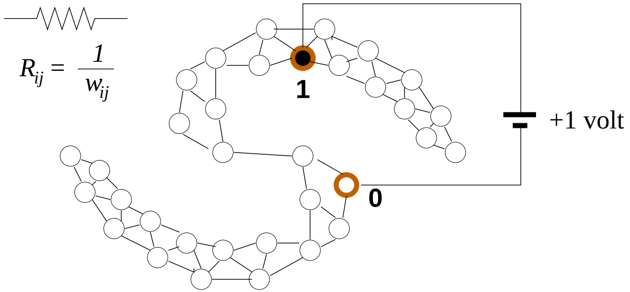
- the mean of a Gaussian random field
- average of neighbors $f(x_i) = \frac{\sum_{j \sim i} w_{ij} f(x_j)}{\sum_{j \sim i} w_{ij}}, \forall x_i \in X_u$

An electric network interpretation

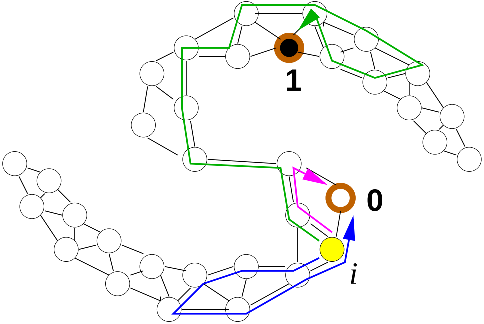
- Edges are resistors with conductance w_{ij}
- 1 volt battery connects to labeled points $y = 0, 1$
- The voltage at the nodes is the harmonic function f

Implied similarity: similar voltage if many paths exist



A random walk interpretation

- Randomly walk from node i to j with probability $\frac{w_{ij}}{\sum_k w_{ik}}$
- Stop if we hit a labeled node
- The harmonic function $f = Pr(\text{hit label 1}|\text{start from } i)$



An algorithm to compute harmonic function

One iterative way to compute the harmonic function:

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1. Initially, set $f(x_i) = y_i$ for $i = 1 \ldots l$, and $f(x_j)$ arbitrarily (e.g., 0) for $x_j \in X_u$.
2. Repeat until convergence: Set $f(x_i) = \frac{\sum_{j \sim i} w_{ij} f(x_j)}{\sum_{j \sim i} w_{ij}}, \forall x_i \in X_u$, i.e., the average of neighbors. Note $f(X_l)$ is fixed.

The graph Laplacian

We can also compute f in closed form using the graph Laplacian.

- $n \times n$ weight matrix W on $X_l \cup X_u$
  - symmetric, non-negative
- Diagonal degree matrix D: $D_{ii} = \sum_{j=1}^{n} W_{ij}$
- Graph Laplacian matrix Δ

$$\Delta = D - W$$

- The energy can be rewritten as

$$\sum_{i \sim j} w_{ij}(f(x_i) - f(x_j))^2 = f^\top \Delta f$$

Harmonic solution with Laplacian

The harmonic solution minimizes energy subject to the given labels

$$\min_f \ \infty \sum_{i=1}^{l} (f(x_i) - y_i)^2 + f^\top \Delta f$$

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The normalized Laplacian $\mathcal{L} = D^{-1/2} \Delta D^{-1/2} = I - D^{-1/2} W D^{-1/2}$, or $\Delta^p, \mathcal{L}^p$ are often used too ($p > 0$).

Local and Global consistency

- Allow $f(X_l)$ to be different from Y_l, but penalize it

$$\min_f \sum_{i=1}^{l} (f(x_i) - y_i)^2 + \lambda f^\top \Delta f$$

Manifold regularization

The graph-based algorithms so far are transductive. Manifold regularization is inductive.

- defines function in a RKHS: $f(x) = h(x) + b, h(x) \in \mathcal{H}_K$
- views the graph as a random sample of an underlying manifold
- regularizer prefers low energy $f_{1:n}^\top \Delta f_{1:n}$

$$\min_f \sum_{i=1}^{l} (1 - y_i f(x_i))_+ + \lambda_1 \|h\|^2_{\mathcal{H}_K} + \lambda_2 f_{1:n}^\top \Delta f_{1:n}$$

Graph spectrum and SSL

Assumption: labels are "smooth" on the graph, characterized by the graph spectrum (eigen-values/vectors $\{(\lambda_i, \phi_i)\}_{i=1}^{l+u}$ of the Laplacian L):

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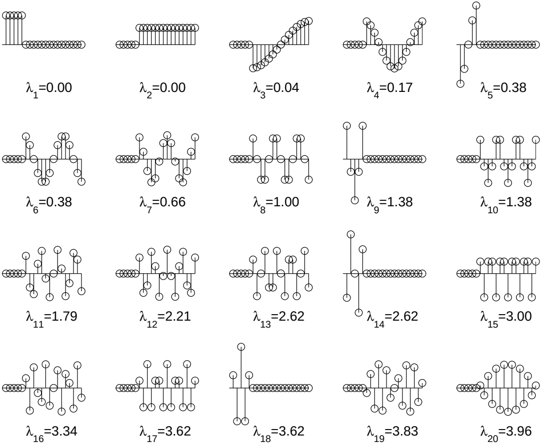
- graph regularizer $\mathbf{f}^\top L \mathbf{f} = \sum_{i=1}^{l+u} a_i^2 \lambda_i$
- smooth function $\mathbf{f}$ uses smooth basis (those with small λ_i)

Example graph spectrum

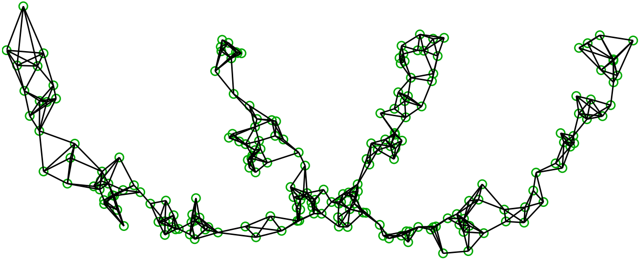
The graph

Eigenvalues and eigenvectors of the graph Laplacian



When the graph assumption is wrong

"colliding two moons"



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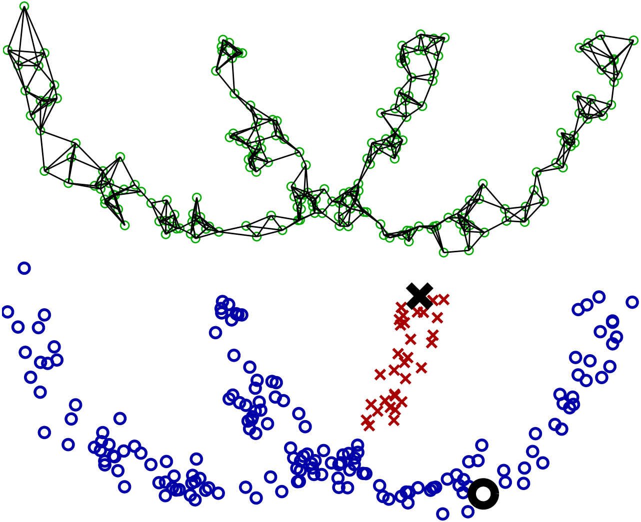
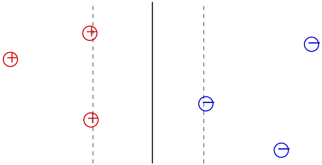


Outline

1. Part I
   - What is SSL?
   - Mixture Models
   - Co-training and Multiview Algorithms
   - Manifold Regularization and Graph-Based Algorithms
   - S3VMs and Entropy Regularization
2. Part II
   - Theory of SSL
   - Online SSL
   - Multimanifold SSL
   - Human SSL

Semi-supervised Support Vector Machines

SVMs



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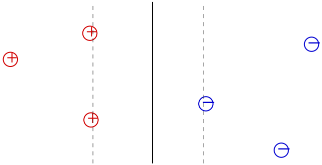
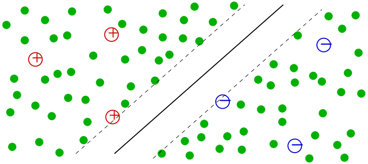


Semi-supervised SVMs (S3VMs) = Transductive SVMs (TSVMs)



Assumption: Unlabeled data from different classes are separated with large margin.

Standard soft margin SVMs

Try to keep labeled points outside the margin, while maximizing the margin:

$$\min_{h,b,\xi} \sum_{i=1}^{l} \xi_i + \lambda \|h\|^2_{\mathcal{H}_K}$$

$$\text{subject to } \; y_i(h(x_i) + b) \geq 1 - \xi_i \quad , \forall i = 1 \dots l$$

$$\xi_i \geq 0$$

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Equivalent to

$$\min_{f} \sum_{i=1}^{l} (1 - y_i f(x_i))_+ + \lambda \|h\|^2_{\mathcal{H}_K}$$

$y_i f(x_i)$ known as the margin, $(1 - y_i f(x_i))_+$ the hinge loss

The S3VM objective function

To incorporate unlabeled points,

- assign putative labels sign$(f(x))$ to $x \in X_u$

The S3VM objective function

To incorporate unlabeled points,

- assign putative labels $\text{sign}(f(x))$ to $x \in X_u$
- the hinge loss on unlabeled points becomes

$$(1 - \text{sign}(f(x))f(x_i))_+ = (1 - |f(x_i)|)_+$$

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To incorporate unlabeled points,

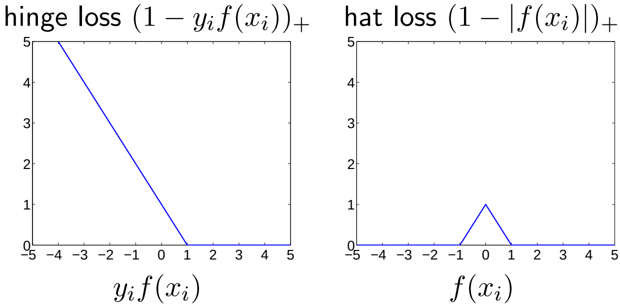
- assign putative labels $\text{sign}(f(x))$ to $x \in X_u$
- the hinge loss on unlabeled points becomes

$$(1 - \text{sign}(f(x))f(x_i))_+ = (1 - |f(x_i)|)_+$$

S3VM objective:

$$\min_f \sum_{i=1}^{l} (1 - y_i f(x_i))_+ + \lambda_1 \|h\|^2_{\mathcal{H}_K} + \lambda_2 \sum_{i=l+1}^{n} (1 - |f(x_i)|)_+$$

The hat loss on unlabeled data



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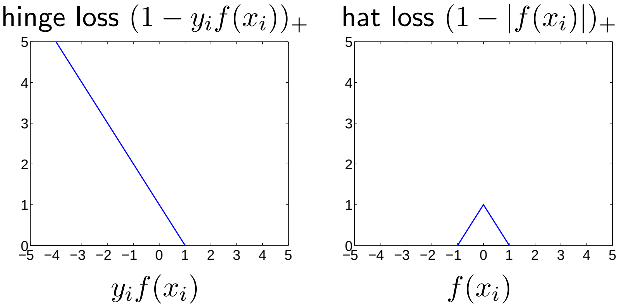

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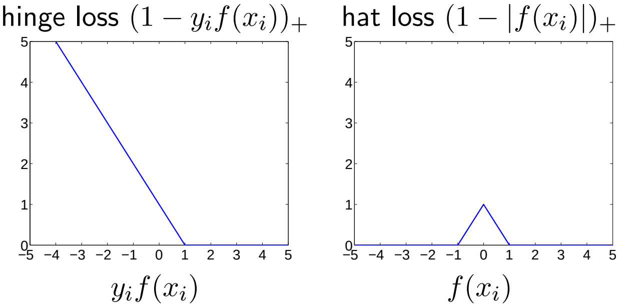

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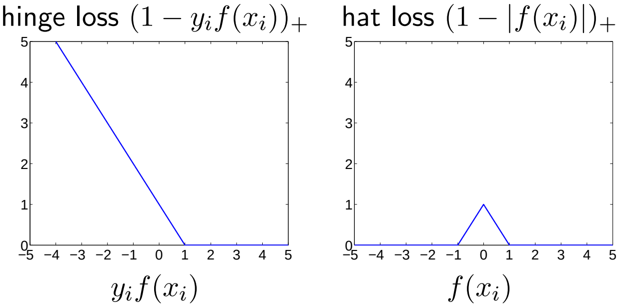

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- Relaxed: $\frac{1}{n-l} \sum_{i=l+1}^{n} f(x_i) = \frac{1}{l} \sum_{i=1}^{l} y_i$.

The S3VM algorithm

$$\min_f \quad \sum_{i=1}^{l}(1-y_i f(x_i))_+ + \lambda_1\|h\|^2_{\mathcal{H}_K} + \lambda_2 \sum_{i=l+1}^{n}(1-|f(x_i)|)_+$$

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- SVM objective is convex
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- SVM objective is convex
- Semi-supervised SVM objective is non-convex
- Optimization approaches: SVM^{light}, ∇S3VM, continuation S3VM, deterministic annealing, CCCP, Branch and Bound, SDP convex relaxation, etc.

Logistic regression

The probabilistic counter part of SVMs.

- $p(y|\mathbf{x}) = 1/\left(1 + \exp(-yf(\mathbf{x}))\right)$ where $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

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Logistic regression does not use unlabeled data.

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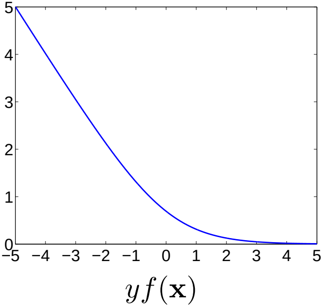
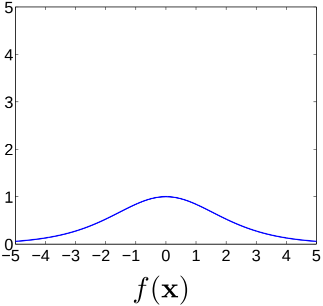
Entropy regularization



(a) the logistic loss



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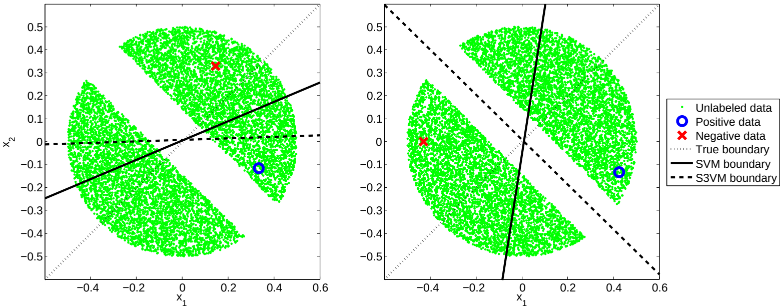
When the large margin assumption is wrong



S3VM in local minimum

S3VM in wrong gap

SVM error: 0.26 ± 0.13
S3VM error: 0.34 ± 0.19

Outline

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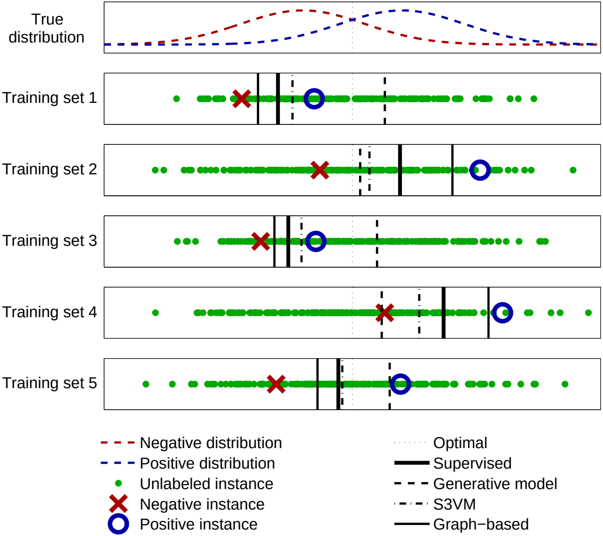
SSL does not always help



Wrong SSL assumption can make SSL worse than SL!

A computational theory for SSL

(Theoretic guarantee of Balcan & Blum)

Recall in supervised learning

- labeled data $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{l} \stackrel{\text{i.i.d.}}{\sim} P(\mathbf{x}, y)$, where P unknown

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- it turns out we can *bound* $e(f_{\mathcal{D}})$ without the knowledge of P.

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&\leq \sum_{\{f\in\mathcal{F}:e(f)>\epsilon\}} Pr_{\mathcal{D}\sim P}\left(\{\hat{e}(f) = 0\}\right)
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$$

- last step is union bound $Pr(A \cup B) \leq Pr(A) + Pr(B)$

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Probably (i.e., on at least $1-|\mathcal{F}|e^{-\epsilon l}$ fraction of random draws of the training sample), the function $f_{\mathcal{D}}$, picked because $\hat{e}(f_{\mathcal{D}})=0$, is approximately correct (i.e., has true error $e(f_{\mathcal{D}}) \le \epsilon$).

Simple sample complexity for SL

Theorem Assume $\mathcal{F}$ is finite. Given any $\epsilon > 0, \delta > 0$, if we see l training instances where

$$l = \frac{1}{\epsilon}\left(\log|\mathcal{F}| + \log\frac{1}{\delta}\right)$$

then with probability at least $1-\delta$, all $f \in \mathcal{F}$ with zero training error $\hat{e}(f) = 0$ have $e(f) \le \epsilon$.

- ϵ controls the error of the learned function
- δ controls the confidence of the bound
- proof: setting $\delta = |\mathcal{F}|e^{-\epsilon l}$

A Finite, Doubly Realizable PAC bound for SSL

Plan: make $|\mathcal{F}|$ smaller

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Theorem (finite, doubly realizable) Assume $\mathcal{F}$ is finite. Given any $\epsilon > 0, \delta > 0$, if we see l labeled and u unlabeled training instances where

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then with probability at least $1-\delta$, all $f \in \mathcal{F}$ with $\hat{e}(f) = 0$ and $\hat{e}_U(f) = 0$ have $e(f) \le \epsilon$.

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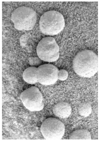
Discussions on the PAC bound for SSL

- Good news: can require less labeled data than SL
- This particular theorem requires finite $\mathcal{F}$, and doubly realizable f with $\hat{e}(f) = 0$ and $\hat{e}_U(f) = 0$
- More general theorems in (Balcan & Blum 2008):
  - infinite $\mathcal{F}$ is OK: extensions of the VC-dimension
  - agnostic, does not require either realizability: both $e(f)$ and $e_U(f)$ may be non-zero and unknown
  - also tighter ϵ-cover based bounds
- Most SSL algorithms (e.g. S3VMs) empirically minimize $\hat{e}(f) + \hat{e}_U(f)$: not necessarily justified in theory
- Incompatibility functions arbitrary. Serves as regularization. There are good and bad incompatibility functions. Example: "inverse S3VM" prefers to cut through dense unlabeled data

$$\Xi_{\text{inv}}(f, \mathbf{x}) = 1 - \Xi_{\text{S3VM}}(f, \mathbf{x})$$

Outline

Life-long learning

x_1	x_2	$\ldots$	x_{1000}	$\ldots$	$x_{1000000}$	$\ldots$
		$\ldots$		$\ldots$		$\ldots$
$y_1 = 0$	-	-	$y_{1000} = 1$	$\ldots$	$y_{1000000} = 0$	$\ldots$

- $n \to \infty$ examples arrive sequentially, cannot store them all
- most examples unlabeled
- no iid assumption, $p(x, y)$ can change over time

This is how children learn, too

x_1	x_2	$\ldots$	x_{1000}	$\ldots$	$x_{1000000}$	$\ldots$
		$\ldots$		$\ldots$		$\ldots$
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4. Learner updates to f_{t+1} based on x_t and y_t (if given). Repeat.

Online manifold regularization

- Recall (batch) manifold regularization risk:

$$
\begin{aligned}
J(f) \quad = \quad & \frac{1}{l} \sum_{t=1}^{T} \delta(y_t) c(f(x_t), y_t) + \frac{\lambda_1}{2} \|f\|_K^2 \\
& + \frac{\lambda_2}{2T} \sum_{s,t=1}^{T} (f(x_s) - f(x_t))^2 w_{st}
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- batch risk = average instantaneous risks $J(f) = \frac{1}{T}\sum_{t=1}^{T} J_t(f)$

Online convex programming

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- If no adversary (iid), the average classifier $\bar{f} = 1/T \sum_{t=1}^{T} f_t$ is good: $J(\bar{f}) \to J(f^*)$.

Sparse approximation by buffering

The algorithm is impractical as $T \to \infty$:

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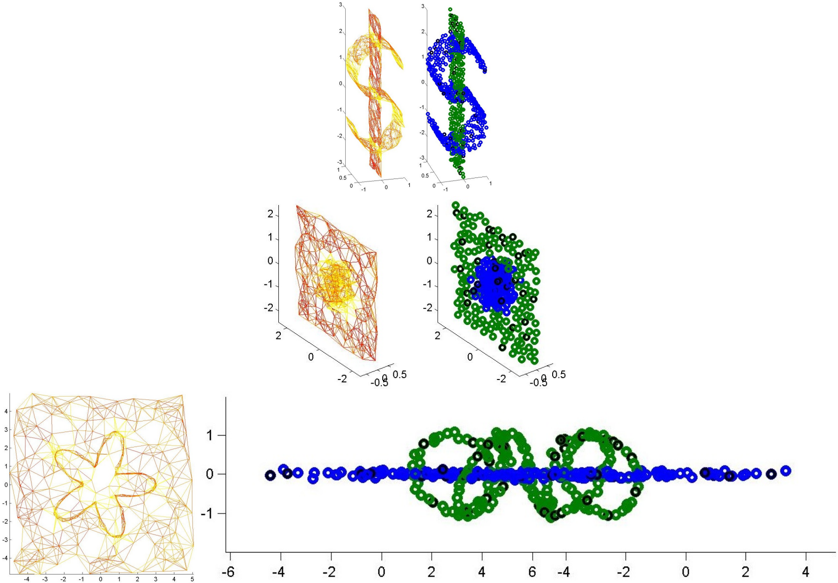
- dynamic graph on instances in the buffer

Outline

Multiple, intersecting manifolds

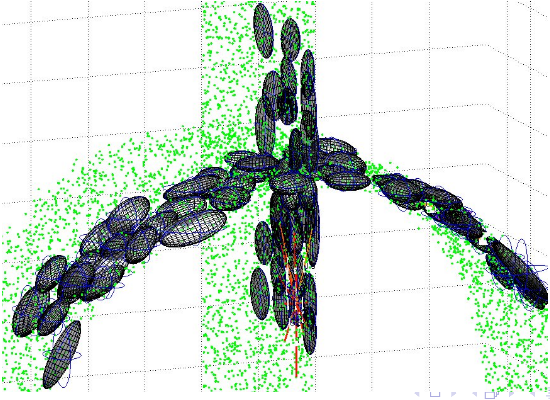


Building Blocks: Local Covariance Matrix

For a sparse subset of points x, the local covariance matrix of the neighbors

$$\Sigma_x = \frac{1}{m-1} \sum_j (x_j - \mu_x)(x_j - \mu_x)^\top$$

captures local geometry.



A Distance on Covariance Matrices

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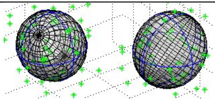
- $H(p,q)$ symmetric, in $[0,1]$
- Let $p = N(0, \Sigma_1), q = N(0, \Sigma_2)$. We define

$$H(\Sigma_1, \Sigma_2) \equiv H(p,q) = \sqrt{1 - 2^{\frac{d}{2}} \frac{|\Sigma_1|^{\frac{1}{4}} |\Sigma_2|^{\frac{1}{4}}}{|\Sigma_1 + \Sigma_2|^{\frac{1}{2}}}}$$

(computed in common subspace)

Hellinger Distance

	Comment	$H(\Sigma_1, \Sigma_2)$
	similar	0.02

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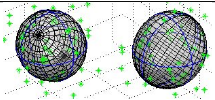
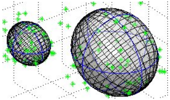
	similar	0.02
	density	0.28

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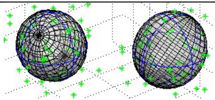
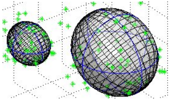
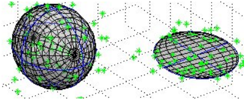
	similar	0.02
	density	0.28
	dimension	1

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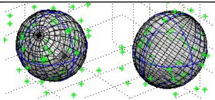
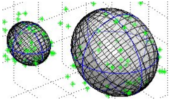
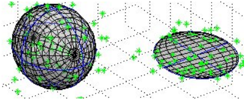
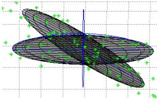
	similar	0.02
	density	0.28
	dimension	1
	orientation*	1

* smoothed version: $\Sigma + \epsilon I$

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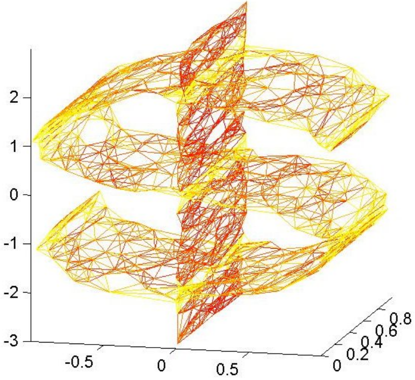
- Combines locality and shape. Red=large w, yellow=small w



- Manifold Regularization on the graph

Outline

Do we learn from both labeled and unlabeled data?

Learning exists long before machine learning. Do humans perform semi-supervised learning?

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Learning exists long before machine learning. Do humans perform semi-supervised learning?

- We discuss two human experiments:
  1. One-class classification [Zaki & Nosofsky 2007]
  2. Binary classification [Zhu et al. 2007]

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- participants shown training sample $\{(\mathbf{x}_i, y_i = 1)\}_{i=1}^{l}$, all from one class.

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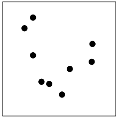
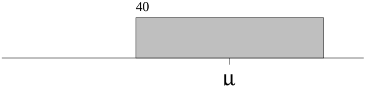
- if $\mathcal{X}_1$ is fixed after training, then test data won't affect classification.
- Zaki & Nosofsky showed this is not true.

The Zaki & Nosofsky 2007 experiment



(a) a stimulus



(b) training distribution

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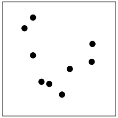

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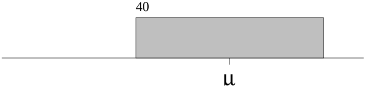

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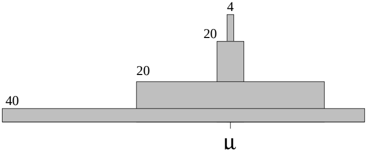
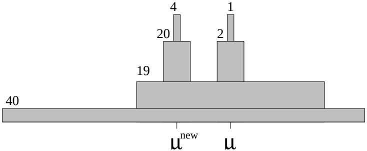
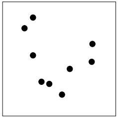


(c) condition 1 test distribution



(d) condition 2 test distribution

The Zaki & Nosofsky 2007 experiment



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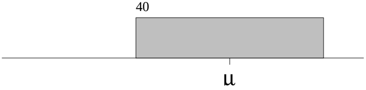

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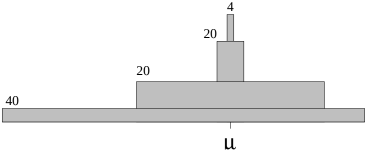

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$$\hat{p}(y=1|\mu) > \hat{p}(y=1|\text{low})$$
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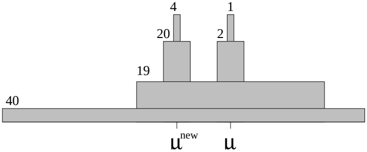
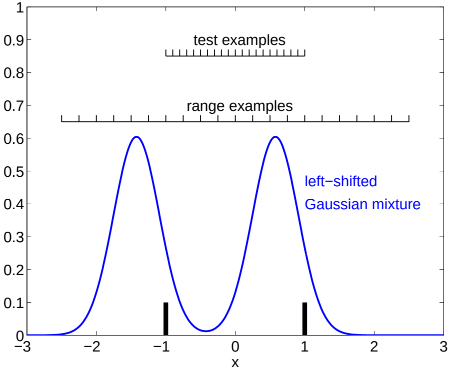


(d) condition 2 test distribution

$$\hat{p}(y=1|\mu^{\text{new}}) > \hat{p}(y=1|\text{low}^{\text{new}})$$
$$> \hat{p}(y=1|\mu) \approx \hat{p}(y=1|\text{low})$$
$$\approx \hat{p}(y=1|\text{high}) \gg \hat{p}(y=1|\text{random})$$

Zhu et al. 2007: mixture model?



blocks

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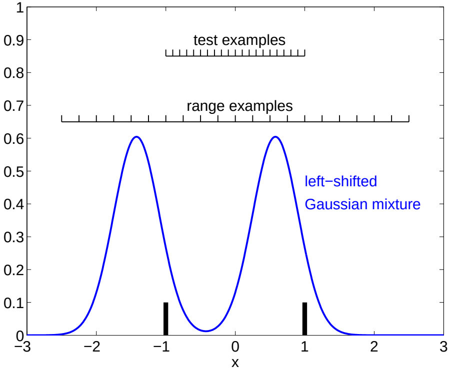

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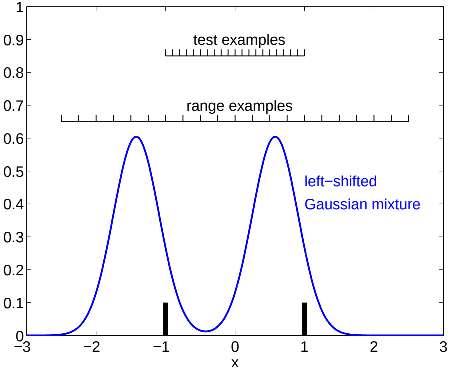

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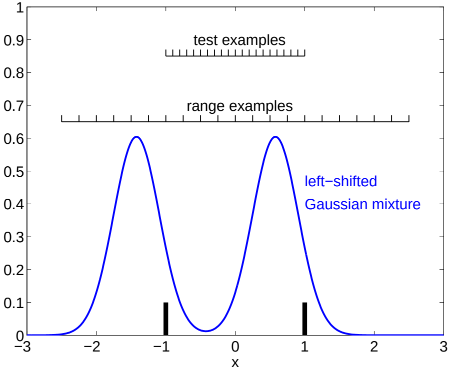

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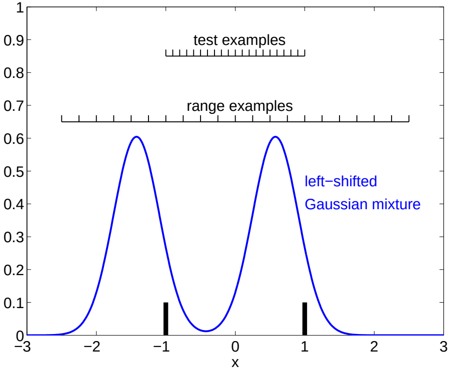
4. test 2: same as test 1

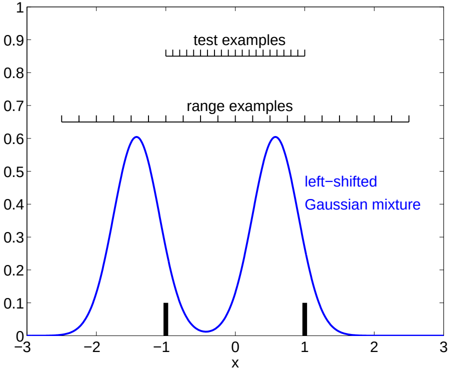
Zhu et al. 2007: mixture model?



blocks

1. 20 labeled points at $x = -1, 1$
2. test 1: 21 test examples in grid $[-1, 1]$
3. 690 examples $\sim$ bimodal distribution, plus 63 range examples in $[-2.5, 2.5]$
4. test 2: same as test 1

Zhu et al. 2007: mixture model?



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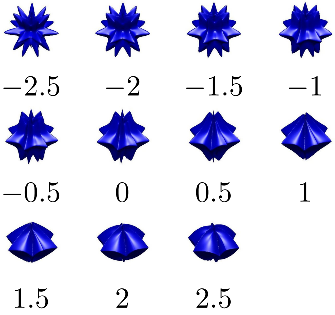
4. test 2: same as test 1

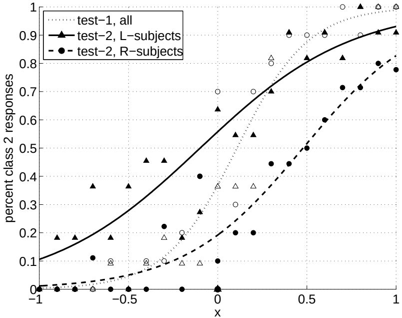
12 participants left-offset, 10 right-offset. Record their decisions and response times.

Visual stimuli

Stimuli parametrized by a continuous scalar x. Some examples:



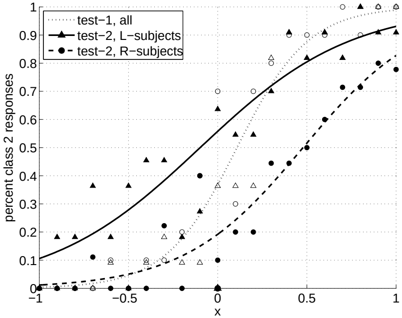
Observation 1: unlabeled data affects decision boundary



average decision boundary

- after seeing labeled data: $x = 0.11$

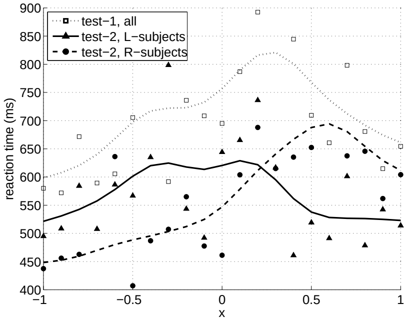
Observation 1: unlabeled data affects decision boundary



average decision boundary

- after seeing labeled data: $x = 0.11$
- after seeing labeled and unlabeled data: L-subjects $x = -0.10$, R-subjects $x = 0.48$

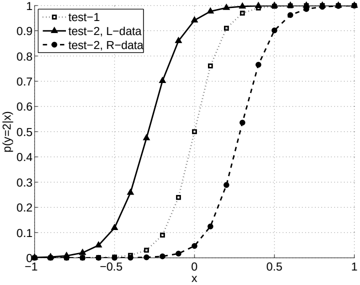
Observation 2: unlabeled data affects reaction time



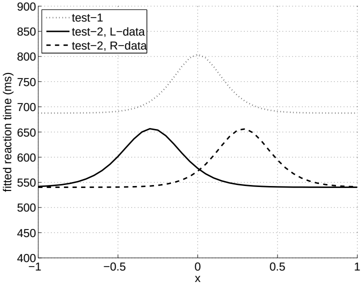
longer reaction time → harder example → closer to decision boundary.
Reaction times too suggest decision boundary shift.

Model fitting

We can fit human behavior with a GMM.



boundary shift



reaction time $t = aH(x) + b$

- Humans and machines both perform semi-supervised learning.
- Understanding natural learning may lead to new machine learning algorithms.

References

See the references in

Xiaojin Zhu and Andrew B. Goldberg. *Introduction to Semi-Supervised Learning*. Morgan & Claypool, 2009.