

Tutorial on Semi-Supervised Learning

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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: $x=\text{animal}$, $y=\text{concept}$ (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

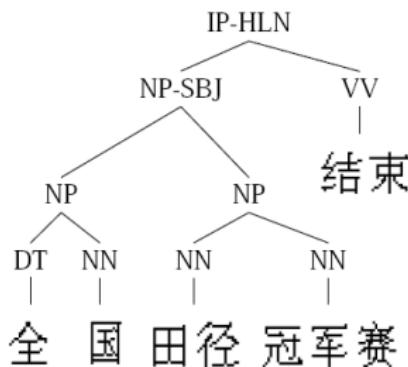
film ⇒ f ih_n uh_g1_n m

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 $\{(x_{n+1\dots}, y_{n+1\dots})\}$, **not available** during training

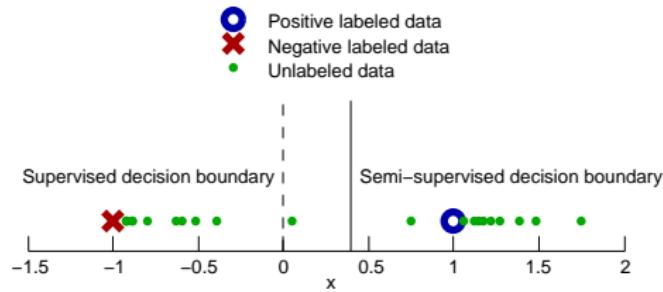
Semi-supervised vs. transductive learning

- **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 $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$.

Semi-supervised vs. transductive learning

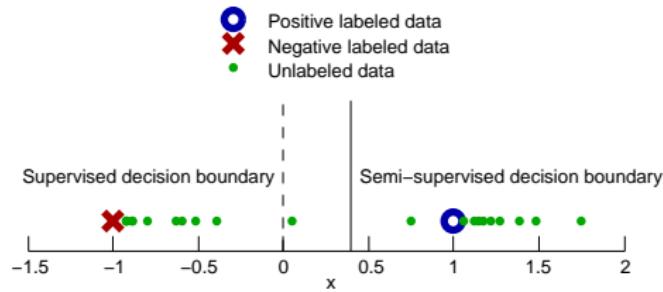
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- **Transductive learning:** Given $\{(\mathbf{x}_i, y_i)\}_{i=1}^l, \{\mathbf{x}_j\}_{j=l+1}^{l+u}$, learn $f : \mathcal{X}^{l+u} \mapsto \mathcal{Y}^{l+u}$ so that f is expected to be a good predictor on the unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$.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



- assuming each class is a coherent group (e.g. Gaussian)
- with and without unlabeled data: decision boundary shift

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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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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

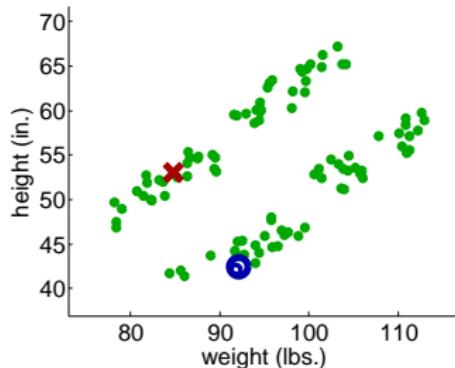
Self-training example: Propagating 1-Nearest-Neighbor

An instance of self-training.

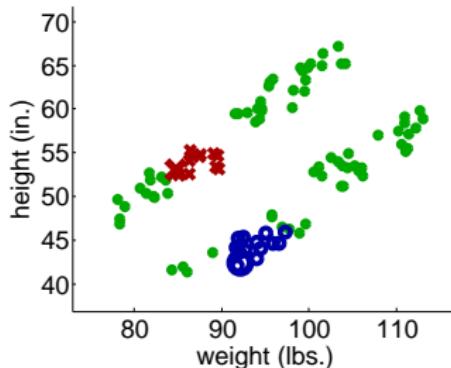
Input: labeled data $\{(\mathbf{x}_i, y_i)\}_{i=1}^l$, unlabeled data $\{\mathbf{x}_j\}_{j=l+1}^{l+u}$, distance function $d()$.

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 $\mathbf{x} = \operatorname{argmin}_{\mathbf{x} \in U} \min_{\mathbf{x}' \in L} d(\mathbf{x}, \mathbf{x}')$.
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 .

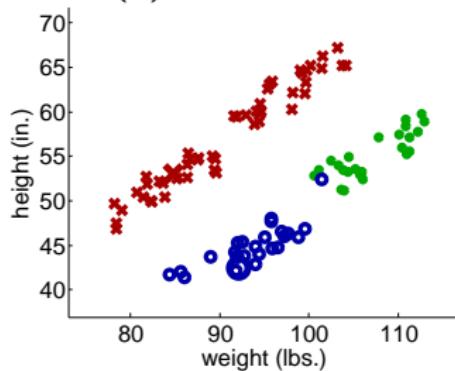
Propagating 1-Nearest-Neighbor: now it works



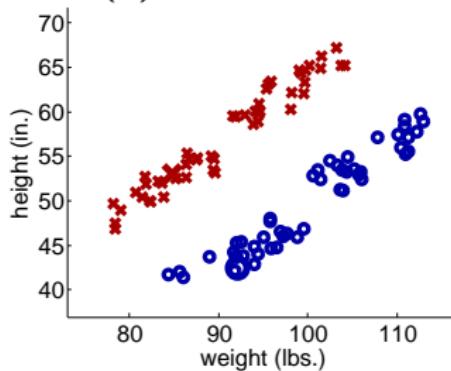
(a) Iteration 1



(b) Iteration 25

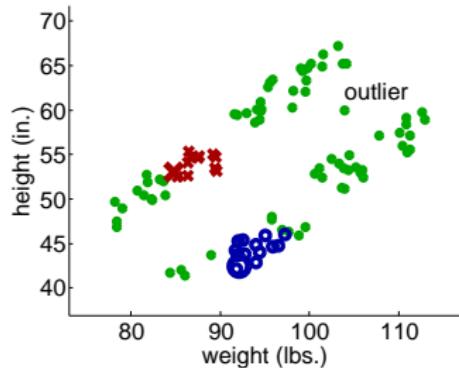


(c) Iteration 74

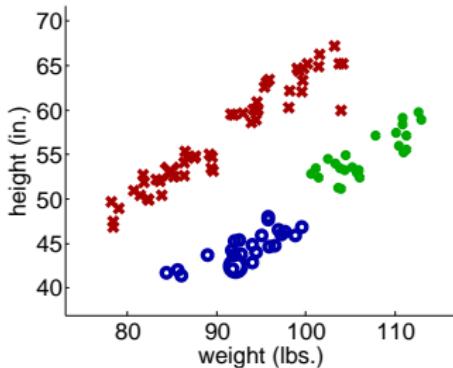


(d) Final labeling of all instances

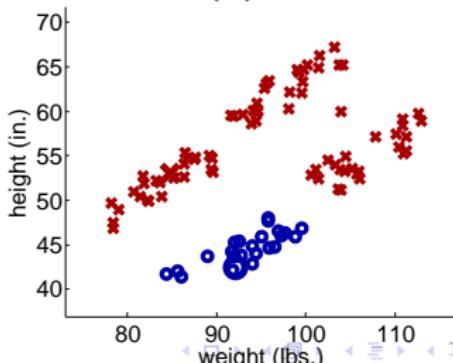
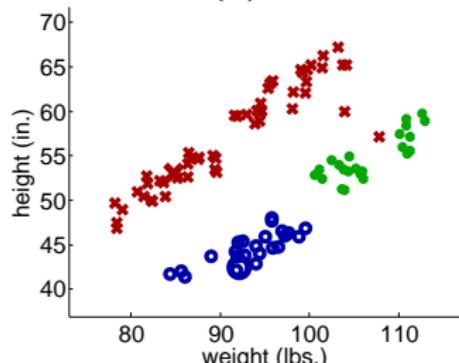
Propagating 1-Nearest-Neighbor: now it doesn't But with a single outlier...



(a)



(b)



Outline

1 Part I

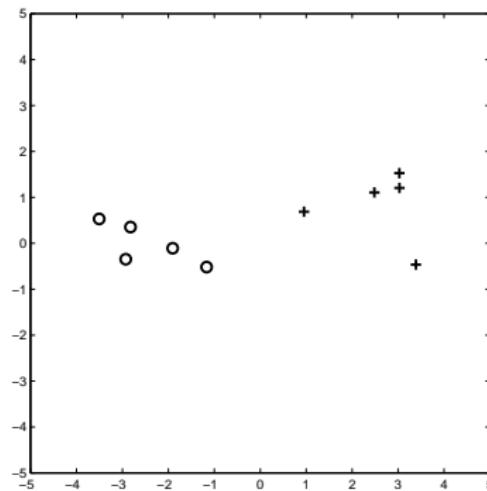
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A simple example of generative models

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: $\theta = \{w_1, w_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$

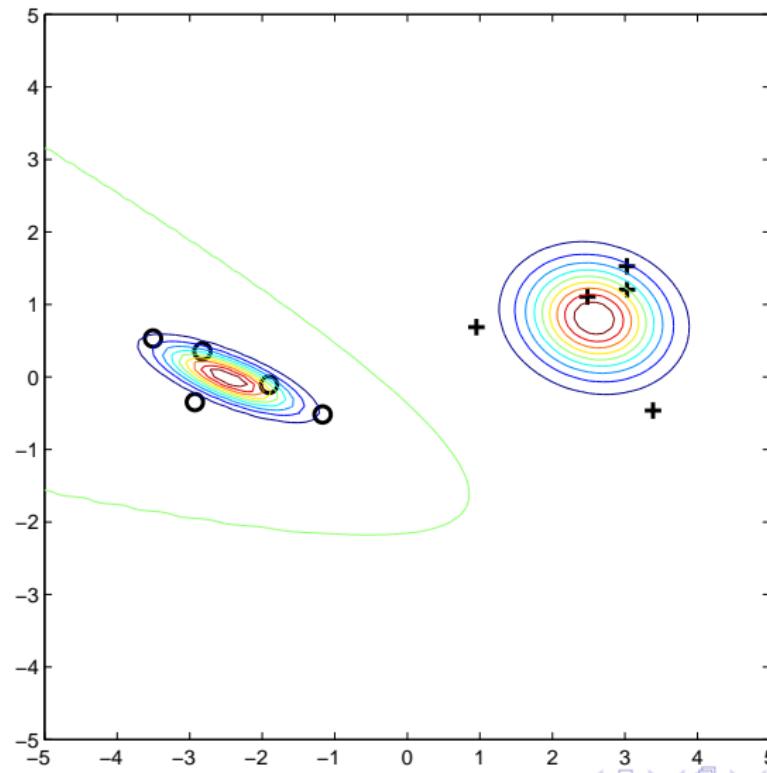
The GMM:

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

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

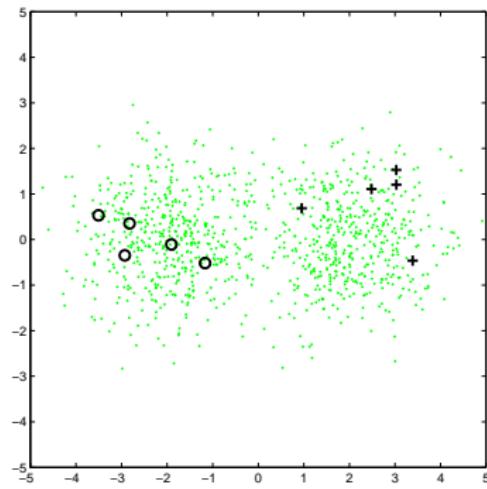
A simple example of generative models

The most likely model, and its decision boundary:



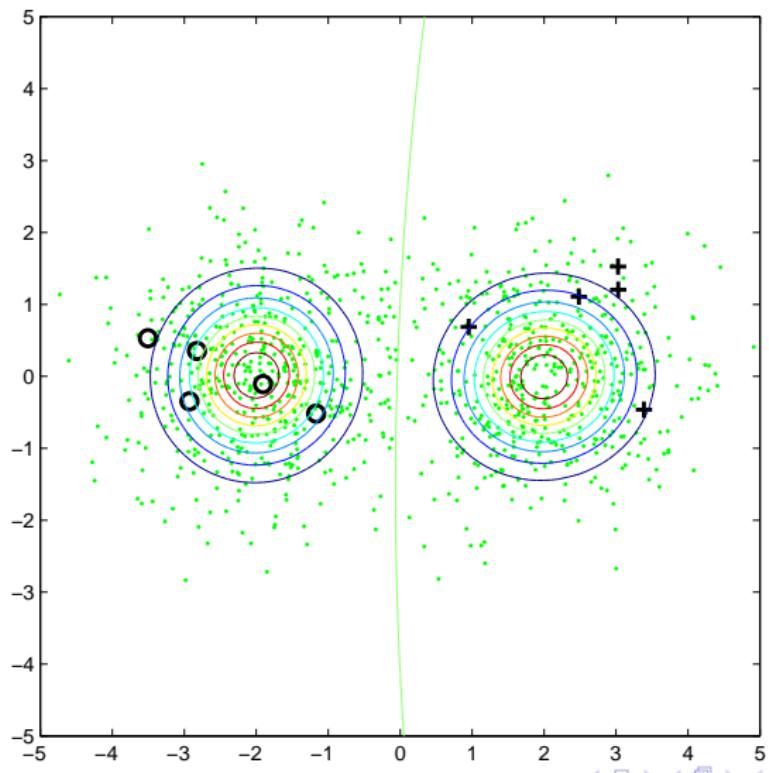
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Adding unlabeled data:



A simple example of generative models

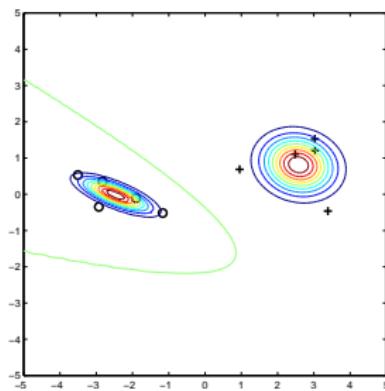
With unlabeled data, the most likely model and its decision boundary:



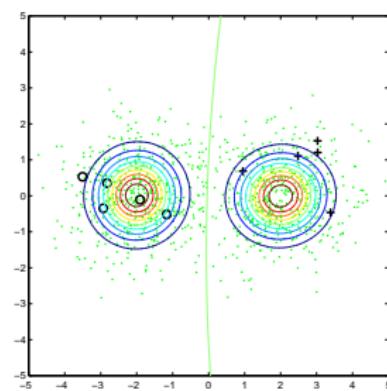
A simple example of generative models

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

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

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- with both labeled and unlabeled data

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

- ▶ 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
- ▶ Σ_c =sample cov of class c

repeat:

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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 $x \in X_u$
- ▶ label $p(y = 1|x, \theta)$ -fraction of x with class 1
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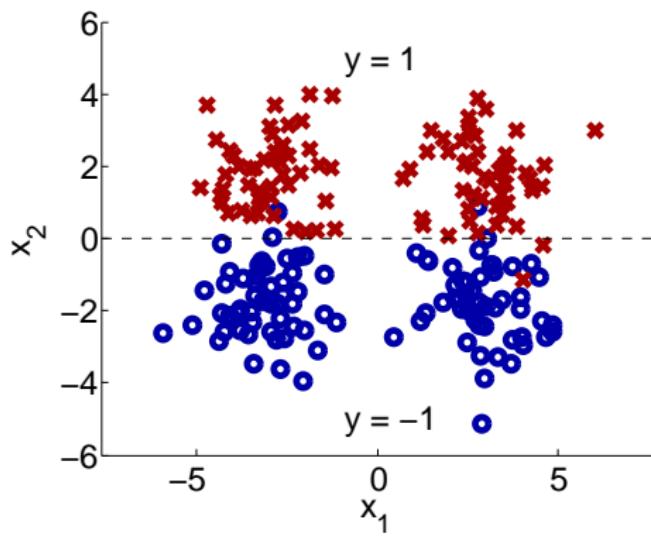
Can be viewed as a special form of self-training.

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.

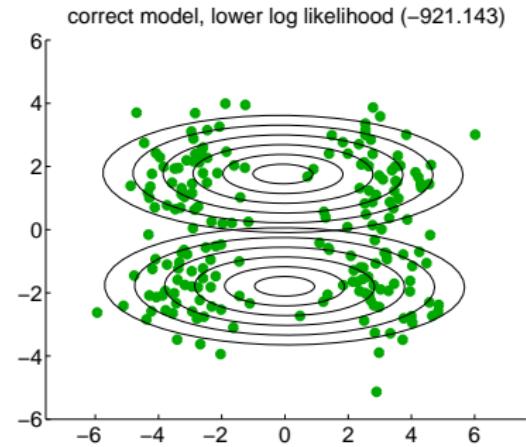
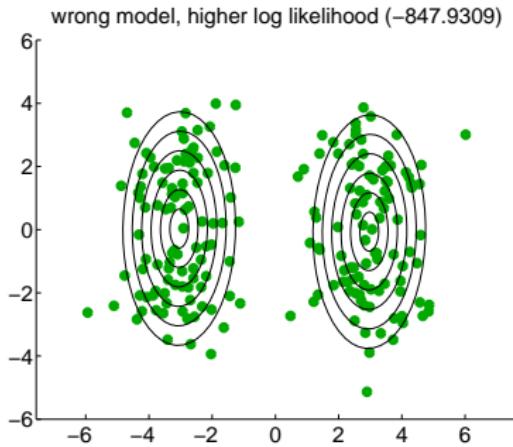
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- When the assumption is wrong:

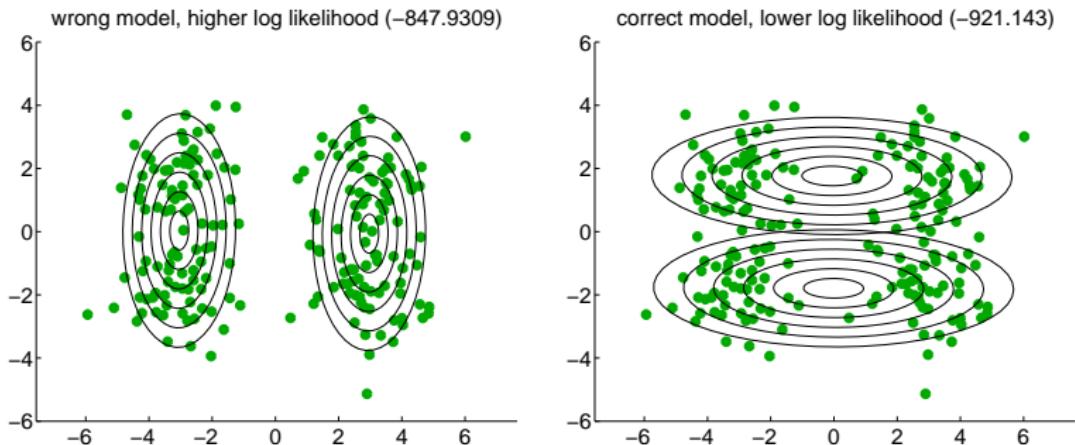


For example, classifying text by topic vs. by genre.

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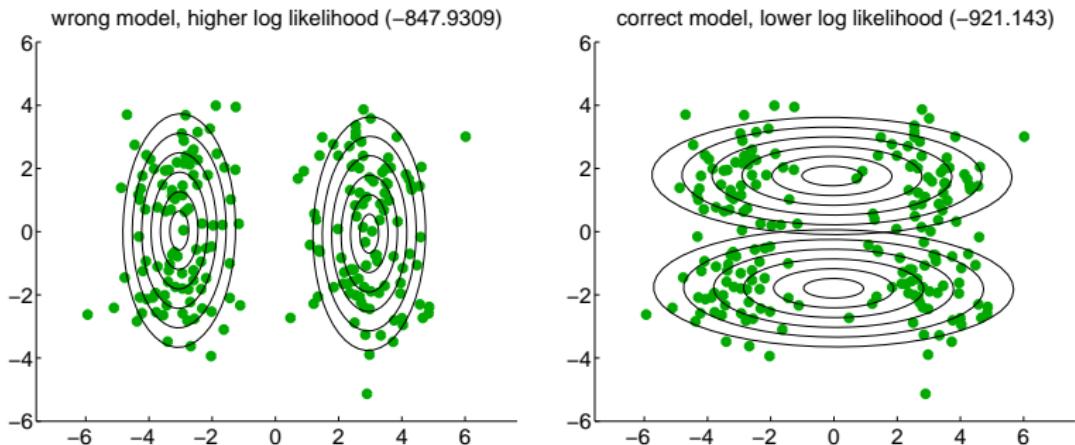
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Heuristics to lessen the danger

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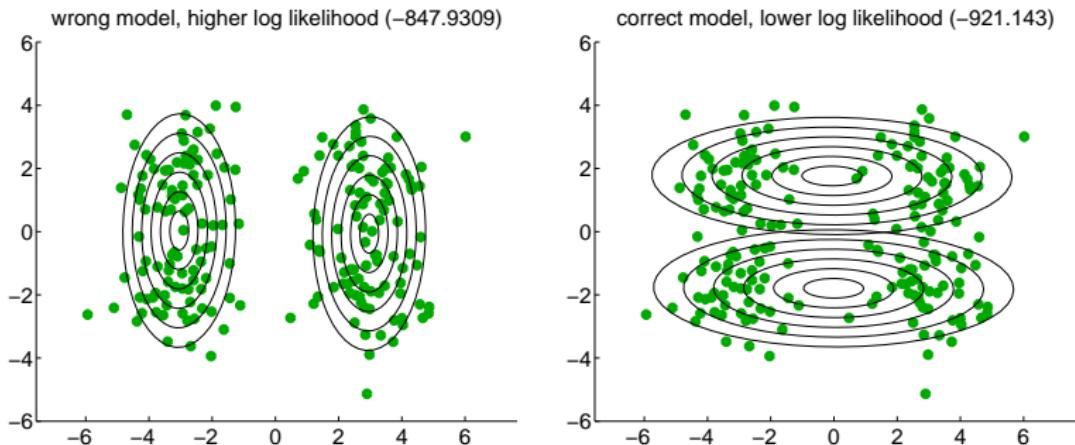


Heuristics to lessen the danger

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

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Other

dangers: identifiability, EM local optima

Related: cluster-and-label

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

Related: cluster-and-label

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Related: cluster-and-label

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2. For each cluster, let S be the labeled instances in it:

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Output: labels on unlabeled data y_{l+1}, \dots, y_{l+u} .

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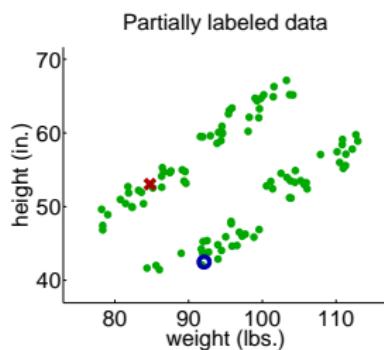
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But again: **SSL sensitive to assumptions**—in this case, that the clusters coincide with decision boundaries. If this assumption is incorrect, the results can be poor.

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

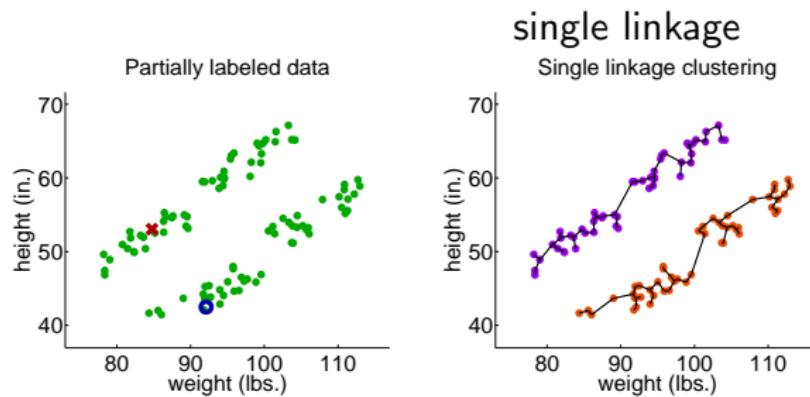
Example: \mathcal{A} =Hierarchical Clustering, \mathcal{L} =majority vote.

single linkage



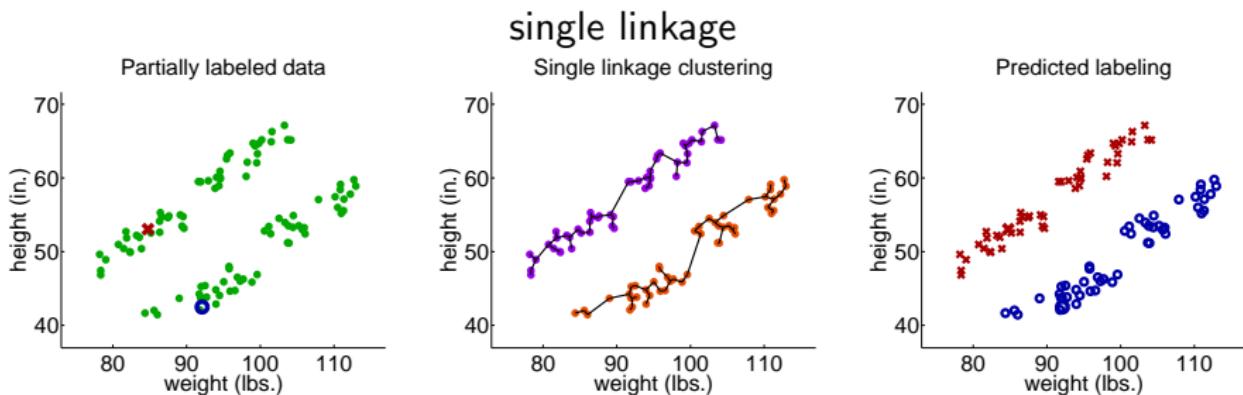
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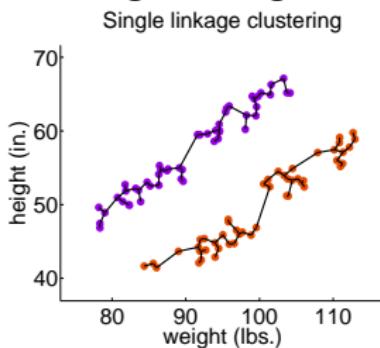
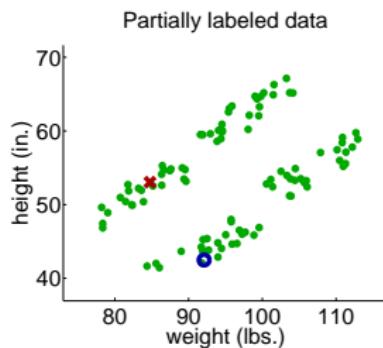
Example: \mathcal{A} =Hierarchical Clustering, \mathcal{L} =majority vote.



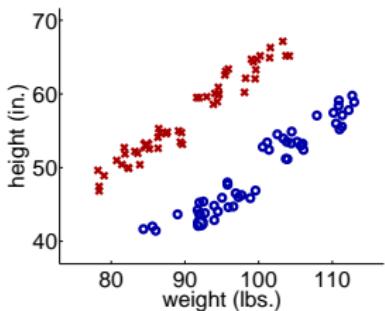
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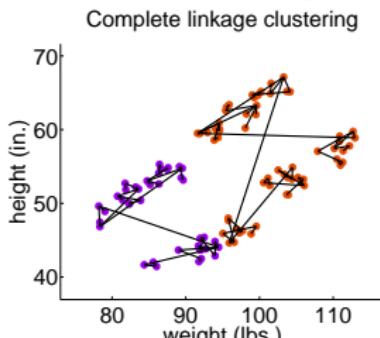
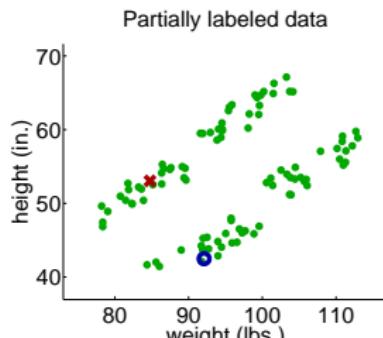
single linkage



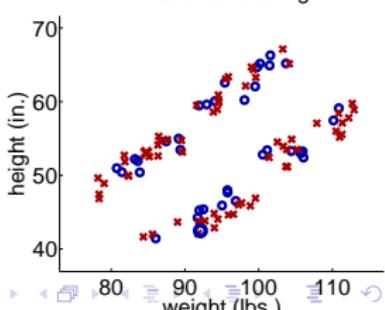
Predicted labeling



complete linkage



Predicted labeling



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
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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

Co-training assumptions

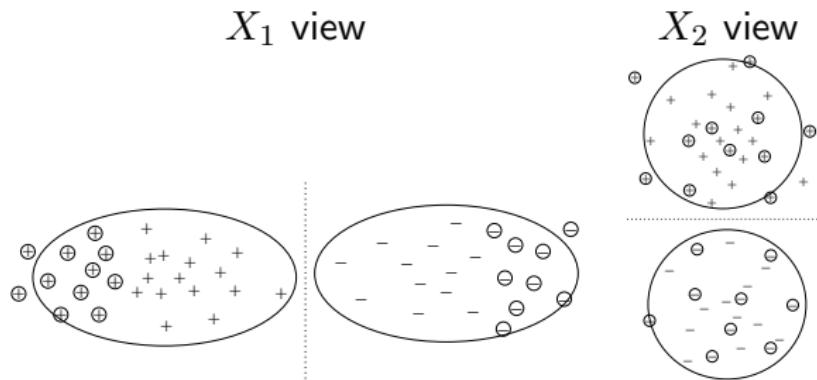
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- $x^{(1)}$ and $x^{(2)}$ are conditionally independent given the class



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 $f^* = \operatorname{argmin}_{f \in \mathcal{F}} \hat{R}(f) + \lambda \Omega(f)$

Multiview learning

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

$$\operatorname{argmin}_{f_1, \dots, f_k} \sum_{v=1}^k \left(\sum_{i=1}^l c(\mathbf{x}_i, y_i, f_v(\mathbf{x}_i)) + \lambda_1 \Omega_{SL}(f_v) \right) \\ + \lambda_2 \sum_{u,v=1}^k \sum_{i=l+1}^{l+u} c(\mathbf{x}_i, f_u(\mathbf{x}_i), f_v(\mathbf{x}_i))$$

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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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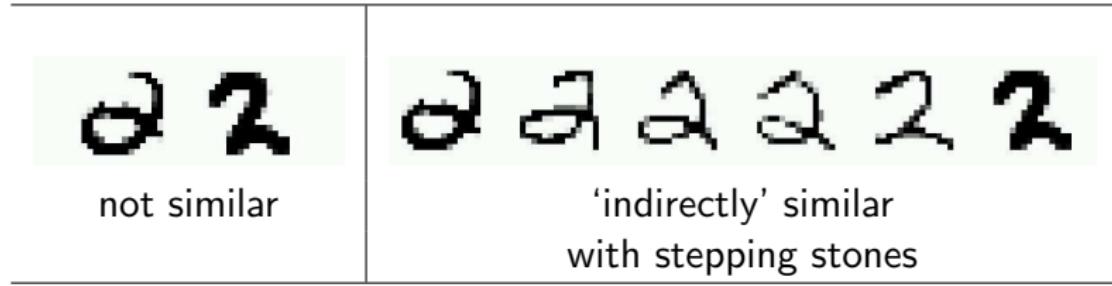
Unlabeled data as stepping stones

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			•		•	•			
⋮									
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airport						•			
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Another example

Handwritten digits recognition with pixel-wise Euclidean distance



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$$w = \exp(-\|x_i - x_j\|^2/\sigma^2)$$

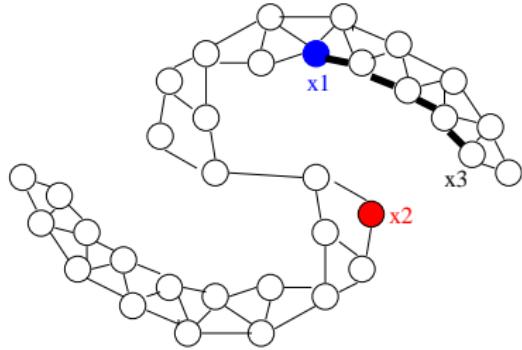
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 - **Assumption** Instances connected by heavy edge tend to have the same label.



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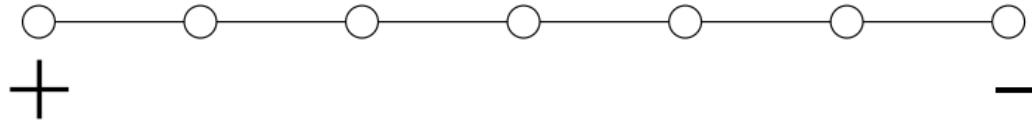
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- Mincut computes the **modes** of a discrete Markov random field, but there might be multiple modes



The harmonic function

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

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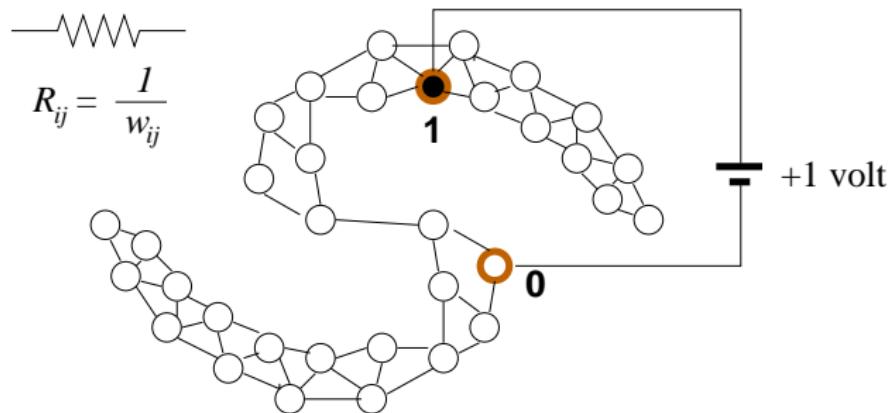
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- the **mean** of a Gaussian random field
- average of neighbors $f(x_i) = \frac{\sum_{j \sim i} w_{ij} f(x_j)}{\sum_{j \sim i} w_{ij}}, \forall x_i \in X_u$

An electric network interpretation

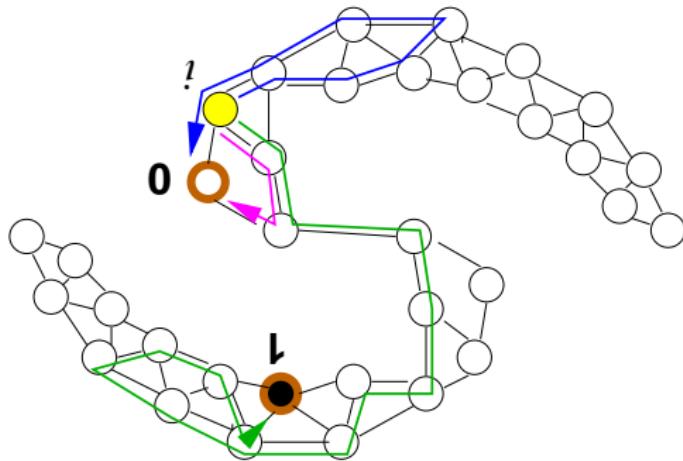
- Edges are resistors with conductance w_{ij}
- 1 volt battery connects to labeled points $y = 0, 1$
- The voltage at the nodes is the harmonic function f

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:

- ① Initially, set $f(x_i) = y_i$ for $i = 1 \dots l$, and $f(x_j)$ arbitrarily (e.g., 0) for $x_j \in X_u$.

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- 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

$$\min_f \frac{1}{2} \|f\|_2^2 + \lambda f^\top \Delta f$$

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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 Δ^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 $f_{1:n}^\top \Delta f_{1:n}$

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

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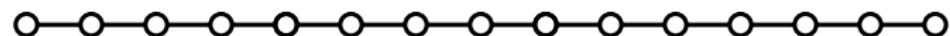
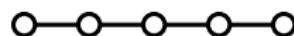
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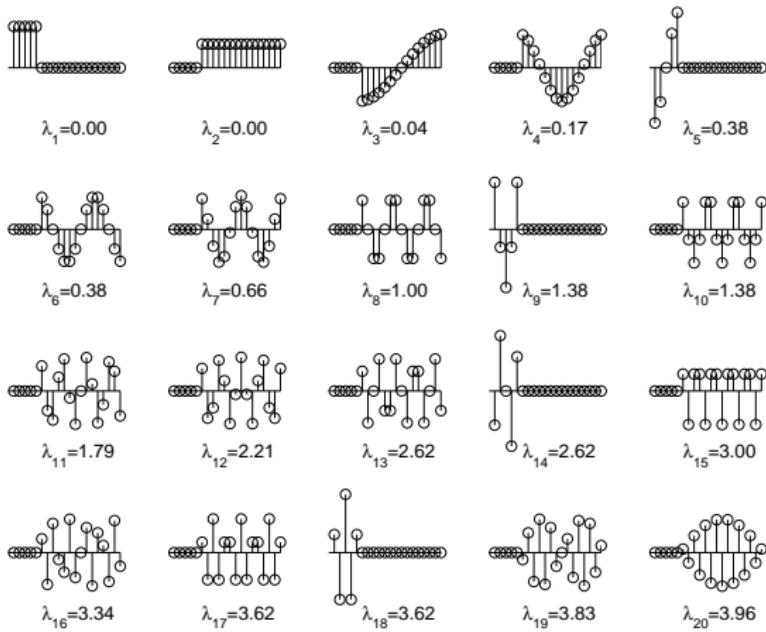
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- graph regularizer $\mathbf{f}^\top L \mathbf{f} = \sum_{i=1}^{l+u} a_i^2 \lambda_i$
- smooth function \mathbf{f} uses smooth basis (those with small λ_i)

Example graph spectrum

The graph

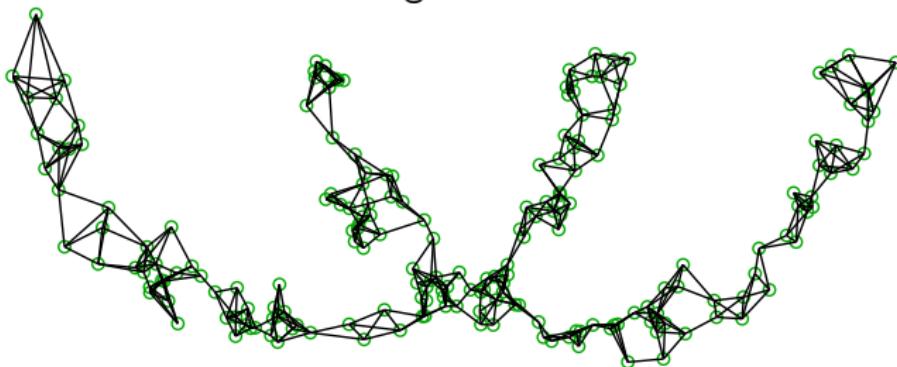


Eigenvalues and eigenvectors of the graph Laplacian



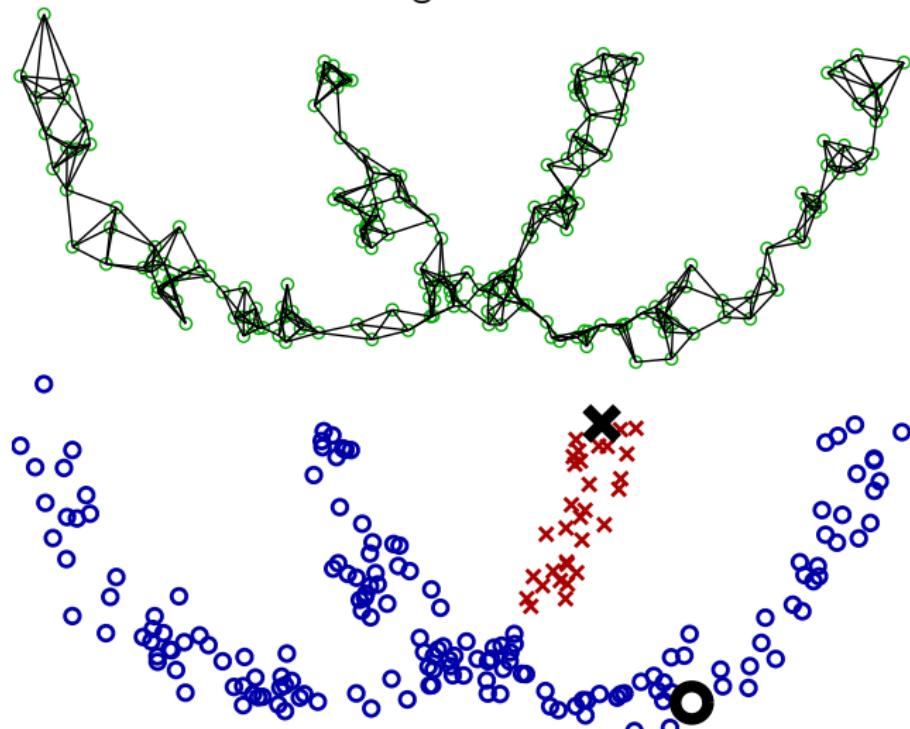
When the graph assumption is wrong

“colliding two moons”



When the graph assumption is wrong

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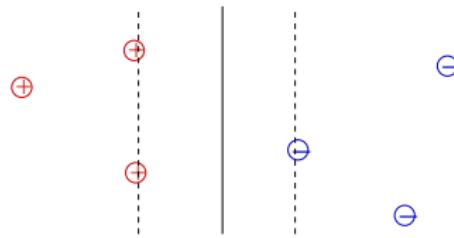
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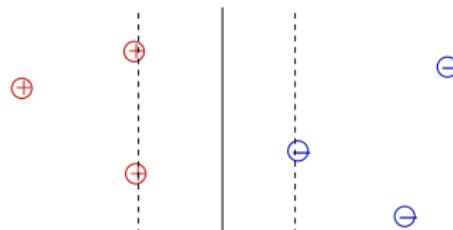
Semi-supervised Support Vector Machines

SVMs

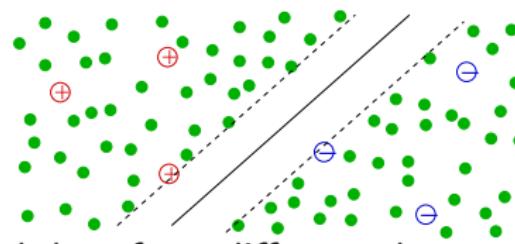


Semi-supervised Support Vector Machines

SVMs



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:

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

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

$$\xi_i \geq 0$$

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$$\xi_i \geq 0$$

Equivalent to

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

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

The S3VM objective function

To incorporate unlabeled points,

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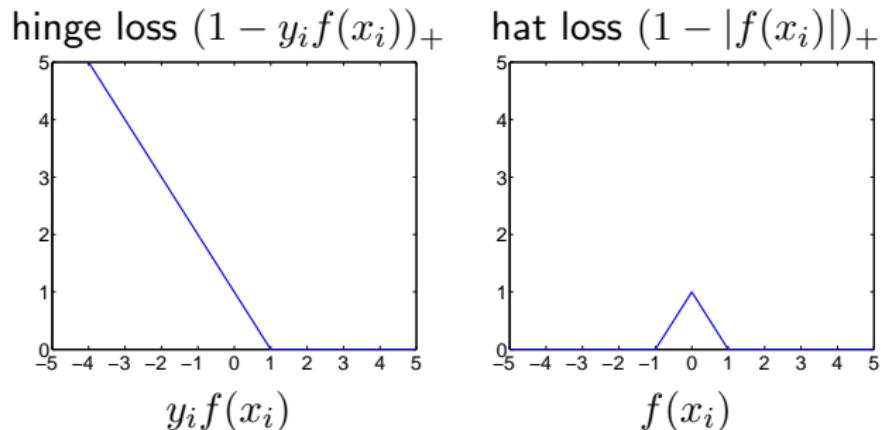
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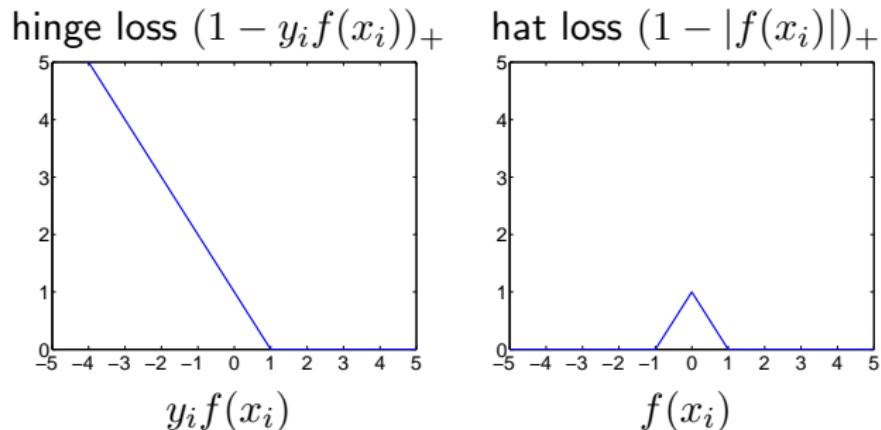
$$\min_f \sum_{i=1}^l (1 - y_i f(x_i))_+ + \lambda_1 \|h\|_{\mathcal{H}_K}^2 + \lambda_2 \sum_{i=l+1}^{\textcolor{red}{n}} (1 - |f(x_i)|)_+$$

The hat loss on unlabeled data



Prefers $f(x) \geq 1$ or $f(x) \leq -1$, i.e., unlabeled instance away from decision boundary $f(x) = 0$.

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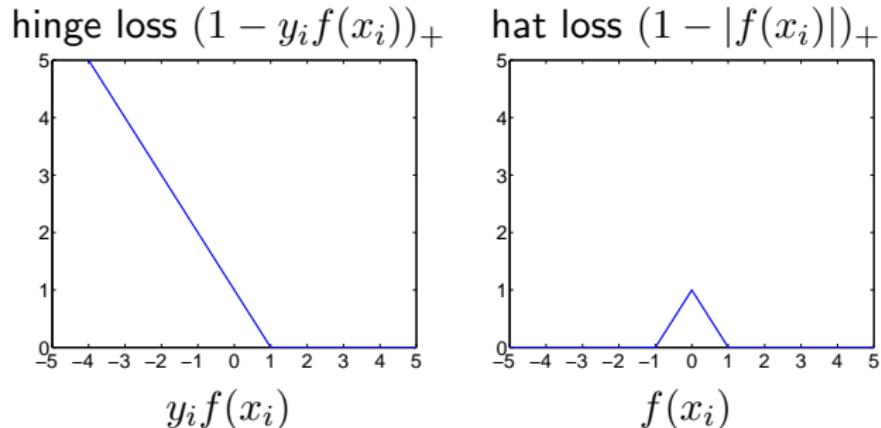


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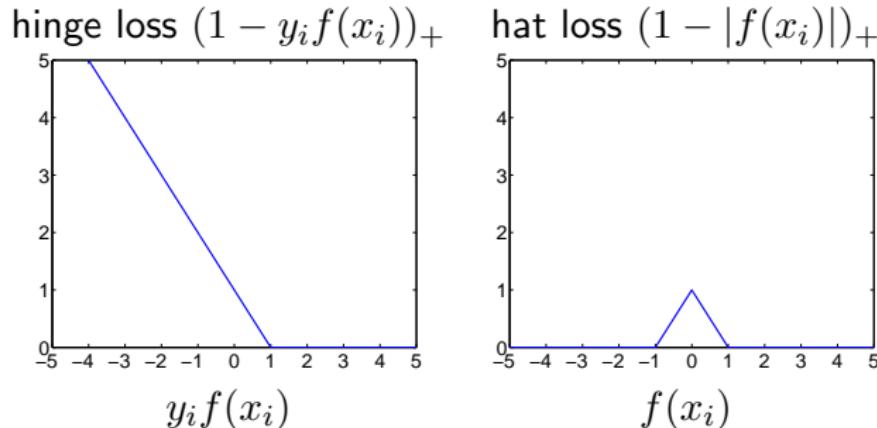


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- Relaxed: $\frac{1}{n-l} \sum_{i=l+1}^n f(x_i) = \frac{1}{l} \sum_{i=1}^l y_i$.

The S3VM algorithm

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Computational difficulty

- SVM objective is convex
- Semi-supervised SVM objective is **non-convex**

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Computational difficulty

- 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.

- $p(y|\mathbf{x}) = 1 / (1 + \exp(-yf(\mathbf{x})))$ 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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- Assumption: if the two classes are well-separated, then $p(y|x)$ on any unlabeled instance should be close to 0 or 1.

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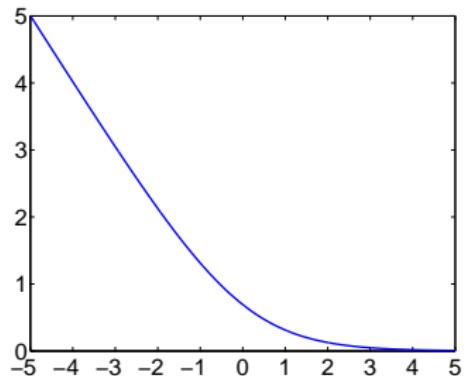
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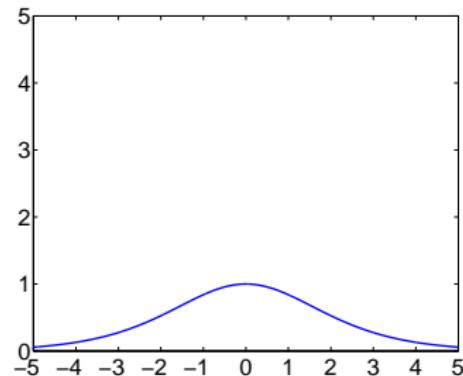
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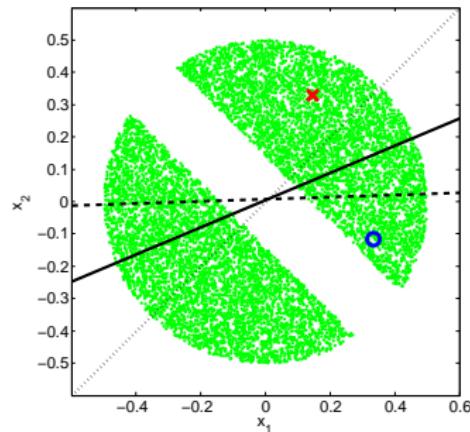


(a) the logistic loss

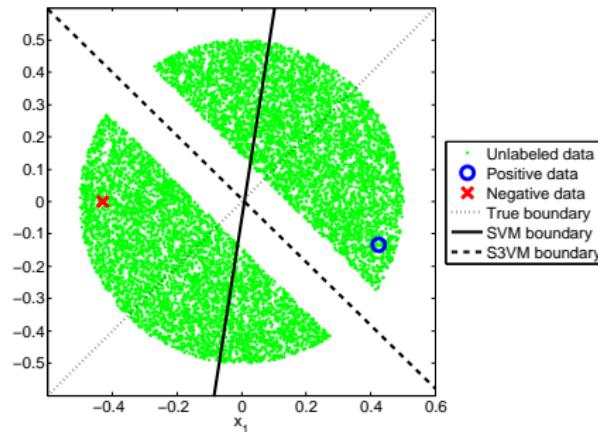


(b) the entropy regularizer

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

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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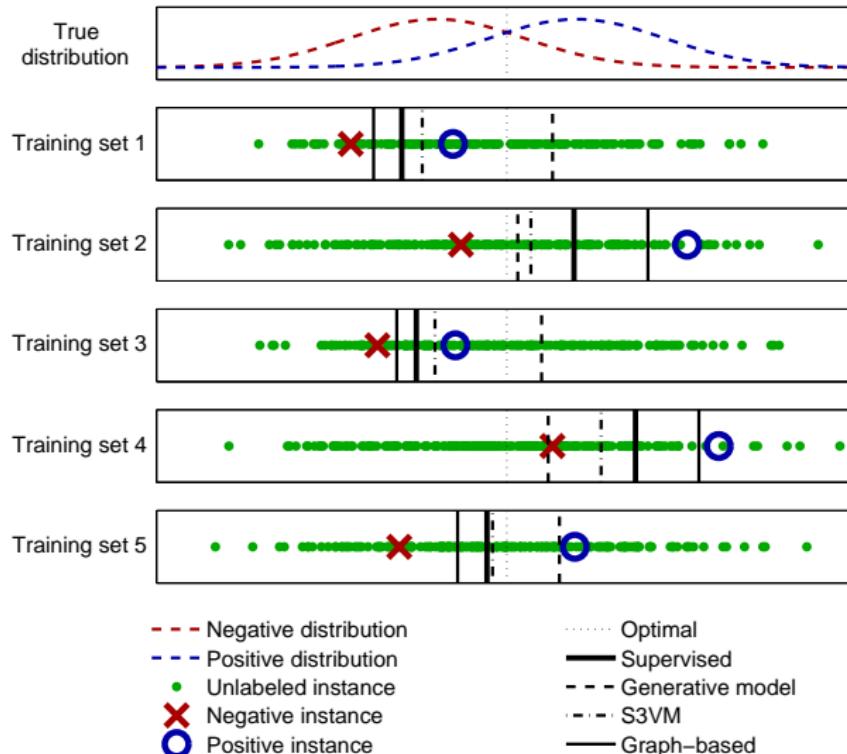
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SSL does not always help



Wrong SSL assumption can make SSL worse than SL!

A computational theory for SSL

(Theoretic guarantee of Balcan & Blum)

Recall in supervised learning

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 $e(f_{\mathcal{D}}) = \mathbb{E}_{(\mathbf{x}, y) \sim P} [f_{\mathcal{D}}(\mathbf{x}) \neq y]$?
- it turns out we can *bound* $e(f_{\mathcal{D}})$ without the knowledge of P .

PAC bound for SL

- training error minimizer f_D is a random variable (of D)

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

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 $e(f) \leq \epsilon$.

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

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

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- **incompatibility** $\Xi(f, \mathbf{x}) : \mathcal{F} \times \mathcal{X} \mapsto [0, 1]$ between a function f and an unlabeled instance \mathbf{x}

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- example: S3VM wants $|f(\mathbf{x})| \geq \gamma$. Define

$$\Xi_{S3VM}(f, \mathbf{x}) = \begin{cases} 1, & \text{if } |f(\mathbf{x})| < \gamma \\ 0, & \text{otherwise.} \end{cases}$$

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- sample unlabeled data error $\hat{e}_U(f) = \frac{1}{u} \sum_{i=l+1}^{l+u} \Xi(f, \mathbf{x}_i)$

PAC bound for SSL

- by a similar argument, after $u = \frac{1}{\epsilon} (\log |\mathcal{F}| + \log \frac{2}{\delta})$ unlabeled data, with probability at least $1 - \delta/2$, all $f \in \mathcal{F}$ with $\hat{e}_U(f) = 0$ have $e_U(f) \leq \epsilon$.

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- i.e., if $\hat{e}_U(f) = 0$, then $f \in \mathcal{F}(\epsilon) \equiv \{f \in \mathcal{F} : e_U(f) \leq \epsilon\}$
- apply the SL PAC bound on the (much smaller) $\mathcal{F}(\epsilon)$

PAC bound for SSL

- by a similar argument, after $u = \frac{1}{\epsilon} (\log |\mathcal{F}| + \log \frac{2}{\delta})$ unlabeled data, with probability at least $1 - \delta/2$, all $f \in \mathcal{F}$ with $\hat{e}_U(f) = 0$ have $e_U(f) \leq \epsilon$.
- i.e., if $\hat{e}_U(f) = 0$, then $f \in \mathcal{F}(\epsilon) \equiv \{f \in \mathcal{F} : e_U(f) \leq \epsilon\}$
- apply the SL PAC bound on the (much smaller) $\mathcal{F}(\epsilon)$

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

$$l = \frac{1}{\epsilon} \left(\log |\mathcal{F}(\epsilon)| + \log \frac{2}{\delta} \right) \text{ and } u = \frac{1}{\epsilon} \left(\log |\mathcal{F}| + \log \frac{2}{\delta} \right),$$

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

Discussions on the PAC bound for SSL

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- requires less labeled data than SL
- but conditions stringent: needs f with $\hat{e}(f) = 0$ and $\hat{e}_U(f) = 0$
- SSL algorithms (e.g. S3VMs) try to empirically minimize both errors
- incompatibility functions *arbitrary*. Example: “inverse S3VM” prefers to cut through dense unlabeled data

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

against intuition?

Outline

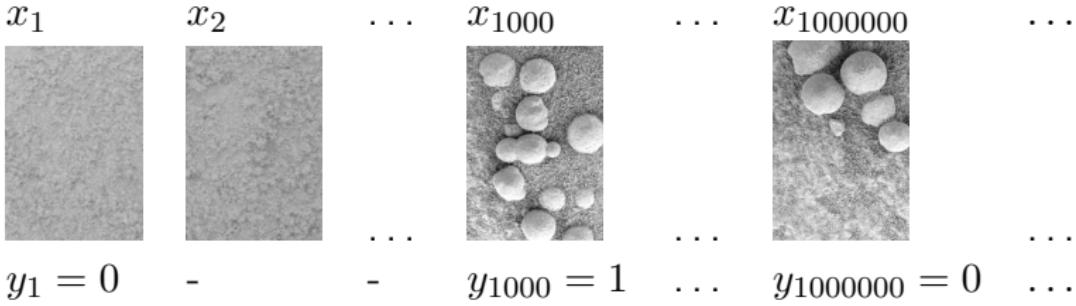
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- **Online SSL**
- Multimanifold SSL
- Human SSL

Life-long learning



- $n \rightarrow \infty$ 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

...

 x_{1000}

...

 $x_{1000000}$

...

 $y_1 = 0$

-

...

 $y_{1000} = 1$

...

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New paradigm: online semi-supervised learning

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- ③ **With small probability**, adversary reveals y_t ; otherwise it abstains (unlabeled)
- 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:

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

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- batch risk = average instantaneous risks $J(f) = \frac{1}{T} \sum_{t=1}^T J_t(f)$

Online convex programming

- Instead of minimizing convex $J(f)$, reduce convex $J_t(f)$ at each step

$$t: f_{t+1} = f_t - \eta_t \left. \frac{\partial J_t(f)}{\partial f} \right|_{f_t}$$

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

Sparse approximation by buffering

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

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- dynamic graph on instances in the buffer

Outline

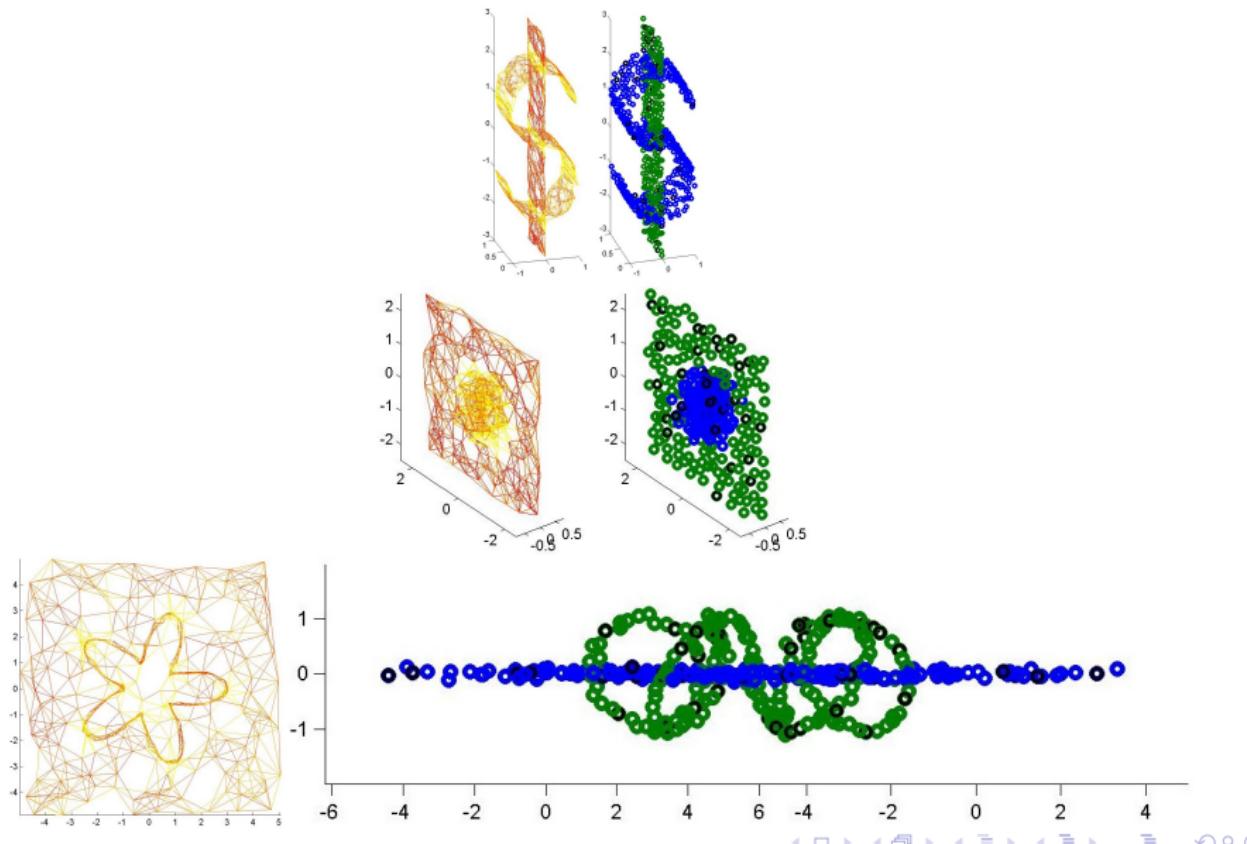
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Multiple, intersecting manifolds

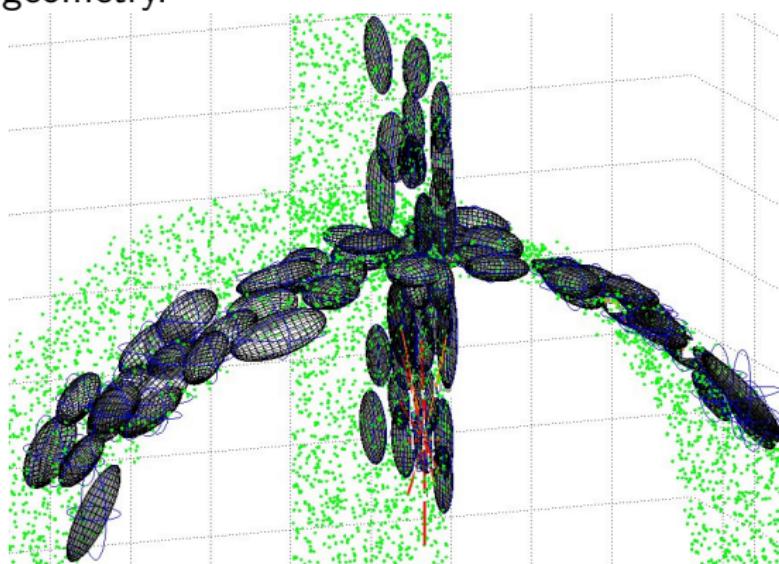


Building Blocks: Local Covariance Matrix

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

- Hellinger distance

$$H^2(p, q) = \frac{1}{2} \int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx$$

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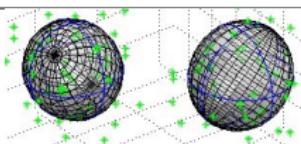
$$H^2(p, q) = \frac{1}{2} \int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx$$

- $H(p, q)$ 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)

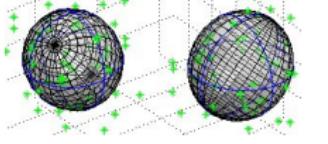
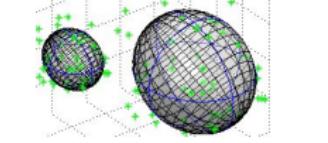
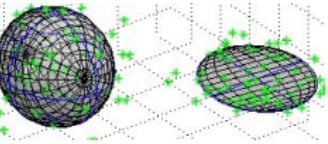
Hellinger Distance

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

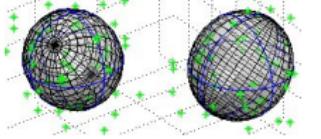
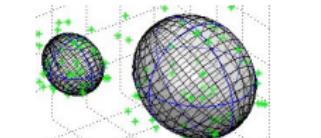
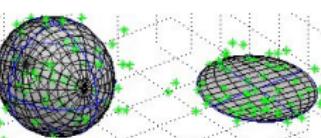
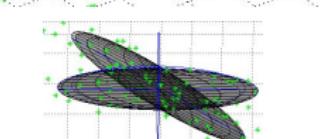
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	orientation* 1

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

A Sparse Graph

- KNN graph use Mahalanobis distance to trace the manifold

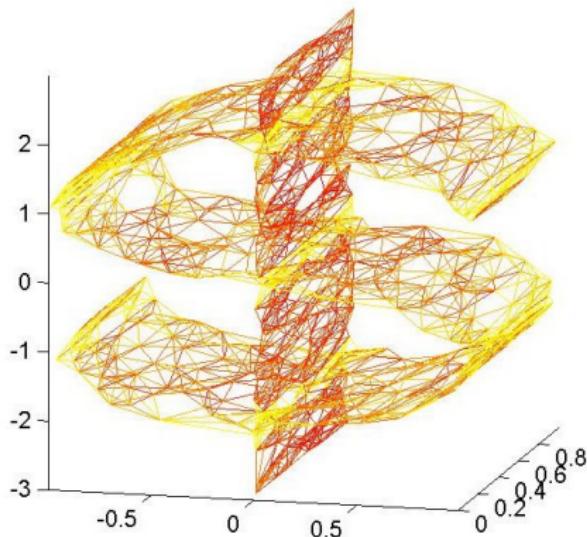
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- Combines locality and shape. Red=large w , yellow=small w



- Manifold Regularization on the graph

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Do we learn from both labeled and unlabeled data?

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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]

Zaki & Nosofsky 2007: self training?

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

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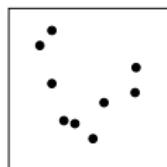
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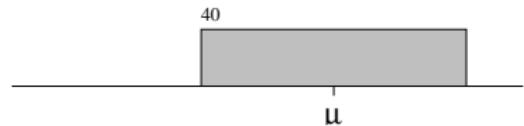
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- if \mathcal{X}_1 is fixed after training, then test data won't affect classification.
- Zaki & Nosofsky showed this is not true.

The Zaki & Nosofsky 2007 experiment

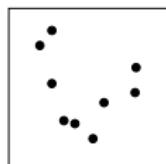


(a) a stimulus

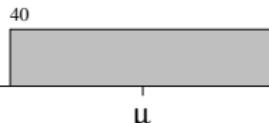


(b) training distribution

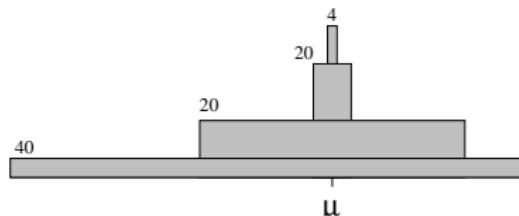
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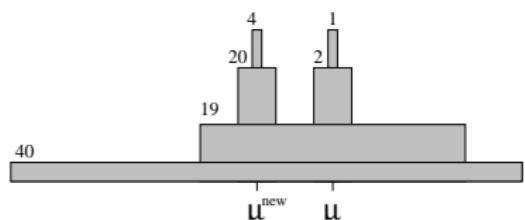
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(c) condition 1 test distribution

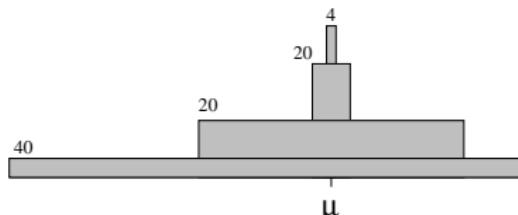


(d) condition 2 test distribution

The Zaki & Nosofsky 2007 experiment

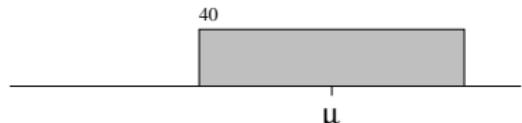


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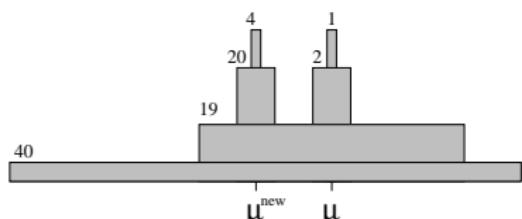


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$$\begin{aligned} \hat{p}(y = 1|\mu) &> \hat{p}(y = 1|\text{low}) \\ &> \hat{p}(y = 1|\text{high}) \gg \hat{p}(y = 1|\text{random}) \end{aligned}$$



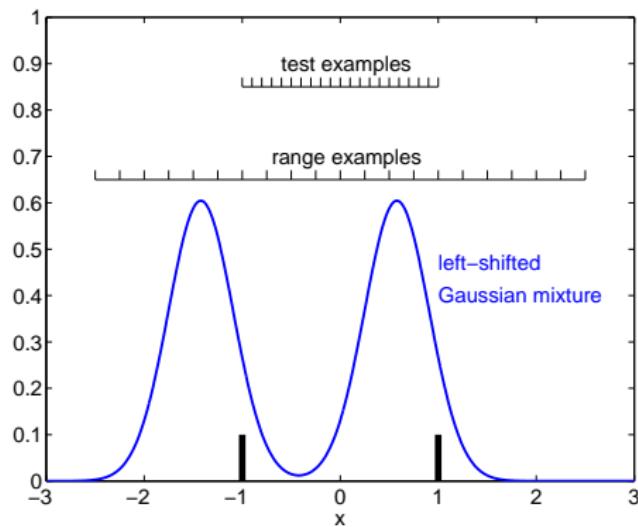
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$$\begin{aligned} \hat{p}(y = 1|\mu^{\text{new}}) &> \hat{p}(y = 1|\text{low}^{\text{new}}) \\ &> \hat{p}(y = 1|\mu) \approx \hat{p}(y = 1|\text{low}) \\ &\approx \hat{p}(y = 1|\text{high}) \gg \hat{p}(y = 1|\text{random}) \end{aligned}$$

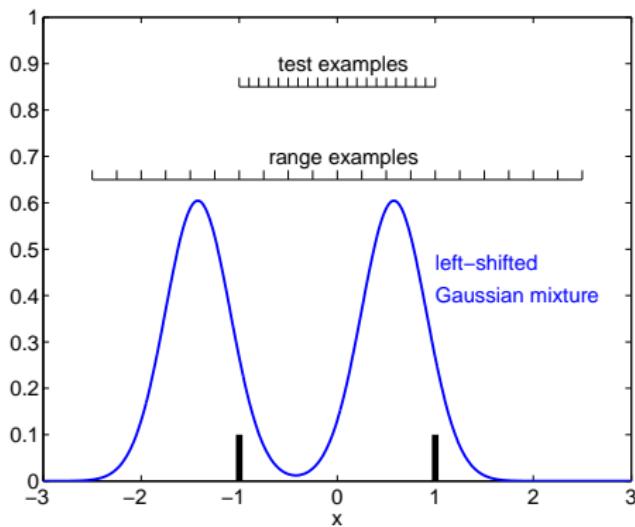
Zhu et al. 2007: mixture model?



blocks

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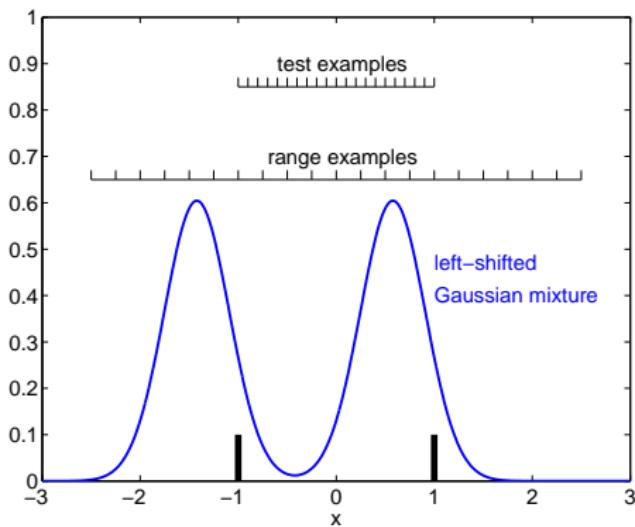
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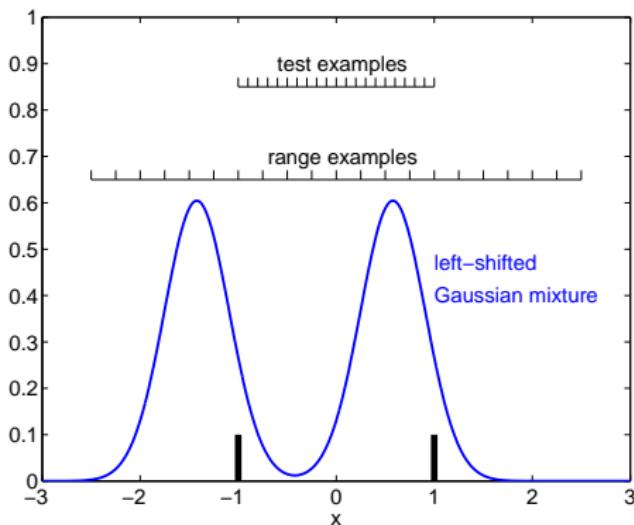
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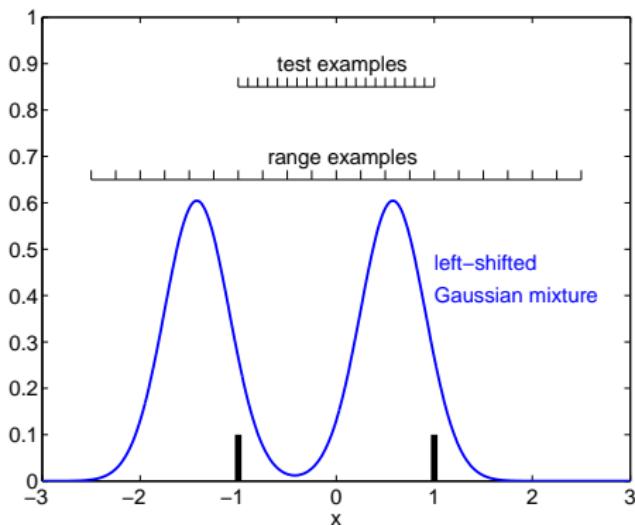
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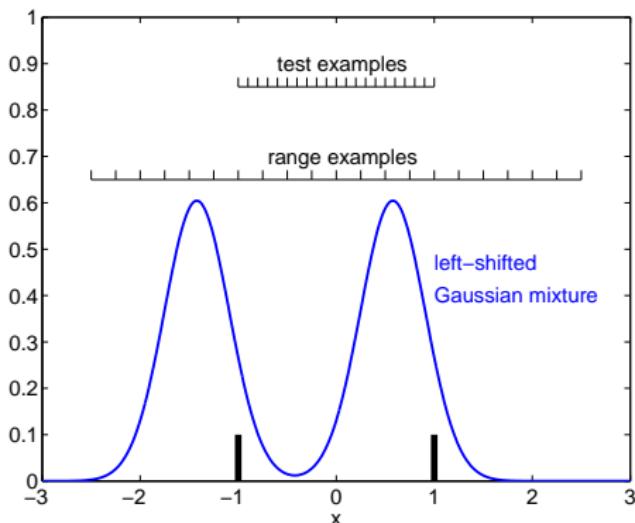
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- ➍ test 2: same as test 1

Zhu et al. 2007: mixture model?



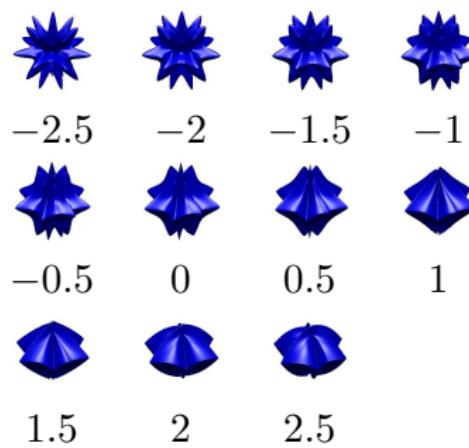
blocks

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

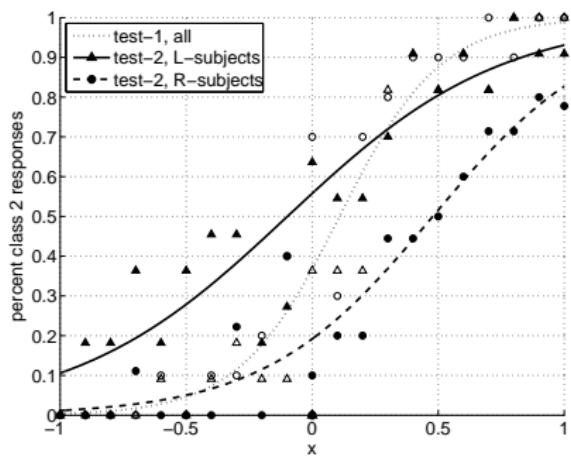
12 participants left-offset, 10 right-offset. Record their decisions and response times.

Visual stimuli

Stimuli parametrized by a continuous scalar x . Some examples:



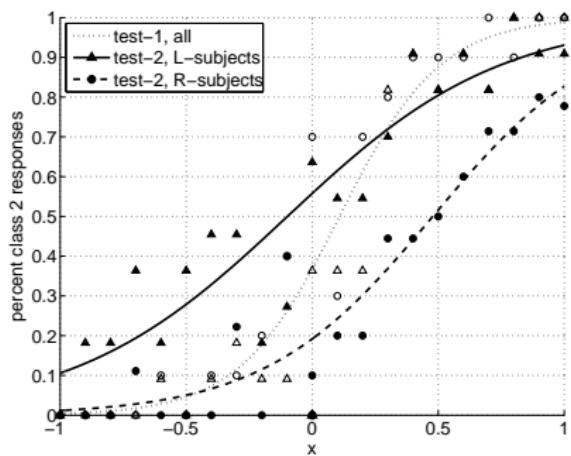
Observation 1: unlabeled data affects decision boundary



average decision boundary

- after seeing labeled data: $x = 0.11$

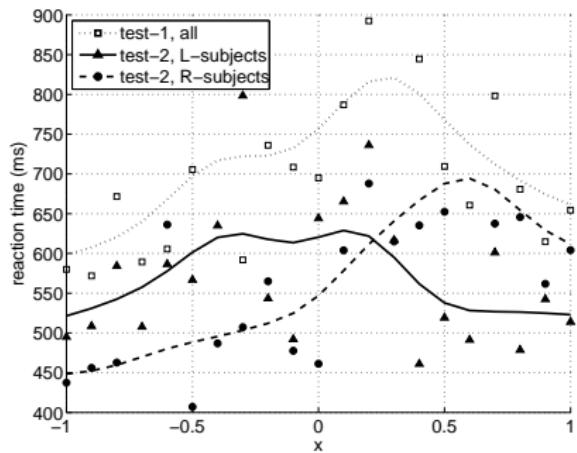
Observation 1: unlabeled data affects decision boundary



average decision boundary

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

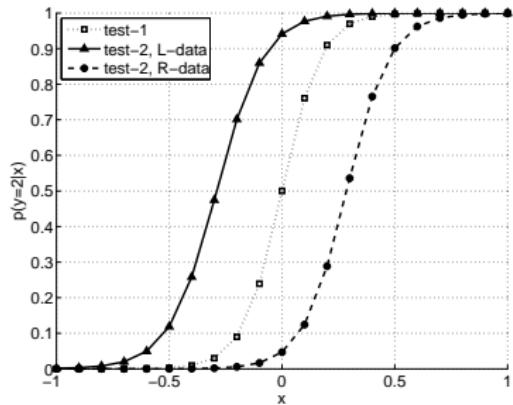
Observation 2: unlabeled data affects reaction time



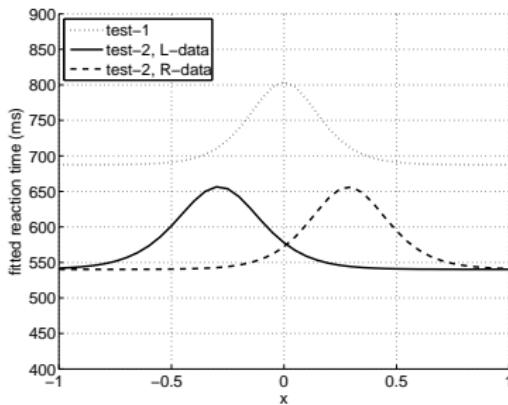
longer reaction time → harder example → closer to decision boundary.
 Reaction times too suggest decision boundary shift.

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.