

Semi-Supervised Learning: A Brief Survey



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Outline

- Introduction to Semi-Supervised Learning
- Semi-Supervised Learning Algorithms
 - Self-training
 - Co-training
 - Multiview Learning
 - Fuzziness based Semi-Supervised Learning
 - EM with generative mixture models
 - Semi-supervised support vector machine and Entropy regularization
 - Graph-based SSL
- Which semi-supervised learning method should I use?
- Some Challenges for Future Research

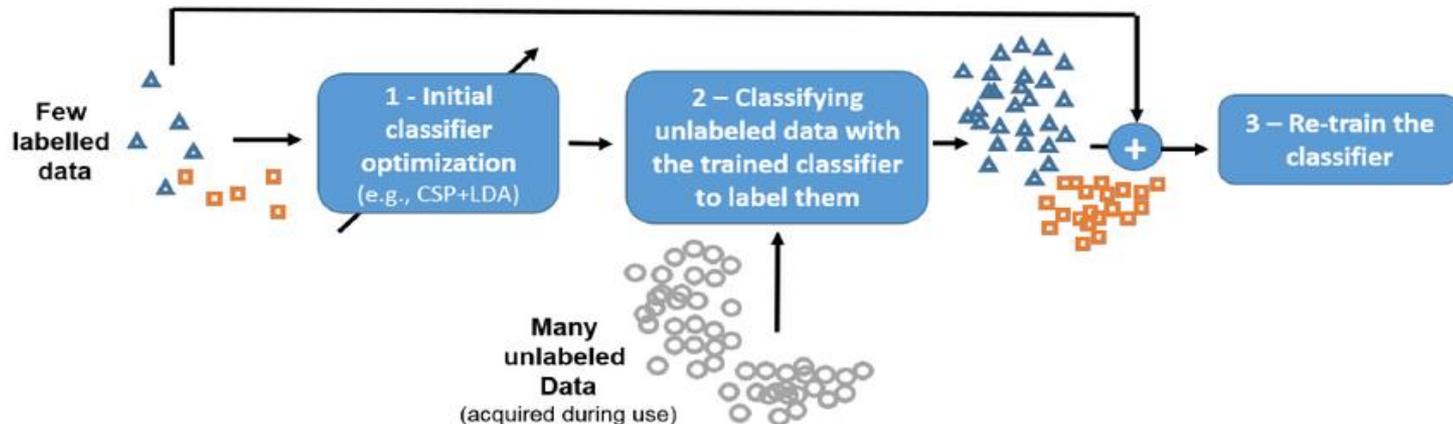
Disclaimer:

Some of the pictures and slides are taken from Xiaojin Zhu's(University of Wisconsin, Madison, USA) presentation slides.

Introduction to Semi-Supervised Learning

The Traditional View:

- Labeled instances are difficult to get
 - Expensive and time consuming to obtain.
 - They require the effort of experienced human annotator.
- Unlabeled data is cheap
- **Semi-supervised learning** is a class of supervised learning tasks and techniques that also make use of unlabeled data for training
- 1965, Scudder



Introduction to Semi-Supervised Learning

- Why Semi-supervised learning?
- The learning problem
 - Goal: Using both labeled and unlabeled data to build better learners, then using each one alone.

Notation:

- input features x , label y
- learner $f : \mathcal{X} \mapsto \mathcal{Y}$
- labeled data $(X_l, Y_l) = \{(x_{1:l}, y_{1:l})\}$
- unlabeled data $X_u = \{x_{l+1:n}\}$
- usually $l \ll n$

How can X_u help?

Introduction to Semi-Supervised Learning

- The landscape

supervised learning (classification, regression)

$$\{(x_{1:n}, y_{1:n})\}$$



semi-supervised classification/regression

$$\{(x_{1:l}, y_{1:l}), x_{l+1:n}\}$$



semi-supervised clustering $\{x_{1:n}, \text{must-}, \text{cannot-links}\}$

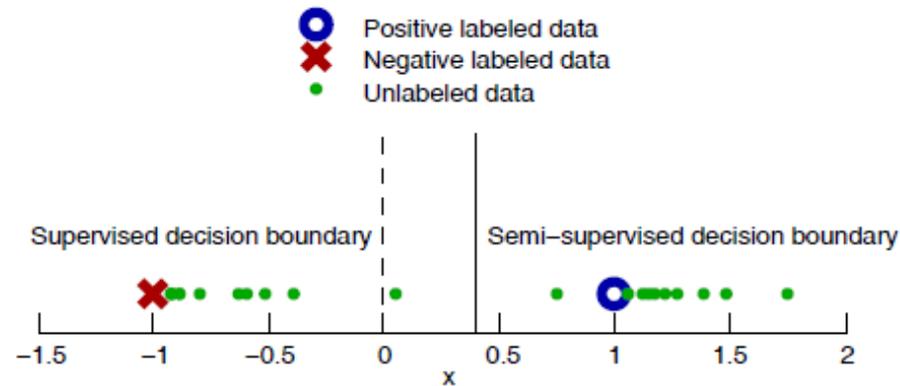


unsupervised learning (clustering) $\{x_{1:n}\}$

transduction (limited to $x_{1:n}$) \leftrightarrow induction (unseen data)

Introduction to Semi-Supervised Learning

How can unlabeled data ever help?



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

Semi-Supervised Learning Algorithms- Self-training

Self-training:

1. Train f from (X_l, Y_l)
 2. Predict on $x \in X_u$
 3. Add $(x, f(x))$ to labeled data
 4. Repeat
- Variations in Self-training
 - Add a few most confident $(x, f(x))$ to labeled data
 - Add all $(x, f(x))$ to labeled data
 - Add all $(x, f(x))$ to labeled data, weigh each by confidence

Semi-Supervised Learning Algorithms-Self-training

Self-training example: image categorization

1. Train a naïve Bayes classifier on the two initial labeled images



2. Classify unlabeled data, sort by confidence $\log p(y = \text{astronomy} | x)$



Semi-Supervised Learning Algorithms-Self-training

Self-training example: image categorization

3. Add the most confident images and **predicted** labels to labeled data



4. Re-train the classifier and repeat



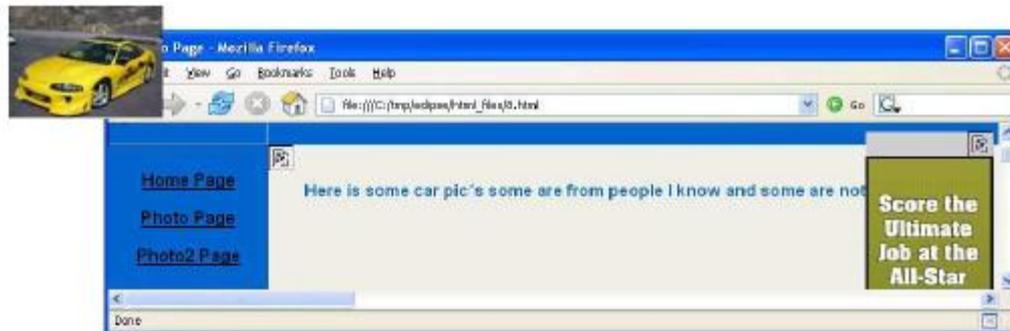
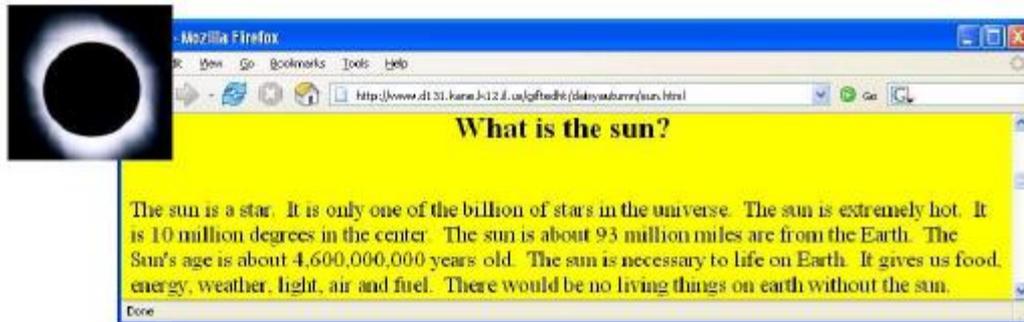
Semi-Supervised Learning Algorithms-Self-training

- Advantages of Self-training
 - The simplest semi-supervised learning method.
 - A wrapper method, applies to existing (complex) classifiers.
 - Often used in real tasks like natural language processing.
- Disadvantages of Self-training
 - Early mistakes could reinforce themselves.
 - ▶ Heuristic solutions, e.g. “un-label” an instance if its confidence falls below a threshold.
 - Cannot say too much in terms of convergence.
 - ▶ But there are special cases when self-training is equivalent to the Expectation-Maximization (EM) algorithm.
 - ▶ There are also special cases (e.g., linear functions) when the closed-form solution is known.

Co-training

Co-training

Two views of an item: image and HTML text



Co-training

Feature split

Each instance is represented by two sets of features $x = [x^{(1)}; x^{(2)}]$

- $x^{(1)}$ = image features
- $x^{(2)}$ = web page text
- This is a natural feature split (or multiple views)

Co-training idea:

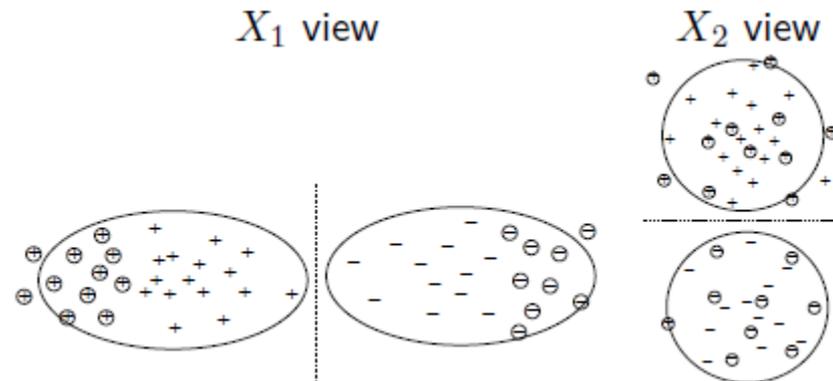
- Train an image classifier and a text classifier
- The two classifiers teach each other

Co-training

Co-training assumptions

Assumptions

- feature split $x = [x^{(1)}; x^{(2)}]$ exists
- $x^{(1)}$ or $x^{(2)}$ alone is sufficient to train a good classifier
- $x^{(1)}$ and $x^{(2)}$ are conditionally independent given the class



Co-training

Co-training algorithm

Co-training algorithm

- 1 Train two classifiers: $f^{(1)}$ from $(X_l^{(1)}, Y_l)$, $f^{(2)}$ from $(X_l^{(2)}, Y_l)$.
- 2 Classify X_u with $f^{(1)}$ and $f^{(2)}$ separately.
- 3 Add $f^{(1)}$'s k -most-confident $(x, f^{(1)}(x))$ to $f^{(2)}$'s labeled data.
- 4 Add $f^{(2)}$'s k -most-confident $(x, f^{(2)}(x))$ to $f^{(1)}$'s labeled data.
- 5 Repeat.

Co-training

Pros and cons of co-training

Pros

- Simple wrapper method. Applies to almost all existing classifiers
- Less sensitive to mistakes than self-training

Cons

- Natural feature splits may not exist
- Models using BOTH features should do better

Co-training

Variants of co-training

Co-EM: add all, not just top k

- Each classifier probabilistically label X_u
- Add (x, y) with weight $P(y|x)$

Fake feature split

- create random, artificial feature split
- apply co-training

Multiview: agreement among multiple classifiers

- no feature split
- train multiple classifiers of different types
- classify unlabeled data with all classifiers
- add majority vote label

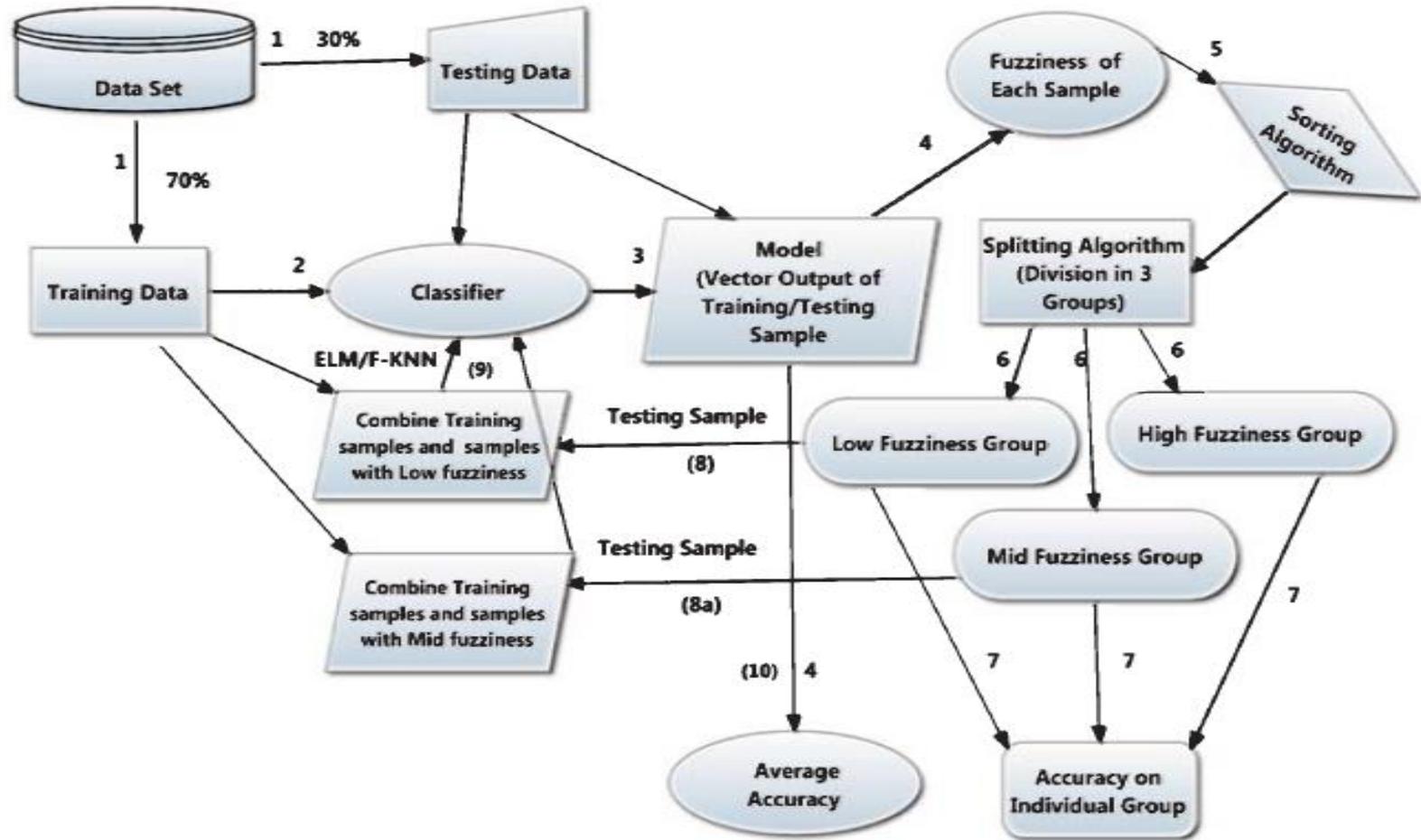
Multiview Learning

A regularized risk minimization framework to encourage multi-learner agreement:

$$\min_f \sum_{v=1}^M \left(\sum_{i=1}^l c(y_i, f_v(x_i)) + \lambda_1 \|f\|_K^2 \right) + \lambda_2 \sum_{u,v=1}^M \sum_{i=l+1}^n (f_u(x_i) - f_v(x_i))^2$$

M learners. $c()$ is the loss function, e.g., hinge loss.

Fuzziness based semi-supervised learning



- **EM with generative mixture models**

Fuzzy Cluster

- In hard clustering methods
 - Every data object is assigned to exactly one cluster
- Some applications may need for fuzzy or soft cluster assignment
 - Ex. An e-game could belong to both entertainment and software
- Example: Popularity of cameras is defined as a fuzzy mapping

Camera	Sales (units)
<i>A</i>	50
<i>B</i>	1320
<i>C</i>	860
<i>D</i>	270

$$\text{Pop}(o) = \begin{cases} 1 & \text{if 1,000 or more units of } o \text{ are sold} \\ \frac{i}{1000} & \text{if } i \text{ (} i < 1000 \text{) units of } o \text{ are sold} \end{cases}$$

- Then, $A(0.05)$, $B(1)$, $C(0.86)$, $D(0.27)$

Fuzzy (Soft) Clustering

- Example: Let cluster features be
 - C_1 :“digital camera” and “lens”
 - C_2 : “computer“

Review-id	Keywords
R_1	digital camera, lens
R_2	digital camera
R_3	lens
R_4	digital camera, lens, computer
R_5	computer, CPU
R_6	computer, computer game

$$M = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ \frac{2}{3} & \frac{1}{3} \\ 0 & 1 \\ 0 & 1 \end{bmatrix}$$

- Fuzzy clustering
 - k fuzzy clusters C_1, \dots, C_k , represented as a partition matrix $M = [w_{ij}]$
 - P1: for each object o_i and cluster C_j , $0 \leq w_{ij} \leq 1$ (fuzzy set)
 - P2: for each object o_i , $\sum_{j=1}^k w_{ij} = 1$, equal participation in the clustering
 - P3: for each cluster C_j , $0 < \sum_{i=1}^n w_{ij} < n$ ensures there is no empty cluster

- Let c_1, \dots, c_k as the center of the k clusters

- For an object o_i , sum of the squared error (SSE), p is a parameter:

- For a cluster C_j , SSE:
$$SSE(C_j) = \sum_{i=1}^n w_{ij}^p \text{dist}(o_i, c_j)^2 \quad SSE(o_i) = \sum_{j=1}^k w_{ij}^p \text{dist}(o_i, c_j)^2$$

- Measure how well a clustering fits the data:

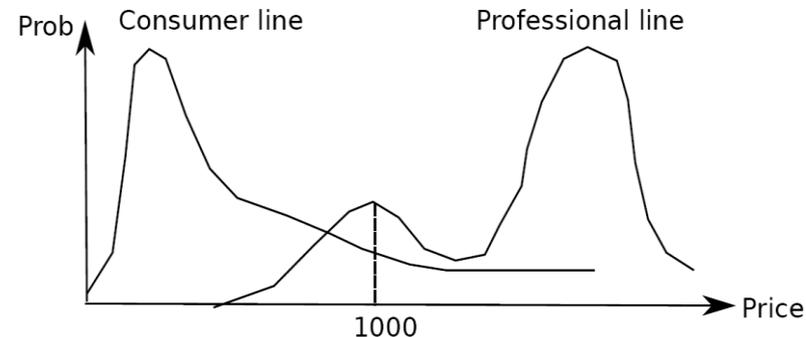
$$SSE(C) = \sum_{i=1}^n \sum_{j=1}^k w_{ij}^p \text{dist}(o_i, c_j)^2$$

Probabilistic Model-Based Clustering

- Cluster analysis is to find hidden categories.
- A hidden category (i.e., *probabilistic cluster*) is a distribution over the data space, which can be mathematically represented using a probability density function (or distribution function).

- Ex. 2 categories for digital cameras sold

- consumer line vs. professional line
- density functions f_1, f_2 for C_1, C_2
- obtained by probabilistic clustering



- A **mixture model** assumes that a set of observed objects is a mixture of instances from multiple probabilistic clusters, and conceptually each observed object is generated independently
- **Our task:** infer a set of k probabilistic clusters that is most likely to generate D using the above data generation process

Probabilistic Model-Based Clustering

- A set \mathbf{C} of k probabilistic clusters C_1, \dots, C_k with probability density functions f_1, \dots, f_k , respectively, and their probabilities $\omega_1, \dots, \omega_k$.
- Probability of an object o generated by cluster C_j is $P(o|C_j) = \omega_j f_j(o)$
- Probability of o generated by the set of cluster \mathbf{C} is $P(o|\mathbf{C}) = \sum_{j=1}^k \omega_j f_j(o)$
- Since objects are assumed to be generated independently, for a data set $D = \{o_1, \dots, o_n\}$, we have,

$$P(D|\mathbf{C}) = \prod_{i=1}^n P(o_i|\mathbf{C}) = \prod_{i=1}^n \sum_{j=1}^k \omega_j f_j(o_i)$$

- Task: Find a set \mathbf{C} of k probabilistic clusters s.t. $P(D|\mathbf{C})$ is maximized
- However, maximizing $P(D|\mathbf{C})$ is often intractable since the probability density function of a cluster can take an arbitrarily complicated form
- To make it computationally feasible (as a compromise), assume the probability density functions being some parameterized distributions

Univariate Gaussian Mixture Model

- $O = \{o_1, \dots, o_n\}$ (n observed objects), $\Theta = \{\theta_1, \dots, \theta_k\}$ (parameters of the k distributions), and $P_j(o_i | \theta_j)$ is the probability that o_i is generated from the j -th distribution using parameter θ_j , we have

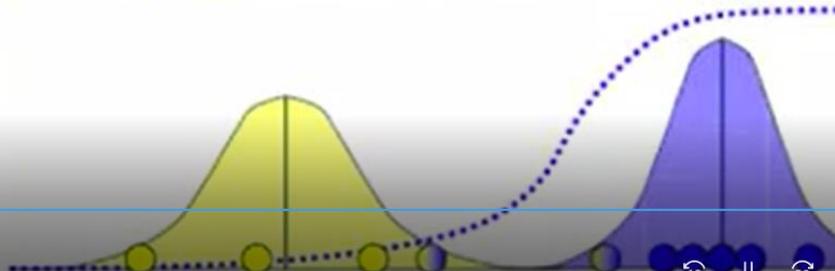
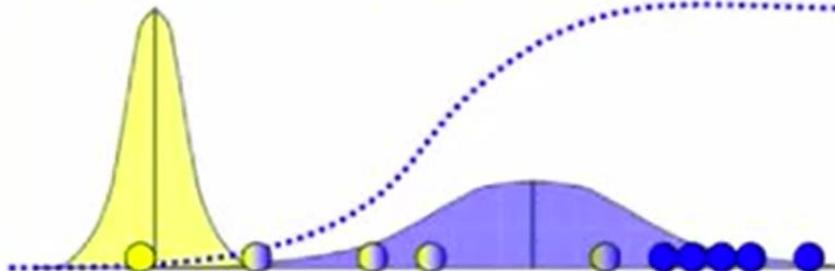
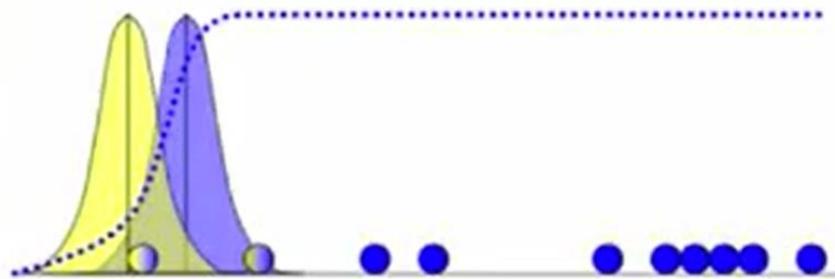
$$P(o_i | \Theta) = \sum_{j=1}^k \omega_j P_j(o_i | \Theta_j) \quad P(\mathbf{O} | \Theta) = \prod_{i=1}^n \sum_{j=1}^k \omega_j P_j(o_i | \Theta_j)$$

- Univariate Gaussian mixture model
 - Assume the probability density function of each cluster follows a 1-d Gaussian distribution. Suppose that there are k clusters.
 - The probability density function of each cluster are centered at μ_j with standard deviation σ_j , $\theta_j = (\mu_j, \sigma_j)$, we have

$$P(o_i | \Theta_j) = \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma_j^2}} \quad P(o_i | \Theta) = \sum_{j=1}^k \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma_j^2}}$$
$$P(\mathbf{O} | \Theta) = \prod_{i=1}^n \sum_{j=1}^k \frac{1}{\sqrt{2\pi}\sigma_j} e^{-\frac{(o_i - \mu_j)^2}{2\sigma_j^2}}$$

Univariate Gaussian Mixture Model

EM: 1-d example



$$P(x_i | b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right)$$

$$b_i = P(b | x_i) = \frac{P(x_i | b)P(b)}{P(x_i | b)P(b) + P(x_i | a)P(a)}$$

$$a_i = P(a | x_i) = 1 - b_i$$

$$\mu_b = \frac{b_1 x_1 + b_2 x_2 + \dots + b_n x_n}{b_1 + b_2 + \dots + b_n}$$

$$\sigma_b^2 = \frac{b_1 (x_1 - \mu_b)^2 + \dots + b_n (x_n - \mu_b)^2}{b_1 + b_2 + \dots + b_n}$$

$$\mu_a = \frac{a_1 x_1 + a_2 x_2 + \dots + a_n x_n}{a_1 + a_2 + \dots + a_n}$$

$$\sigma_a^2 = \frac{a_1 (x_1 - \mu_a)^2 + \dots + a_n (x_n - \mu_a)^2}{a_1 + a_2 + \dots + a_n}$$

could also estimate priors:

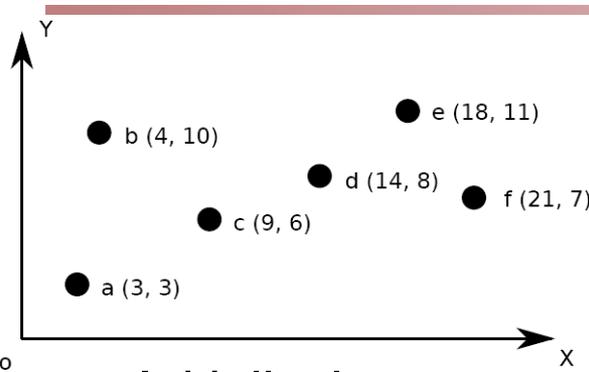
$$P(b) = (b_1 + b_2 + \dots + b_n) / n$$

$$P(a) = 1 - P(b)$$

The EM (Expectation Maximization) Algorithm

- The k-means algorithm has two steps at each iteration:
 - **Expectation Step** (E-step): Given the current cluster centers, each object is assigned to the cluster whose center is closest to the object: An object is *expected to belong to the closest cluster*
 - **Maximization Step** (M-step): Given the cluster assignment, for each cluster, the algorithm *adjusts the center* so that *the sum of distance* from the objects assigned to this cluster and the new center is minimized
- **The (EM) algorithm:** A framework to approach maximum likelihood or maximum a posteriori estimates of parameters in statistical models.
 - **E-step** assigns objects to clusters according to the current fuzzy clustering or parameters of probabilistic clusters
 - **M-step** finds the new clustering or parameters that maximize the sum of squared error (SSE) or the expected likelihood

Fuzzy Clustering Using the EM Algorithm



Iteration	E-step	M-step
1	$M^T = \begin{bmatrix} 1 & 0 & 0.48 & 0.42 & 0.41 & 0.47 \\ 0 & 1 & 0.52 & 0.58 & 0.59 & 0.53 \end{bmatrix}$	$c_1 = (8.47, 5.12),$ $c_2 = (10.42, 8.99)$
2	$M^T = \begin{bmatrix} 0.73 & 0.49 & 0.91 & 0.26 & 0.33 & 0.42 \\ 0.27 & 0.51 & 0.09 & 0.74 & 0.67 & 0.58 \end{bmatrix}$	$c_1 = (8.51, 6.11),$ $c_2 = (14.42, 8.69)$
3	$M^T = \begin{bmatrix} 0.80 & 0.76 & 0.99 & 0.02 & 0.14 & 0.23 \\ 0.20 & 0.24 & 0.01 & 0.98 & 0.86 & 0.77 \end{bmatrix}$	$c_1 = (6.40, 6.24),$ $c_2 = (16.55, 8.64)$

- Initially, let $c_1 = a$ and $c_2 = b$

- 1st E-step: assign o to c_1 , w. wt = $\frac{\frac{1}{dist(o,c_1)^2}}{\frac{1}{dist(o,c_1)^2} + \frac{1}{dist(o,c_2)^2}} = \frac{dist(o,c_2)^2}{dist(o,c_1)^2 + dist(o,c_2)^2}$
 - $w_{c,c_1} = \frac{41}{45+41} = 0.48$

- 1st M-step: recalculate the centroids according to the partition matrix, minimizing the sum of squared error (SSE)

$$c_j = \frac{\sum_{\text{each point } o} w_{o,c_j}^2 o}{\sum_{\text{each point } o} w_{o,c_j}^2} \quad c_1 = \left(\frac{1^2 \times 3 + 0^2 \times 4 + 0.48^2 \times 9 + 0.42^2 \times 14 + 0.41^2 \times 18 + 0.47^2 \times 21}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2}, \frac{1^2 \times 3 + 0^2 \times 10 + 0.48^2 \times 6 + 0.42^2 \times 8 + 0.41^2 \times 11 + 0.47^2 \times 7}{1^2 + 0^2 + 0.48^2 + 0.42^2 + 0.41^2 + 0.47^2} \right) = (8.47, 5.12)$$

- Iteratively calculate this until the cluster centers converge or the change is small enough

Computing Mixture Models with EM

- Given n objects $\mathbf{O} = \{o_1, \dots, o_n\}$, we want to mine a set of parameters $\Theta = \{\theta_1, \dots, \theta_k\}$ s.t., $P(\mathbf{O}|\Theta)$ is maximized, where $\theta_j = (\mu_j, \sigma_j)$ are the mean and standard deviation of the j -th univariate Gaussian distribution
- We initially assign random values to parameters θ_j , then iteratively conduct the E- and M- steps until converge or sufficiently small change
- At the E-step, for each object o_i , calculate the probability that o_i belongs to each distribution,

$$P(\Theta_j|o_i, \Theta) = \frac{P(o_i|\Theta_j)}{\sum_{l=1}^k P(o_i|\Theta_l)}$$

- At the M-step, adjust the parameters $\theta_j = (\mu_j, \sigma_j)$ so that the expected likelihood $P(\mathbf{O}|\Theta)$ is maximized

$$\mu_j = \sum_{i=1}^n o_i \frac{P(\Theta_j|o_i, \Theta)}{\sum_{l=1}^k P(\Theta_j|o_l, \Theta)} = \frac{\sum_{i=1}^n o_i P(\Theta_j|o_i, \Theta)}{\sum_{i=1}^n P(\Theta_j|o_i, \Theta)} \quad \sigma_j = \sqrt{\frac{\sum_{i=1}^n P(\Theta_j|o_i, \Theta)(o_i - \mu_j)^2}{\sum_{i=1}^n P(\Theta_j|o_i, \Theta)}}$$

Advantages and Disadvantages of Mixture Models

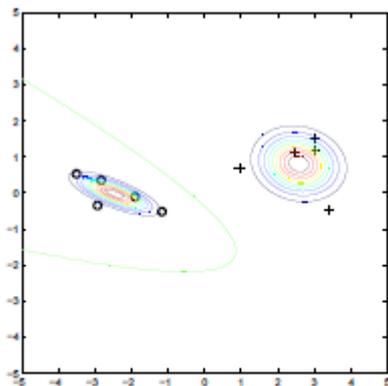
- Strength
 - Mixture models are more general than partitioning and fuzzy clustering
 - Clusters can be characterized by a small number of parameters
 - The results may satisfy the statistical assumptions of the generative models
- Weakness
 - Converge to local optimal (overcome: run multi-times w. random initialization)
 - Computationally expensive if the number of distributions is large, or the data set contains very few observed data points
 - Need large data sets
 - Hard to estimate the number of clusters

EM with generative mixture model

The MLE of θ without and with X_u is different.

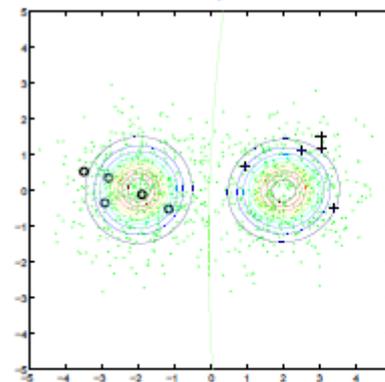
labeled data only

$$\begin{aligned} & \log p(X_l, Y_l | \theta) \\ &= \sum_{i=1}^l \log p(y_i | \theta) p(x_i | y_i, \theta) \end{aligned}$$



labeled and unlabeled

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



In principle X_u is useful for other generative models too.

Generative model for semi-supervised learning

Assumption

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

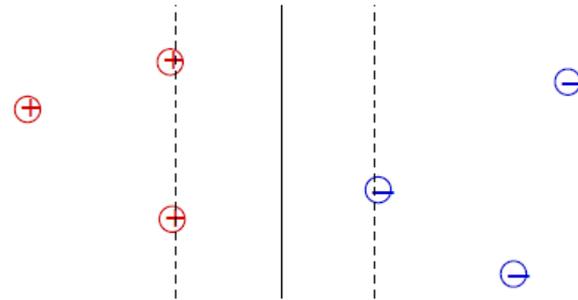
- joint and marginal likelihood

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

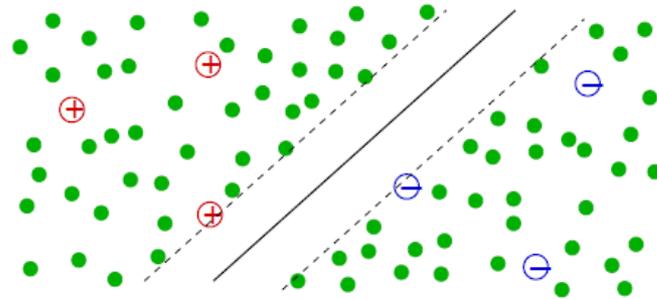
- find the maximum likelihood estimate (MLE) of θ , the maximum a posteriori (MAP) estimate, or be Bayesian
- common mixture models used in semi-supervised learning:
 - ▶ Mixture of Gaussian distributions (GMM) – image classification
 - ▶ Mixture of multinomial distributions (Naïve Bayes) – text categorization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

Semi-supervised Support Vector Machines

SVMs



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



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

Semi-supervised Support Vector Machines

S3VMs

Assumption

Unlabeled data from different classes are separated with large margin.

S3VM idea:

- Enumerate all 2^u possible labeling of X_u
- Build one standard SVM for each labeling (and X_l)
- Pick the SVM with the largest margin

Advantages and Disadvantages of SVMs

- Advantages
 - Applicable wherever SVMs are applicable.
 - Clear mathematical framework.
- Disadvantages
 - Optimization is difficult.
 - Can be trapped in bad local optima.
 - More modest assumption than generative model or graph-based methods, potentially lesser gain.

Entropy Regularization

- Assumption: if the two classes are well-separated, then $p(y|x)$ on any unlabeled instance should be close to 0 or 1.
- Entropy $H(p) = -p \log p - (1 - p) \log(1 - p)$ should be small
- entropy regularizer $\Omega(f) = \sum_{j=l+1}^{l+u} H(p(y = 1|\mathbf{x}_j, \mathbf{w}, b))$
- semi-supervised logistic regression

$$\min_{\mathbf{w}, b} \sum_{i=1}^l \log(1 + \exp(-y_i f(\mathbf{x}_i))) + \lambda_1 \|\mathbf{w}\|^2$$
$$+ \lambda_2 \sum_{j=l+1}^{l+u} H(1 / (1 + \exp(-f(\mathbf{x}_j))))$$

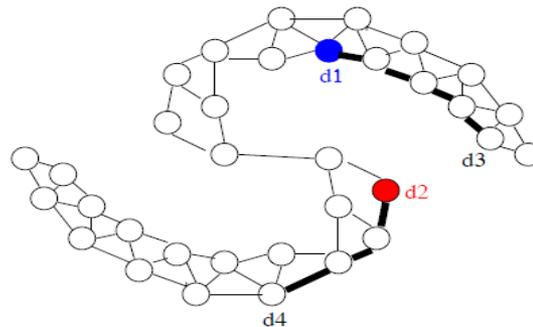
- The probabilistic counter part of S3VMs.

Graph-based semi-supervised learning

- Assumption
 - A graph is given on the labeled and unlabeled data. Instances connected by heavy edge tend to have the same label.

The graph

- Nodes: $X_l \cup X_u$
- Edges: similarity weights computed from features, e.g.,
 - ▶ k -nearest-neighbor graph, unweighted (0, 1 weights)
 - ▶ fully connected graph, weight decays with distance
 $w = \exp(-\|x_i - x_j\|^2 / \sigma^2)$
- Want: **implied** similarity via all paths



Graph-based semi-supervised learning

- Some graph-based algorithms
 - Mincut
 - Harmonic
 - Local and global consistency
 - Manifold regularization

Graph-based semi-supervised learning

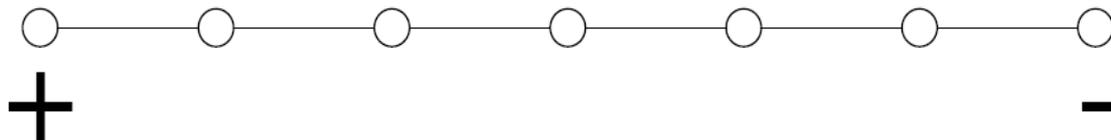
■ The mincut algorithm

The graph mincut problem:

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

$$\min_{Y \in \{0,1\}^n} \infty \sum_{i=1}^l (y_i - Y_{li})^2 + \sum_{ij} w_{ij} (y_i - y_j)^2$$

- Combinatorial problem, but has polynomial time solution.
- Mincut computes the **modes** of a Boltzmann machine
- There might be multiple modes
- One solution is to randomly perturb the weights, and average the results.



The harmonic function

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

- $f(x_i) = y_i$ for $i = 1 \dots l$
- f minimizes the energy

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

- 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 algorithm to compute harmonic function

One way to compute the harmonic function is:

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

This can be viewed as a special case of self-training too.

Problems with harmonic function

Harmonic solution has two issues

- It fixes the given labels Y_l
 - ▶ What if some labels are wrong?
 - ▶ Want to be flexible and disagree with given labels occasionally
- It cannot handle new test points directly
 - ▶ f is only defined on X_u
 - ▶ We have to add new test points to the graph, and find a new harmonic solution

Local and global consistency

- Allow $f(X_l)$ to be different from Y_l , but penalize it
- Introduce a balance between labeled data fit and graph energy

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

Manifold regularization

Manifold regularization solves the two issues

- Allows but penalizes $f(X_l) \neq Y_i$ using hinge loss
- Automatically applies to new test data
 - ▶ Defines function in kernel K induced RKHS:
 $f(x) = h(x) + b, h(x) \in \mathcal{H}_K$
- Still prefers low energy $f_{1:n}^\top \Delta f_{1:n}$

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

Manifold regularization algorithm

- 1 Input: kernel K , weights λ_1, λ_2 , (X_l, Y_l) , X_u
- 2 Construct similarity graph W from X_l, X_u , compute graph Laplacian Δ
- 3 Solve the optimization problem for $f(x) = h(x) + b, h(x) \in \mathcal{H}_K$

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

- 4 Classify a new test point x by $\text{sign}(f(x))$

Pros and Cons of Graph-based SSL

- Pros
 - Clear mathematical framework.
 - Performance is strong if the graph happens to fit the task
 - The (pseudo) inverse of the Laplacian can be viewed as a kernel matrix
 - Can be extended to directed graphs
- Cons
 - Performance is bad if the graph is bad
 - Sensitive to graph structure and edge weights

Which semi-supervised learning method should I use?

Ideally, one should use a method whose assumptions fit the problem structure.

- Do the classes produce well clustered data?

If yes, EM with generative mixture models may be a good choice.

- Do the features naturally split into two sets?

If yes, co-training may be appropriate.

- Is it true that two points with similar features tend to be in the same class?

If yes, graph-based methods can be used.

- Already using SVM?

Transductive SVM is a natural extension.

- Is the existing supervised classifier complicated and hard to modify?

Self-training is a practical wrapper method.

Future Direction

- Real SSL tasks
 - What tasks can be dramatically improved by SSL, so that new functionalities are enabled?
- New SSL assumptions

Generative models, multiview, graph methods, S3VMs

$$\sum_{i=1}^l \log p(y_i|\theta)p(x_i|y_i, \theta) + \lambda \sum_{i=l+1}^n \log \left(\sum_{y=1}^c p(y|\theta)p(x_i|y, \theta) \right)$$
$$\min_f \sum_{v=1}^M \left(\sum_{i=1}^l c(y_i, f_v(x_i)) + \lambda_1 \|f\|_K^2 \right) + \lambda_2 \sum_{u,v=1}^M \sum_{i=l+1}^n (f_u(x_i) - f_v(x_i))^2$$
$$\min_f \sum_{i=1}^l c(y_i, f(x_i)) + \lambda_1 \|f\|_K^2 + \lambda_2 \sum_{i,j=1}^n w_{ij} (f(x_i) - f(x_j))^2$$
$$\min_f \sum_{i=1}^l (1 - y_i f(x_i))_+ + \lambda_1 \|f\|_K^2 + \lambda_2 \sum_{i=l+1}^n (1 - |f(x_i)|)_+$$

Future Direction

What other assumptions can we make on unlabeled data? For example:

- label dissimilarity $y_i \neq y_j$

$$\sum_{i,j} w_{ij} (f(x_i) - s_{ij} f(x_j))^2$$

w_{ij} edge confidence; $s_{ij} = 1$: same label, -1 : different labels

- order preference $y_i - y_j \geq d$ for regression

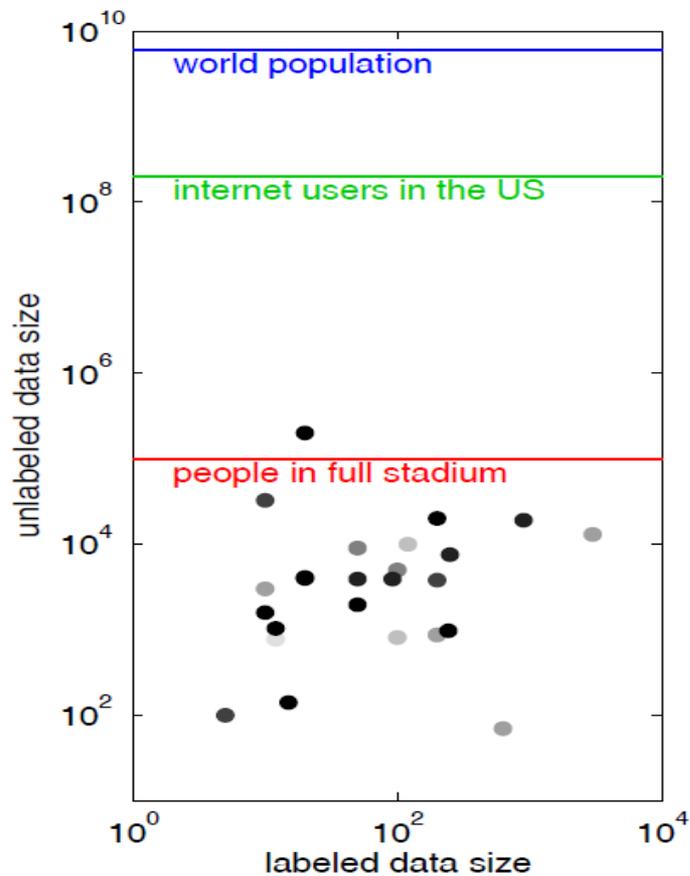
$$(d - (f(x_i) - f(x_j)))_+$$

New assumptions may lead to new SSL algorithms.

Future Direction

- Efficiency on huge unlabeled datasets

Some recent SSL datasets as reported in research papers:



Future Direction

Safe SSL

- How do we know that we are making the right model assumptions?
- Which semi-supervised learning method should I use?
- If I have labeled AND unlabeled data, I should do at least as well as only having the labeled data.

How can we make sure that SSL is “safe”?

References

- ① Olivier Chapelle, Alexander Zien, Bernhard Schölkopf (Eds.). (2006). *Semi-supervised learning*. MIT Press.
- ② Xiaojin Zhu (2005). *Semi-supervised learning literature survey*. TR-1530. University of Wisconsin-Madison Department of Computer Science.
- ③ Matthias Seeger (2001). *Learning with labeled and unlabeled data*. Technical Report. University of Edinburgh.

... and the references therein.

Thank you