Topics in Machine Learning Theory

Semi-Supervised Learning

Avrim Blum

Semi-Supervised Learning

- The main models we have been studying (PAC, mistake-bound) are for supervised learning.
  - Given labeled examples $S = \{(x_i, y_i)\}$, try to learn a good prediction rule.
- Unfortunately, labeled data is often expensive.
- On the other hand, unlabeled data is often plentiful and cheap.
  - Documents, images, OCR, web-pages, protein sequences, …

Can we use unlabeled data to help?

Semi-Supervised Learning

- Two scenarios: active learning and semi-supervised learning.
  - Active learning: have ability to ask for labels of unlabeled points of interest.
    - Can you do better than just ask for labels on random subset?
  - Semi-supervised learning: no querying. Just have lots of additional unlabeled data.
    - Will look today at SSL. This is the most puzzling one since unclear what unlabeled data can do for you.

Semi-Supervised Learning

Given a set L of labeled data and set U of unlabeled data. Can we use U to help?

- What can the unlabeled data possibly do for us?
- Abstract high-level answer we will get to is:
  - Going back to "Occam's razor", unlabeled data can help us improve our notion of what is simpler than what, by identifying regularities that appear in the data.
- But first:
  - Discuss several methods that have been developed for using unlabeled data to help.
  - Then will give an extension of PAC model to make sense of what's going on.

Plan for today

Methods:

- Co-training
- Transductive SVM
- Graph-based methods

Model:

- Augmented PAC model for SSL.

There's also a book "Semi-supervised learning" on the topic.

Co-training

[B&Mitchell'98] motivated by [Yarowsky'95]

Yarowsky's Problem & Idea:

- Some words have multiple meanings (e.g., "plant"). Want to identify which meaning was intended in any given instance.
- Standard approach: learn function from local context to desired meaning, using labeled data. "…nuclear power plant generated…"
- Idea: use fact that in most documents, multiple uses have same meaning. Use to transfer confident predictions over.

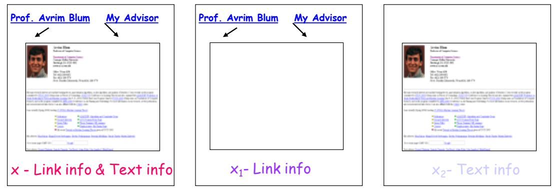
Co-training

Actually, many problems have a similar characteristic.

- Examples x can be written in two parts (x_1,x_2).
- Either part alone is in principle sufficient to produce a good classifer.
- E.g., speech+video, image and context, web page contents and links.
- So if confident about label for x_1, can use to impute label for x_2, and vice versa. Use each classifier to help train the other.

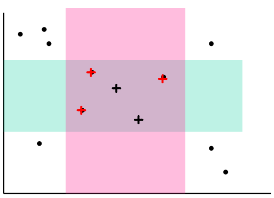
Example: classifying webpages

- Co-training: Agreement between two parts
  - examples contain two sets of features, i.e. an example is $x=\langle x_1, x_2\rangle$ and the belief is that the two parts of the example are sufficient and consistent, i.e. $\exists\ c_1, c_2$ such that $c_1(x_1)=c_2(x_2)=c(x)$



Example: intervals

Suppose $x_1 \in R$, $x_2 \in R$. $c_1 = [a_1,b_1]$, $c_2 = [a_2,b_2]$



Co-Training Theorems

- [BM98] if x_1, x_2 are independent given the label: $D = p(D_1^+ \times D_2^+) + (1-p)(D_1^- \times D_2^-)$, and if C is learnable from noisy data, then can learn from an initial "weakly-useful" h_1 plus unlabeled data.
- Def: h is weakly-useful if
  $$\Pr[h(x)=1|c(x)=1] > \Pr[h(x)=1|c(x)=0] + \varepsilon.$$
  (same as weak hyp if target c is balanced)
- E.g., say "syllabus" appears on 1/3 of course pages but only 1/6 of non-course pages.
- Idea: use as a noisy label of other view. (helpful trick: balance data so observed labels are 50/50)

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- [BB] in some cases (e.g., LTFs), you can use this to learn from a single labeled example.
  - Pick random hyperplane and boost (using above).
  - Repeat process multiple times.
  - Get 4 kinds of hyps: {close to c, close to $\neg$c, close to 1, close to 0}
  - Just need one labeled example to choose right one.

Co-Training Theorems

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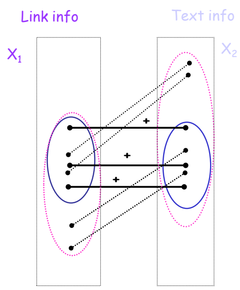
- [BB] in some cases (e.g., LTFs), you can use this to learn from a single labeled example.
- [BBY] if don't want to assume independence, and C is learnable from positive data only, then suffices for D^+ to have expansion.

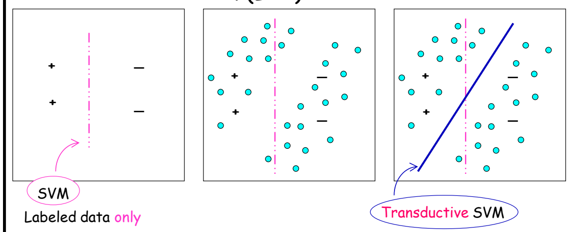
Co-Training and expansion

Want initial sample to expand to full set of positives after limited number of iterations.



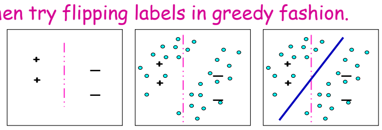
Transductive SVM [Joachims99]

- Suppose we believe target separator goes through low density regions of the space/large margin.
- Aim for separator with large margin wrt labeled and unlabeled data. (L+U)



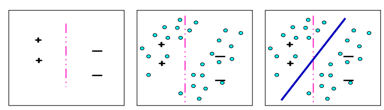
Transductive SVM [Joachims99]

- Suppose we believe target separator goes through low density regions of the space/large margin.
- Aim for separator with large margin wrt labeled and unlabeled data. (L+U)
- Unfortunately, optimization problem is now NP-hard. Algorithm instead does local optimization.
  - Start with large margin over labeled data. Induces labels on U.
  - Then try flipping labels in greedy fashion.



Transductive SVM [Joachims99]

- Suppose we believe target separator goes through low density regions of the space/large margin.
- Aim for separator with large margin wrt labeled and unlabeled data. (L+U)
- Unfortunately, optimization problem is now NP-hard. Algorithm instead does local optimization.
  - Also, recent work on polynomial-time approximation algorithms. ("furthest hyperplane problem")

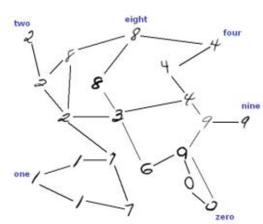


Graph-based methods

- Suppose we believe that very similar examples probably have the same label.
- If you have a lot of labeled data, this suggests a Nearest-Neighbor type of alg.
- If you have a lot of unlabeled data, suggests a graph-based method.

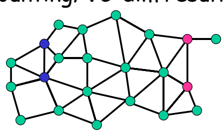
Graph-based methods

- Transductive approach. (Given L + U, output predictions on U).
- Construct a graph with edges between very similar examples.
- Solve for:
  - Minimum cut
  - Minimum "soft-cut" [ZhuGhahramaniLafferty]
  - Spectral partitioning



Graph-based methods

- Suppose just two labels: 0 & 1.
- Solve for labels f(x) for unlabeled examples x to minimize:
  - $\sum_{e=(u,v)}|f(u)-f(v)|$ [soln = minimum cut]
  - $\sum_{e=(u,v)}(f(u)-f(v))^2$ [soln = electric potentials]
- In case of min-cut, can use counting/VC-dim results to get confidence bounds.
  - VC-dimension of class of cuts of size k is $O(k/\lambda_{min})$, where λ_{min} is the minimum nontrivial cut in the graph. [Kleinberg]



How can we think about these approaches to using unlabeled data in a PAC-style model?

PAC-SSL Model [BB]

- Augment the notion of a concept class C with a notion of compatibility χ between a concept and the data distribution.
  - "learn C" becomes "learn (C,χ)" (i.e. learn class C under compatibility notion χ)
- Express relationships that one hopes the target function and underlying distribution will possess.
- Idea: use unlabeled data & the belief that the target is compatible to reduce C down to just {the highly compatible functions in C}.
  - Or, order the functions in C by compatibility.

PAC-SSL Model [BB]

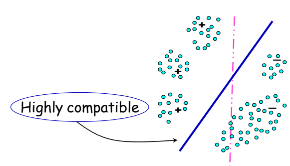
- Augment the notion of a concept class C with a notion of compatibility χ between a concept and the data distribution.
  - "learn C" becomes "learn (C,χ)" (i.e. learn class C under compatibility notion χ)
- To do this, need to be able to estimate compatibility of h with D from unlabeled data.
- Require that the degree of compatibility be something that can be estimated from a finite sample.

PAC-SSL Model [BB]

- Augment the notion of a concept class C with a notion of compatibility χ between a concept and the data distribution.
  - "learn C" becomes "learn (C,χ)" (i.e. learn class C under compatibility notion χ)
- Require χ to be an expectation over individual examples:
  - $\chi(h,D)=E_{x\sim D}[\chi(h, x)]$ = compatibility of h with D, $\chi(h,x) \in [0,1]$
  - $err_{unl}(h)=1-\chi(h, D)$ = incompatibility of h with D (unlabeled error rate of h)

Margins, Compatibility

- Margins: belief is that should exist a large margin separator.

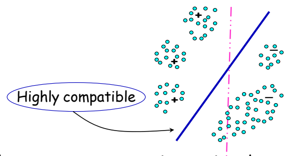


- Incompatibility of h and D (unlabeled error rate of h): the probability mass within distance γ of h.
- Can be written as an expectation over individual examples $\chi(h,D)=E_{x\sim D}[\chi(h,x)]$ where:
  - $\chi(h,x)=0$ if $dist(x,h) < \gamma$
  - $\chi(h,x)=1$ if $dist(x,h) > \gamma$

$$err_{unl}(h) = \Pr_{x\sim D}[dist(x,h) < \gamma]$$

Margins, Compatibility

- Margins: belief is that should exist a large margin separator.



- If do not want to commit to γ in advance, define $\chi(h,x)$ to be a smooth function of dist(x,h), e.g.:

$$\chi(h,x) = 1 - e^{\left[-\frac{dist(x,h)}{2\sigma^2}\right]} \qquad err_{unl}(h) = E_{x\sim D}\left[e^{\left[-\frac{dist(x,h)}{2\sigma^2}\right]}\right]$$

- Illegal notion of compatibility: the largest γ s.t. D has probability mass exactly zero within distance γ of h.

Co-Training, Compatibility

- Co-training: examples come as pairs $\langle x_1, x_2\rangle$ and the goal is to learn a pair of functions $\langle h_1, h_2\rangle$
- Hope is that the two parts of the example are consistent.
- Legal (and natural) notion of compatibility:
  - the compatibility of $\langle h_1, h_2\rangle$ and D:

$$\Pr_{\langle x_1,x_2\rangle \in D}[h_1(x_1) = h_2(x_2)]$$

  - can be written as an expectation over examples:

$$\chi(\langle h_1,h_2\rangle, \langle x_1,x_2\rangle) = 1 \text{ if } h_1(x_1) = h_2(x_2)$$

$$\chi(\langle h_1,h_2\rangle, \langle x_1,x_2\rangle) = 0 \text{ if } h_1(x_1) \neq h_2(x_2)$$

Sample Complexity - Uniform convergence bounds

Finite Hypothesis Spaces, Doubly Realizable Case

- Define $C_{D,\chi}(\varepsilon) = \{h \text{ in } C : err_{unl}(h) < \varepsilon\}$.

Theorem

If we see

$$m_u \geq \frac{1}{\varepsilon}\left[\ln|C| + \ln\frac{2}{\delta}\right]$$

unlabeled examples and

$$m_l \geq \frac{1}{\varepsilon}\left[\ln|C_{D,\chi}(\varepsilon)| + \ln\frac{2}{\delta}\right]$$

labeled examples, then with probability $\geq 1-\delta$, all $h \in C$ with $\widehat{err}(h) = 0$ and $\widehat{err}_{unl}(h) = 0$ have $err(h) \leq \varepsilon$.

- Bound the # of labeled examples as a measure of the helpfulness of D with respect to χ
  - a helpful distribution is one in which $C_{D,\chi}(\varepsilon)$ is small

Example

- Every variable is a positive indicator or negative indicator. No example has both kinds.
  - Algorithm: create graph on variables. Put an edge between two variables if any example has both of them.
  - Bad distribution: uniform over unit-vectors $\{e_i\}$.
  - Good distribution:
    - Small number of connected components.
    - Both classes have good "expansion".

More Generally

- Want algorithm that runs in poly time using samples poly in respective bounds.
- E.g., can think of:
  - ln|C| as # bits to describe target without knowing D,
  - $\ln|C_{D,\chi}(\varepsilon)|$ as number of bits to describe target knowing a good approx to D,

  under assumption that target has low unlabeled error rate.
- Can get analogous sample-complexity bounds when target is not perfectly compatible.

Infinite hypothesis spaces / VC-dimension

Infinite Hypothesis Spaces

Assume $\chi(h,x)$ in {0,1} and $\chi(C) = \{\chi_h : h \text{ in } C\}$ where $\chi_h(x) = \chi(h,x)$.

Two issues:

1. If we want uniform convergence of unlabeled error rates (all $h \in C$ have $|\widehat{err}_{unl}(h) - err_{unl}(h)| \leq \epsilon$) then we need unlabeled sample size to be large as a function of VC-dimension of $\chi(C)$.
2. For "size" of highly-compatible set, the max number of ways of splitting m points is not a good measure. Instead:

C[m,D]: expected # of splits of m points from D with concepts in C.

Infinite hypothesis spaces / VC-dimension

Infinite Hypothesis Spaces

Assume $\chi(h,x)$ in {0,1} and $\chi(C) = \{\chi_h : h \text{ in } C\}$ where $\chi_h(x) = \chi(h,x)$.

C[m,D] - expected # of splits of m points from D with concepts in C.

Theorem

$$m_u = O\left(\frac{VCdim\left(\chi(C)\right)}{\varepsilon^2}\log\frac{1}{\varepsilon} + \frac{1}{\varepsilon^2}\log\frac{2}{\delta}\right)$$

unlabeled examples and

$$m_l > \frac{2}{\varepsilon}\left[\log(2s) + \log\frac{2}{\delta}\right]$$

labeled examples, where

$$s = C_{D,\chi}(t + 2\varepsilon)[2m_l, D]$$

are sufficient so that with probability at least $1-\delta$, all $h \in C$ with $\widehat{err}(h) = 0$ and $\widehat{err}_{unl}(h) \le t + \varepsilon$ have $err(h) \le \varepsilon$, and furthermore all $h \in C$ have

$$|err_{unl}(h) - \widehat{err}_{unl}(h)| \le \varepsilon$$

Implication: If $err_{unl}(c^*) \le t$, then with probab. $\ge 1-\delta$, the $h \in C$ that optimizes both $\widehat{err}(h)$ and $\widehat{err}_{unl}(h)$ has $err(h) \le \varepsilon$.

ε-Cover-based bounds

- For algorithms that behave in a specific way:
  - first use the unlabeled data to choose a representative set of compatible hypotheses
  - then use the labeled sample to choose among these

Theorem

If t is an upper bound for $err_{unl}(c^*)$ and p is the size of a minimum ε − cover for $C_{D,\chi}(t + 4\varepsilon)$, then using

$$m_u = O\left(\frac{VCdim\left(\chi(C)\right)}{\varepsilon^2}log\frac{1}{\varepsilon} + \frac{1}{\varepsilon^2}log\frac{2}{\delta}\right)$$

unlabeled examples and

$$m_l = O\left(\frac{1}{\varepsilon}\ln\frac{p}{\delta}\right)$$

labeled examples, we can with probab. $\ge 1-\delta$ identify a hypothesis which is 10ϵ close to c^*.

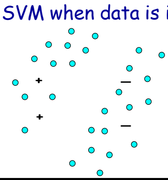
- Can result in much better bound than uniform convergence.

ε-Cover-based bounds

- For algorithms that behave in a specific way:
  - first use the unlabeled data to choose a representative set of compatible hypotheses
  - then use the labeled sample to choose among these

E.g., in case of co-training linear separators with independence assumption:
  - ε-cover of compatible set = {0, 1, c*, ¬c*}

E.g., Transductive SVM when data is in two blobs.



Ways unlabeled data can help in this model

- If the target is highly compatible with D and have enough unlabeled data to estimate χ over all h ∈ C, then can reduce the search space (from C down to just those h ∈ C whose estimated unlabeled error rate is low).
- By providing an estimate of D, unlabeled data can allow a more refined distribution-specific notion of hypothesis space size (such as Annealed VC-entropy or the size of the smallest ε-cover).
- If D is nice so that the set of compatible h ∈ C has a small ε-cover and the elements of the cover are far apart, then can learn from even fewer labeled examples than the 1/ε needed just to verify a good hypothesis.

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