15-859(B) Machine Learning Theory

Semi-Supervised Learning

Avrim Blum
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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.
- However, often labeled data is expensive.
- On the other hand, often unlabeled data is plentiful and cheap.
  - Documents, images, OCR, web-pages, protein sequences, …
- Can we use unlabeled data to help?

Semi-Supervised Learning

- Can we use unlabeled data to help?
- Two scenarios: active learning and semi-supervised learning.
  - Active learning: have ability to ask for labels of unlabeled points of interest.
  - Semi-supervised learning: no querying. Just have lots of additional unlabeled data.

Semi-Supervised Learning

Can we use unlabeled data to help?

- Unlabeled data is missing the most important info! But maybe still has useful regularities that we can use. E.g., OCR.

Semi-Supervised Learning

Can we use unlabeled data to help?

- This is a question a lot of people in ML have been interested in. A number of interesting methods have been developed.

Today:

- Discuss several methods for trying to use unlabeled data to help.
- 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

[Blum&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.

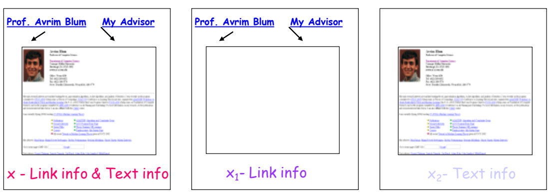
Co-training

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.

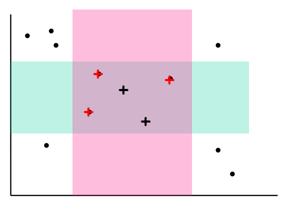
Example: classifying webpages

- 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 SQ-learnable, 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.

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- E.g., say "syllabus" appears on 1/3 of course pages but only 1/6 of non-course pages.
- Use as noisy label. Like classification noise with potentially asymmetric noise rates α, β.
- Can learn so long as $\alpha+\beta < 1-\varepsilon$.

  (helpful trick: balance data so observed labels are 50/50)

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- [BalcanB05] in some cases (e.g., LTFs), you can use this to learn from a single labeled example!

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  - Pick random hyperplane and boost (using above).
  - Repeat process multiple times.
  - Get 4 kinds of hyps: {close to c, close to ¬c, close to 1, close to 0}

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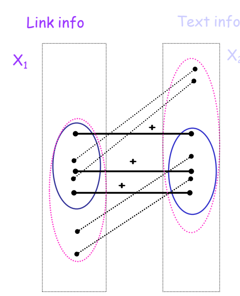
- [BalcanB05] in some cases (e.g., LTFs), you can use this to learn from a single labeled example!

- [BalcanBYang04] if don't want to assume indep, and C is learnable from positive data only, then suffices for D^+ to have expansion.

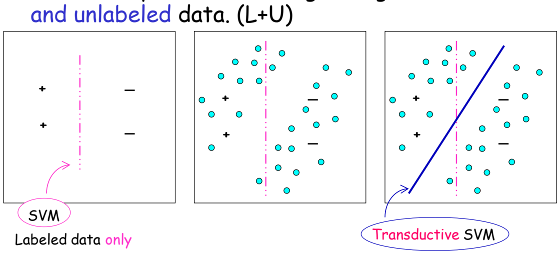
Co-Training and expansion

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



Transductive SVM [Joachims98]

- 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)



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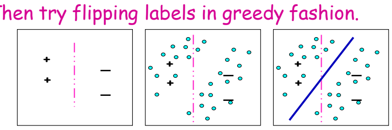
- Unfortunately, optimization problem is now NP-hard. Algorithm instead does local optimization.
  - Start with large margin over labeled data. Induces labels on U.
  - Then try flipping labels in greedy fashion.

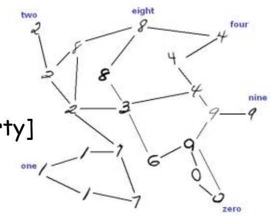


Graph-based methods

- 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.

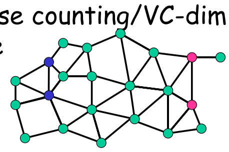
Graph-based methods

- 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.



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

PAC-SSL Model [BalcanB05]

- 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*}.

PAC-SSL Model [BalcanB05]

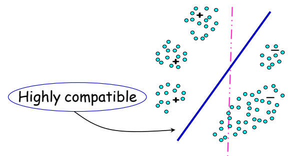
- Augment the notion of a concept class *C* with a notion of compatibility χ between a concept and the data distribution.
  - "learn *C*" becomes "learn (C,χ)" (i.e. learn class *C* under compatibility notion χ)
- To do this, need unlabeled data to allow us to uniformly estimate compatibilities well.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

PAC-SSL Model [BalcanB05]

- 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

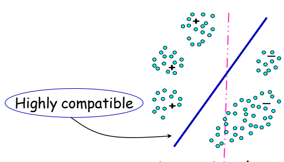
- Margins: belief is that should exist a large margin separator.



- 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 $\chi(h,D)=E_{x \in D}[\chi(h,x)]$ where:
  - $\chi(h,x)=0$ if $dist(x,h) \le \gamma$
  - $\chi(h,x)=1$ if $dist(x,h) \ge \gamma$

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.:

$$\chi(h,x) = 1 - e^{\left[-\frac{dist(x,h)}{2\sigma^2}\right]}$$

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

Theorem

If we see

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

unlabeled examples and

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

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

- 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.

Semi-Supervised Learning
Natural Formalization (PAC_χ)

- We will say an algorithm "PAC_χ-learns" if it 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, and $\ln|C_{D,\chi}(\varepsilon)|$ as number of bits to describe target knowing a good approximation to D, given the assumption that the target has low unlabeled error rate.

Target in C, but not fully compatible

Finite Hypothesis Spaces – c^* not fully compatible:

Theorem

Given $t \in [0,1]$, if we see

$$m_u \geq \frac{2}{\varepsilon^2}\left[\ln|C| + \ln\frac{4}{\delta}\right]$$

unlabeled examples and

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

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

Implication If $err_{unl}(c^*) \leq t$ and $err(c^*) = 0$ then with probability $\geq 1-\delta$ the $h \in C$ that optimizes $\widehat{err}(h)$ and $\widehat{err}_{unl}(h)$ has $err(h) \leq \epsilon$.

Infinite hypothesis spaces / VC-dimension

Infinite Hypothesis Spaces

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

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

Theorem

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

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 $\widehat{err}_{unl}(h) \leq t+\varepsilon$ have $err(h) \leq \varepsilon$, and furthermore all $h \in C$ have

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

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

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

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

unlabeled examples and

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

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

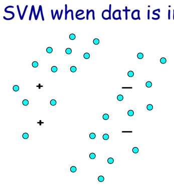
- Can result in much better bound than uniform convergence.

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 $h \in C$, then can reduce the search space (from C down to just those $h \in C$ 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 $h \in C$ has a small ε-cover and the elements of the cover are far apart, then can learn from even fewer labeled examples than the $1/\varepsilon$ needed just to verify a good hypothesis.