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Semi-Supervised Learning under Cluster Assumption

- f(X) is the optimal predictor of Y given P_{XY}
- Data: n labeled points $\stackrel{iid}{\sim} P_{XY}$, m unlabeled points $\stackrel{iid}{\sim} P_X$, $m \gg n$
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- Goal: learn f(X) from data
- The cluster assumption:
 - ▶ *P_X* is a mixture of components in *d*-dim
 - f(X) smooth on each component
 - ▶ γ is the margin (> 0 separation, < 0 overlap), characterizes difficulty of learning problem



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Given a finite labeled data, there are learning problems with small enough γ that SL fails, whereas perfect knowledge of components would yield small error.

Our Contributions

- Benefits of SSL not always revealed through asymptotic analysis and rates
- Instead, we quantify them with finite sample analysis
- We show SSL sometimes helps, sometimes not
- There are cases in which SSL has faster rates than SL

- $f_{m,n}$: predictor learned from m unlabeled and n labeled points
 - m = 0: supervised
 - m > 0: semi-supervised
 - $m = \infty$: oracle (full knowledge of P_X , but not f)

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$$R(f_{m,n}) = \mathbb{E}_{(X,Y) \sim P_{XY}} \left[\ell(f_{m,n}(X), Y) \right]$$

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• $\epsilon_{\infty,n,\gamma} \leq \epsilon_{m,n,\gamma} \leq \epsilon_{0,n,\gamma}$

Mathematical Formalization of Cluster Assumption

- Components (compact support, Lipschitz boundary)
- \bullet Density bounded from below and above, Hölder- α smooth



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p(x)

- Decision sets \mathcal{D} : all intersections of components
- Overall density jumps at decision set boundaries

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• Connectedness is almost as good as knowing the decision sets: Lemma: if $|\gamma| > Cm^{-1/d}$, then for all pairs x_1, x_2 not in a small tube around decision set boundaries, with large probability x_1, x_2 in same decision set if and only if $x_1 \leftrightarrow x_2$

SSL Error

Corollary: if $|\gamma| > Cm^{-1/d}$, then SSL is only "a bit worse" than oracle:

$$\epsilon_{m,n,\gamma} \le \epsilon_{\infty,n,\gamma} + O\left(nm^{-1/d}\right)$$

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- The value of unlabeled data: if $m \gg n$ s.t. $nm^{-1/d} \le \epsilon_{\infty,n,\gamma}$, then SSL is as good as Oracle.
 - if $\epsilon_{\infty,n,\gamma}$ decays polynomially, m must grow polynomially with n
 - if $\epsilon_{\infty,n,\gamma}$ decays exponentially, m must grow exponentially with n

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 - if $\epsilon_{\infty,n,\gamma}$ decays polynomially, m must grow polynomially with n
 - if $\epsilon_{\infty,n,\gamma}$ decays exponentially, m must grow exponentially with n
- If, in addition, Oracle is better than any ordinary SL

$$\epsilon_{\infty,n,\gamma} < \epsilon_{0,n,\gamma}$$

then SSL helps.

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- SL: if $\gamma > cn^{-1/d}$ then $\epsilon_{0,n,\gamma} = n^{-2\alpha/(2\alpha+d)}$, otherwise $\epsilon_{0,n,\gamma} = n^{-1/d}$ (worse: blur across decision sets).



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• SSL: if $|\gamma| > Cm^{-1/d}$ and $m \gg n^{2d}$, then the same as Oracle.



| margin | Oracle | SL | SSL | SSL |
|-------------------------------|----------------------------------|----------------------------------|----------------------------------|--------|
| | $\epsilon_{\infty,n,\gamma}$ | $\epsilon_{0,n,\gamma}$ | $\epsilon_{m,n,\gamma}$ | helps? |
| $n^{-\frac{1}{d}} \le \gamma$ | $n^{-\frac{2\alpha}{2\alpha+d}}$ | $n^{-\frac{2\alpha}{2\alpha+d}}$ | $n^{-\frac{2\alpha}{2\alpha+d}}$ | no |





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Thank you

Backup Slides

Singh, Nowak, Zhu (Wisconsin) Unlabeled data: Now it helps, now it doesn't

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Hölder Smoothness

If f is Hölder- α , then the $k = \lfloor \alpha \rfloor$ Taylor polynomial at x_0 , p_{k,f,x_0} , yields the approximation error bound:

$$|p_{k,f,x_0}(x) - f(x)| \le C|x - x_0|^{\alpha}$$

The Corollary

Even when $|\gamma| > Cm^{-1/d}$, the Lemma may fail for two reasons:

- One of the *n* labeled points or the test point falls in the small uncertain tube.
 - Volume of the tube $O(m^{-1/d})$
 - This is the probability that one point falls in the tube
 - Union bound gives $O(nm^{-1/d})$
 - Risk is bounded
 - The contribution to excess error is $O(nm^{-1/d})$

ullet With probability 1/m connectedness does not imply same decision set

- The contribution to excess error is O(1/m)
- Overall, $O(1/m+nm^{-1/d})\sim O(nm^{-1/d}).$

The lemma does not apply when $|\gamma| \leq Cm^{-1/d}$.