Unsupervised Learning under Latent Label Shift

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- Finding categories in unlabeled data is ill-posed.
 - Multiple ways to group the same data
- What principles can we use to determine the correct groupings?

Unlabeled examples



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Grouping by life stage



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Grouping by species



Instances that shift together group together

• Group together elements that shift together in prevalence across domains



Latent Label Shift (LLS)

• Label Shift Assumption: Class conditional distributions over samples remain domain invariant, while class prevalences may shift.

• For all $d, d' \in [r]$, $p_d(x|y) = p_{d'}(x|y)$

• **Goal:** Estimate $p_d(y)$ and $p_d(y|x)$.



- Consider mixing distribution Q in which domain is a random variable D.
 Then q(x, y|D = d) = p_d(x, y).
- If X takes on finite set of values [m], we model the mixture as the matrix product $Q_{X|D} = Q_{X|Y}Q_{Y|D}$, where
 - $Q_{X|D}$ holds the known marginals over X in each domain
 - $Q_{X|Y}$ holds the unknown class-conditional distributions
 - $Q_{Y|D}$ holds the unknown marginals over Y in each domain.
- Solving for unknown matrices via Non-negative Matrix Factorization (NMF) is not identified in general.

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Isomorphism to Topic Modeling

- Topic modeling considers documents as mixtures of topics.
 - Each topic has a word distribution (invariant over documents).
- LLS with finite set of values for X is isomorphic to topic modeling:
 - A domain is a document.
 - A label is a topic.
 - An example is a word.

• Topic modeling gives us the anchor word condition for identifiability:

• If each label Y has some input X which occurs with nonzero probability only under that label, the solution is identifiable. [Donoho & Stodden, 2003]

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Extension to Continuous Inputs

- No prior identifiability results for continuous X.
- **Our goal**: find a suitable **discretization** of the continuous space.
 - Resulting discrete problem will always satisfy label shift assumption.
 - If the discretized problem satisfies the anchor word assumption, we can apply discrete identifiability conditions to identify the solution.

- In Theorem 2, we give a set of sufficient conditions to identify $p_d(y)$ and $p_d(y|x)$:
 - Anchor subdomain condition: for each label, there is a region of X space with nonzero support in only this label.
 - Access to a domain discriminator: we assume we may query a function which predicts the distribution q(d|x) over domains for any value X.
 - Some other assumptions including rank assumptions on $Q_{Y|D}$.
- Discretization strategy:
 - Push density over X through the domain discriminator.
 - Match point masses in q(d|x) space to distinct discrete values.

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• We outline a practical algorithm to find $p_d(y)$ and $p_d(y|x)$.



1. Sample (input x, source domain d) data pairs



2. Train an estimate of a domain discriminator



3. Push samples through learned estimate



4. Cluster $\hat{q}(d|x)$ vectors into a finite number of clusters



5. Discretize using clusters, build $\widehat{Q}_{c(X)|D}$ matrix



6. Using NMF algorithm, decompose matrix



7. Estimate domain-specific classifier



Output: estimate of label-proportion matrix and domain-specific classifier.



Experiments

- Semi-synthetic experiments on CIFAR-10, CIFAR-20, ImageNet-50, FieldGuide-2, FieldGuide-28
 - Sample $Q_{Y|D}$, assign examples to different domains according to label prevalence, train a domain discriminator and evaluate recovery of labels.
 - Can achieve higher classification accuracy and lower error in recovering $Q_{Y|D}$ than baseline unsupervised approach SCAN, when $Q_{Y|D}$ sufficiently sparse and in datasets with few classes.



- Use domain structure to uncover categories in unlabeled data
- Leverage a strong connection to topic modeling to establish sufficient set of conditions for identifiability.
- Establish experimentally that domain structure aids class discovery.