Semi-supervised and transfer Learning

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Problem formulation of supervised learning.

- Input vector: $oldsymbol{x} = (x_1, x_2, \dots, x_d)^{ op} \in \mathbb{R}^d$
- Output: $y \in \mathbb{R}$
- $(\boldsymbol{x}_i, y_i) \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$
- Labeled data: $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
- Model: $f(x; w) = w^{\top}x$. (Linear model)

Risk: $R(w) = \iint loss(y, f(x; w))p(x, y)dxdy$ Empirical Risk: $R_{emp}(w) = \frac{1}{n} \sum_{i=1}^{n} loss(y_i, f(x_i; w))$ Empirical Risk Minimization (ERM): $\widehat{w} = argmin_w R_{emp}(w)$ Problem formulation of semi-supervised learning.

- $(\boldsymbol{x}_i, y_i) \stackrel{\text{i.i.d.}}{\sim} p(\boldsymbol{x}, y)$
- $\boldsymbol{x}_i \overset{ ext{i.i.d.}}{\sim} p(\boldsymbol{x})$
- Labeled data: $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
- Unlabeled data: $\{oldsymbol{x}_{n+1},oldsymbol{x}_{n+2},\ldots,oldsymbol{x}_{n+m}\}$
- Usually $n \ll m$ and n is small

Semi-supervised learning:

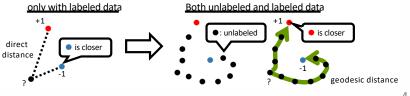
- We have both labeled and unlabeled samples.
- Semi-supervised learning uses both labeled and unlabeled samples.
- The unlabeled samples follow the same distribution of the marginal distribution of p(x,y)

Data generation process

- Input x is generated by a distribution with p(x).
- Output y for x is generated by conditional distribution with probability density p(y|x).

Unlabeled data can be used for capturing p(x)

• input data distribution, input space metric, or better representation.



Semi-supervised learning frameworks

- Weighted maximum likelihood estimation
- Graph-based learning
- Self-training
- Clustering
- Generative models

The original goal of MLE is to maximize:

where P(y|x; w) is a model. Each training instance is equally weighted.

Note, MLE is equivalent to maximize the negative log-likelihood function:

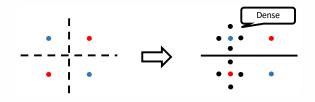
$$L(\boldsymbol{w}) = \log\left(\prod_{i=1}^{n} P(y_i | \boldsymbol{x}_i; \boldsymbol{w})\right) \propto \frac{1}{n} \sum_{i=1}^{n} \log(P(y_i | \boldsymbol{x}_i; \boldsymbol{w}))$$

Weighted maximum likelihood

Weighted maximum likelihood:

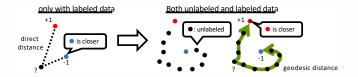
$$\max_{\boldsymbol{w}} \sum_{i=1}^{n} p(\boldsymbol{x}_i) \log(P(y_i | \boldsymbol{x}_i; \boldsymbol{w}))$$

- Each training data instance is weighted by $p(x_i)$.
- p(x) is estimated by using unlabeled data.
- Denser areas are largely weighted
- Training a classifier focusing on the dense areas



Graph-based method

- Basic idea: construct a graph capturing the intrinsic shape of input space, and make prediction on the graph.
- Assumption: Data lie on a manifold in the feature space
- The graph represent adjacency relationships among data
- K-nearest neighbor graph (e.g., $A_{ij} = \{0, 1\}$)
- Edge-weighted graph with e.g., $A_{ij} = \exp(-\|m{x}_i m{x}_j\|_2^2)$

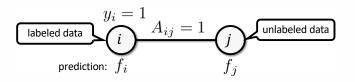


Basic idea: Adjacent instances tend to have the same label. Transductive setting (we have test instances)

$$\min_{f \in \mathbb{R}^{n+m}} \sum_{i=1}^{n} (f_i - y_i)^2 + \lambda \sum_{i=1}^{n+m} \sum_{j=1}^{n+m} A_{ij} (f_i - f_j)^2,$$

where $\lambda > 0$ is the regularization parameter.

- 1st term: (squared) loss function to fit to labeled data.
- 2nd term: regularization function to make adjacent nodes to have similar predictions.



Transfer Learning

Supervised Learning:

- Training $\{(\boldsymbol{x}_i^{\mathsf{tr}}, y_i^{\mathsf{tr}})\}_{i=1}^n \overset{\mathsf{i.i.d.}}{\sim} p_{\mathsf{tr}}(\boldsymbol{x}, y)$
- Test $(x^{\text{te}}, y^{\text{te}}) \stackrel{\text{i.i.d.}}{\sim} p_{\text{te}}(x, y)$ (Not observed during training)
- $p_{tr} = p_{te}$ (Training and test distributions are same)

Semi-supervised Learning:

- Training $\{(\boldsymbol{x}_{i}^{\mathrm{tr}}, y_{i}^{\mathrm{tr}})\}_{i=1}^{n} \stackrel{\text{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y), \\ \{\boldsymbol{x}_{i}^{\mathrm{tr}}\}_{i=n+1}^{n+m} \stackrel{\text{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}).$
- Test $(x^{te}, y^{te}) \stackrel{\text{i.i.d.}}{\sim} p_{te}(x, y)$ (Not observed during training)
- $p_{tr} = p_{te}$ (Training and test distributions are same)

If $p_{tr} \neq p_{te}$, supervised method and semi-supervised method do not perform well. A solution: Transfer Learning!

Unsupervised transfer learning

•
$$\{(\boldsymbol{x}_{i}^{\mathrm{tr}}, y_{i}^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \stackrel{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, \boldsymbol{y}),$$

• $\{m{x}_j^{ ext{te}}\}_{j=1}^{n_{ ext{te}}} \overset{ ext{l.l.d.}}{\sim} p_{ ext{te}}(m{x})$, $n_{ ext{tr}} \ll n_{ ext{te}}$

Supervised transfer learning

•
$$\{(\boldsymbol{x}_i^{\mathsf{tr}}, y_i^{\mathsf{tr}})\}_{i=1}^{n_{\mathsf{tr}}} \stackrel{\text{i.i.d.}}{\sim} p_{\mathsf{tr}}(\boldsymbol{x}, y)$$

• $\{({m x}_j^{ ext{te}},y_j^{ ext{te}})\}_{j=1}^{n_{ ext{te}}} \overset{ ext{i.i.d.}}{\sim} p_{ ext{te}}({m x},y)$, $n_{ ext{te}} \ll n_{ ext{tr}}$

Semi-supervised transfer learning

•
$$\{(\boldsymbol{x}_i^{\mathsf{tr}}, y_i^{\mathsf{tr}})\}_{i=1}^{n_{\mathsf{tr}}} \overset{\text{i.i.d.}}{\sim} p_{\mathsf{tr}}(\boldsymbol{x}, y)$$

- $\{(x_j^{\mathrm{te}}, y_j^{\mathrm{te}})\}_{j=1}^{n_{\mathrm{te}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{te}}(x, y)$, $n_{\mathrm{te}} \ll n_{\mathrm{tr}}$
- $\{x_j^{ ext{te}}\}_{j=n_{ ext{te}}+1}^{n_{ ext{te}}} \overset{ ext{i.i.d.}}{\sim} p_{ ext{te}}(x)$, $n_{ ext{tr}} \ll n_{ ext{te}}$

Unsupervised Transfer Learning

We assume

- It does not need to have test label
- Need some assumption

Standard approaches

- Importance weighted method (e.g., Covariate shift adaptation)
- Subspace based method.

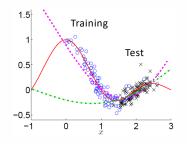
Covariate Shift Adaptation [1]

Problem setup:

•
$$\{(x_i^{tr}, y_i^{tr})\}_{i=1}^{n_{tr}} \stackrel{\text{i.i.d.}}{\sim} p_{tr}(x, y),$$

• $\{x_i^{te}\}_{j=1}^{n_{te}} \stackrel{\text{i.i.d.}}{\sim} p_{te}(x), n_{tr} \ll n_{te}$

Key idea: Learning a function so that error in test data is minimized under the assumption $p_{tr}(y|x) = p_{te}(y|x)$



Covariate Shift Adaptation

The risk for
$$p_{te}(x, y)$$
 can be written as

$$J(w) = \iint L(y, f(x)) p_{te}(x, y) dx dy$$

$$= \iint L(y, f(x)) \frac{p_{te}(x, y)}{p_{tr}(x, y)} p_{tr}(x, y) dx dy$$

$$= \iint L(y, f(x)) \frac{p_{te}(y|x) p_{te}(x)}{p_{tr}(y|x) p_{tr}(x)} p_{tr}(y, x) dx dy$$

$$= \iint L(y, f(x)) \frac{p_{te}(x)}{p_{tr}(x)} p_{tr}(y, x) dx dy$$

$$\approx \frac{1}{n_{tr}} \sum_{i=1}^{n_{tr}} L(y_i^{tr}, f(x_i^{tr})) \frac{p_{te}(x_i^{tr})}{p_{tr}(x_i^{tr})}$$

Actually, it is a weighted maximum likelihood problem. Note $\frac{p_{te}(\boldsymbol{x}_i^{tr})}{p_{tr}(\boldsymbol{x}_i^{tr})}$ is a ratio of probability densities (density-ratio).

Exponentially-flattened Importance weighted empirical risk minimization (IW-ERM) [1]:

$$\min_{f \in \mathcal{F}} \quad \frac{1}{n_{\mathsf{tr}}} \sum_{i=1}^{n_{\mathsf{tr}}} L(y_i^{\mathsf{tr}}, f(\boldsymbol{x}_i^{\mathsf{tr}})) \left(\frac{p_{\mathsf{te}}(\boldsymbol{x}_i^{\mathsf{tr}})}{p_{\mathsf{tr}}(\boldsymbol{x}_i^{\mathsf{tr}})}\right)^{\tau}$$

where 0 $\leq \tau \leq$ 1 is a tuning parameter for stabilizing the covariate shift adaptation.

- $\tau = 0 \rightarrow \text{ERM}$
- $0 < \tau < 1 \rightarrow$ Intermediate
- $\tau = 1 \text{ IW-ERM}$

Setting τ to 0 $<\tau<1$ is practically useful.

Relative Importance weighted empirical risk minimization (RIW-ERM) [2]:

$$\min_{f \in \mathcal{F}} \quad \frac{1}{n_{\mathsf{tr}}} \sum_{i=1}^{n_{\mathsf{tr}}} L(y_i^{\mathsf{tr}}, f(\boldsymbol{x}_i^{\mathsf{tr}})) \frac{p_{\mathsf{te}}(\boldsymbol{x}_i^{\mathsf{tr}})}{(1-\alpha)p_{\mathsf{te}}(\boldsymbol{x}_i^{\mathsf{tr}}) + \alpha p_{\mathsf{tr}}(\boldsymbol{x}_i^{\mathsf{tr}})}$$

where 0 $\leq \tau \leq$ 1 is a tuning parameter for stabilizing the covariate shift adaptation.

- $\alpha = \mathbf{0} \rightarrow \mathsf{ERM}$
- $0 < \alpha < 1 \rightarrow$ Intermediate
- $\alpha = 1$ IW-ERM

$$r_{lpha}(oldsymbol{x}) = rac{p_{\mathsf{te}}(oldsymbol{x})}{(1-lpha)p_{\mathsf{tr}}(oldsymbol{x}) + lpha p_{\mathsf{tr}}(oldsymbol{x})} < rac{1}{1-lpha}$$

The density ratio is bounded above by $1/(1-\alpha)$.

Importance Weighted Least Squares

The importance weighted least squares problem can be written as

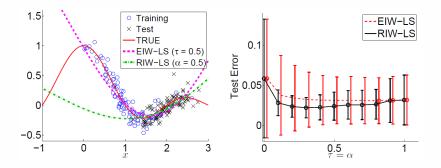
$$\min_{\boldsymbol{w}} \quad J(\boldsymbol{w}) = \frac{1}{n_{\mathsf{tr}}} \sum_{i=1}^{n_{\mathsf{tr}}} r(\boldsymbol{x}_i^{\mathsf{tr}}) \| y_i^{\mathsf{tr}} - \boldsymbol{w}^\top \boldsymbol{x}_i^{\mathsf{tr}} \|_2^2,$$

where r(x) is a weight function (e.g., density-ratio).

Take the derivative w.r.t. w and equating it to zero.

$$egin{aligned} rac{\partial J(oldsymbol{w})}{\partialoldsymbol{w}} &= -rac{2}{n_{ ext{tr}}}\sum_{i=1}^{n_{ ext{tr}}}r(oldsymbol{x}_i^{ ext{tr}})(y_i^{ ext{tr}}-oldsymbol{w}^ opoldsymbol{x}_i^{ ext{tr}})oldsymbol{x}_i^{ ext{tr}} &= oldsymbol{0} \ \widehat{oldsymbol{w}} &= \left(\sum_{i=1}^{n_{ ext{tr}}}r(oldsymbol{x}_i^{ ext{tr}})oldsymbol{x}_i^{ ext{tr}}oldsymbol{x}_i^{ ext{tr}}^ op\right)^{-1}\sum_{i=1}^{n_{ ext{tr}}}r(oldsymbol{x}_i^{ ext{tr}})y_i^{ ext{tr}}oldsymbol{x}_i^{ ext{tr}} \end{aligned}$$

Comparison of EIW-LS and RIW-LS:



Problem formulation:

- $\{(\boldsymbol{x}_i^{\mathsf{tr}}, y_i^{\mathsf{tr}})\}_{i=1}^{n_{\mathsf{tr}}} \overset{\text{i.i.d.}}{\sim} p_{\mathsf{tr}}(\boldsymbol{x}, y)$
- $\{(\pmb{x}_j^{\texttt{te}}, y_j^{\texttt{te}})\}_{j=1}^{n_{\texttt{te}}} \overset{\text{i.i.d.}}{\sim} p_{\texttt{te}}(\pmb{x}, y)$, $n_{\texttt{te}} \ll n_{\texttt{tr}}$

We assume to have a large number of training samples and a small number of paired target labeled samples.

- Frustratingly easy domain adaptation [3].
- Multi-task Learning
- Fine-tuning (Deep Learning)

Naive approach: Pooling training and test samples

$$egin{aligned} J(oldsymbol{w}) &= \iint \mathsf{loss}(y, f(oldsymbol{x}; oldsymbol{w})) p_\mathsf{te}(oldsymbol{x}, oldsymbol{y}) \mathsf{dx}\mathsf{dy} \ &= lpha \iint \mathsf{loss}(y, f(oldsymbol{x}; oldsymbol{w})) p_\mathsf{tr}(oldsymbol{x}, oldsymbol{y}) \mathsf{dx}\mathsf{dy} \ &+ (1-lpha) \iint \mathsf{loss}(y, f(oldsymbol{x}; oldsymbol{w})) p_\mathsf{te}(oldsymbol{x}, oldsymbol{y}) \mathsf{dx}\mathsf{dy} \ &\simeq rac{lpha}{n_\mathsf{tr}} \sum_{i=1}^{n_\mathsf{tr}} \mathsf{loss}(y_i^\mathsf{tr}, f(oldsymbol{x}_i^\mathsf{tr}; oldsymbol{w})) + rac{(1-lpha)}{n_\mathsf{te}} \sum_{j=1}^{n_\mathsf{te}} \mathsf{loss}(y_j^\mathsf{te}, f(oldsymbol{x}_j^\mathsf{te}; oldsymbol{w})) \end{aligned}$$

where $0 \le \alpha \le 1$ is a tuning parameter to control trade off between source and target errors.

Problem formulation:

• Task1:
$$\{(x_i^{(1)}, y_i^{(1)})\}_{i=1}^{n_1} \overset{\text{i.i.d.}}{\sim} p_1(x, y)$$

- ...
- $\mathsf{Task}M$: $\{(oldsymbol{x}_{j}^{(M)}, y_{j}^{(M)})\}_{j=1}^{n_{M}}\overset{\mathrm{i.i.d.}}{\sim}p_{M}(oldsymbol{x}, y)$
- Linear Models: $f_1(x^{(1)}) = w_1^{\top} x^{(1)}, f_2(x^{(2)}) = w_2^{\top} x^{(2)}, \dots, f_M(x^{(M)}) = w_M^{\top} x^{(M)}$

 $\min_{\boldsymbol{w}_1,\ldots,\boldsymbol{w}_M} \quad \sum_{m=1}^M \frac{1}{n_m} \sum_{i=1}^{n_m} \operatorname{loss}(y_i^{(m)}, f_m(\boldsymbol{x}^{(m)})) + \lambda R(\boldsymbol{w}_1,\ldots,\boldsymbol{w}_M).$

where $R(\boldsymbol{w}_1,\ldots,\boldsymbol{w}_M)$ is a regularizer.

- $\lambda = 0$: Independently optimize ws
- $\lambda > 0$: We share some information among models.

Multi-task Learning

Multi-task learning optimization (Graph-Laplacian).

$$\min_{\boldsymbol{w}_1,...,\boldsymbol{w}_M} \quad \sum_{m=1}^M \frac{1}{n_m} \sum_{i=1}^{n_m} \log(y_i^{(m)}, f_m(\boldsymbol{x}_i^{(m)})) + \lambda \sum_{m=1}^M \sum_{m'=1}^M r_{m,m'} \|\boldsymbol{w}_m - \boldsymbol{w}_{m'}\|_2^2.$$

where $r_{m,m'} \ge 0$ is a model parameter (similarity between models). If $r_{m,m'} > 0$, we make w_m and $w_{m'}$ close.

Other approach: Explicitly including shared parameter. We decompose $oldsymbol{w}_m = oldsymbol{w}_0 + oldsymbol{v}_m$

That is

•
$$f_1(x^{(1)}) = (w_0 + v_1)^\top x^{(1)}$$
,
• $f_2(x^{(2)}) = (w_0 + v_2)^\top x^{(2)}$

•
$$f_2(x^{(2)}) = (w_0 + v_2)^+ a$$

•
$$f_M(x^{(M)}) = (w_0 + v_M)^{\top} x^{(M)}$$

where w_0 is a common factor for all models.

For squared-loss, we can write the problem as

$$\min_{\boldsymbol{w}_1,...,\boldsymbol{w}_M} \quad \frac{1}{2} \sum_{m=1}^M \frac{1}{n_m} \sum_{i=1}^{n_m} \left(y_i^{(m)} - (\boldsymbol{w}_0 + \boldsymbol{v}_m)^\top \boldsymbol{x}_i^{(m)} \right)^2 + \lambda (\|\boldsymbol{w}_0\|_2^2 + \sum_{m=1}^M \|\boldsymbol{v}_m\|_2^2)$$

Supervised Transfer Learning: Frustratingly easy domain adaptation

A frustratingly easy feature augmentation approach:

$$oldsymbol{z}^{ extsf{tr}} = (oldsymbol{x}^{ extsf{tr}} oldsymbol{x}^{ extsf{tr}} oldsymbol{0}_{ extsf{d}}^{ op})^{ op}, \hspace{0.2cm} oldsymbol{z}^{ extsf{te}} = (oldsymbol{x}^{ extsf{te}} oldsymbol{0}_{ extsf{d}}^{ op} oldsymbol{0}_{ extsf{d}}^{ op})^{ op}, \hspace{0.2cm} oldsymbol{z}^{ extsf{te}} = (oldsymbol{x}^{ extsf{te}} oldsymbol{0}_{ extsf{d}}^{ op} oldsymbol{0}_{ extsf{d}}^{ op})^{ op}, \hspace{0.2cm} oldsymbol{z}^{ extsf{te}} = (oldsymbol{x}^{ extsf{te}} oldsymbol{0}_{ extsf{d}}^{ op} oldsymbol{0}_{ extsf{d}}^{ op})^{ op},$$

The inner product of z in the same domain is give as

$$oldsymbol{z}^{\mathsf{tr} op}oldsymbol{z}^{\mathsf{tr}}=2oldsymbol{x}^{\mathsf{tr} op}oldsymbol{x}^{\mathsf{te}},\ oldsymbol{z}^{\mathsf{te} op}oldsymbol{z}^{\mathsf{te}}=2oldsymbol{x}^{\mathsf{te} op}oldsymbol{x}^{\mathsf{te}},$$

while we have

$$oldsymbol{z}^{\mathsf{tr}^ op}oldsymbol{z}^{\mathsf{te}} = oldsymbol{x}^{\mathsf{tr}^ op}oldsymbol{x}^{\mathsf{tr}},$$
 ,

Then, we train a supervised learning method with the transformed vectors *z*. Super easy!!!!

Supervised transfer learning can be regarded as a two-task learning problem. First task is for training and second task is for test.

Let us denote the transformed vectors as

$$egin{aligned} oldsymbol{z}^{\mathsf{tr}} &= (oldsymbol{x}^{\mathsf{tr}^ op} \,\,\,oldsymbol{x}^{\mathsf{tr}^ op} \,\,\,oldsymbol{0}_{\mathsf{d}}^ op)^ op \in \mathbb{R}^{3d}, \ oldsymbol{z}^{\mathsf{te}} &= (oldsymbol{x}^{\mathsf{te}^ op} \,\,\,oldsymbol{0}_{\mathsf{d}}^ op \,\,\,oldsymbol{x}^{\mathsf{te}^ op})^ op \in \mathbb{R}^{3d}, \end{aligned}$$

where $\mathbf{0}_{\mathsf{d}} \in \mathbb{R}^d$ is the vector whose elements are all zero.

And, we consider a linear regression problem: The model parameter of the linear model can be written as

$$oldsymbol{w} = (oldsymbol{w}_0^ op \, oldsymbol{v}_1^ op \, oldsymbol{v}_2^ op)^ op \in \mathbb{R}^{3d}$$

Multi-task Learning

$$\begin{split} J(\boldsymbol{w}) &= \frac{1}{2n_{\mathrm{tr}}} \sum_{i=1}^{n_{\mathrm{tr}}} \|y_i^{\mathrm{tr}} - \boldsymbol{z}_i^{\mathrm{tr}^{\top}} \boldsymbol{w}\|_2^2 + \frac{1}{2n_{\mathrm{te}}} \sum_{i=1}^{n_{\mathrm{te}}} \|y_i^{\mathrm{te}} - \boldsymbol{z}_i^{\mathrm{te}^{\top}} \boldsymbol{w}\|_2^2 + \lambda \|\boldsymbol{w}\|_2^2 \\ &= \frac{1}{2} \sum_{m=1}^{M} \frac{1}{n_m} \sum_{i=1}^{n_m} \left(y_i^{(m)} - (\boldsymbol{w}_0 + \boldsymbol{v}_m)^{\top} \boldsymbol{x}_i^{(m)} \right)^2 + \lambda (\|\boldsymbol{w}_0\|_2^2 + \sum_{m=1}^{M} \|\boldsymbol{v}_m\|_2^2), \end{split}$$

where we use

$$egin{aligned} m{w}^ op m{z}^{ ext{tr}} &= (m{w}_0 + m{v}_1)^ op m{x}^{ ext{tr}}, & m{w}^ op m{z}^{ ext{te}} &= (m{w}_0 + m{v}_2)^ op m{x}^{ ext{te}} \ m{x}^{ ext{tr}} &= m{x}^{(1)}, & m{x}^{ ext{te}} &= m{x}^{(2)}, \ \|m{w}\|_2^2 &= \|m{w}_0\|_2^2 + \sum_{m=1}^2 \|m{v}_m\|_2^2. \end{aligned}$$

Frustratingly easy domain adaptation is a multi-task learning.

Summary

- Semi-supervised learning. Use unlabeled samples and assume the data distribution of unlabeled data is same as training.
- Weighted Maximum Likelihood, Graph-based method.
- Transfer Learning. Use samples from test data. Training and test distributions are different.
- Covariate shift adaptation, frustratingly easy domain adaptation.

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