ICLR2023, Kigali, Rwanda

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Importance-Weighting Approach to Distribution Shift Adaptation

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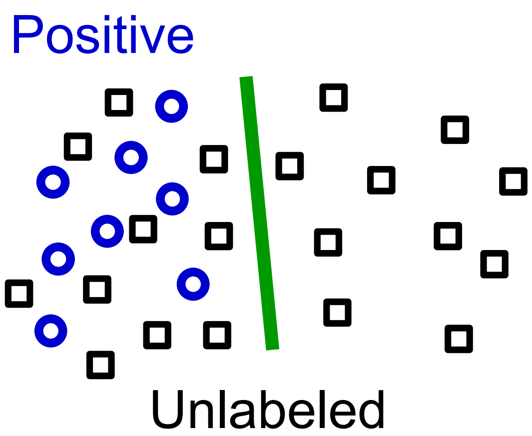
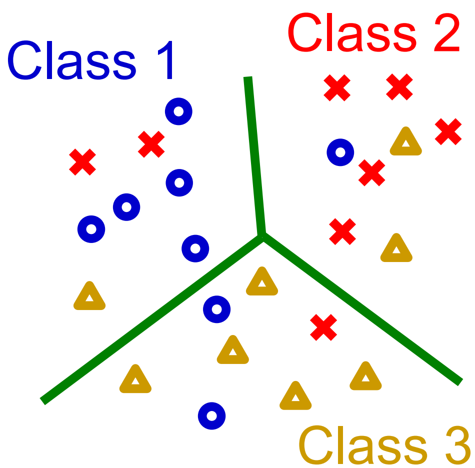
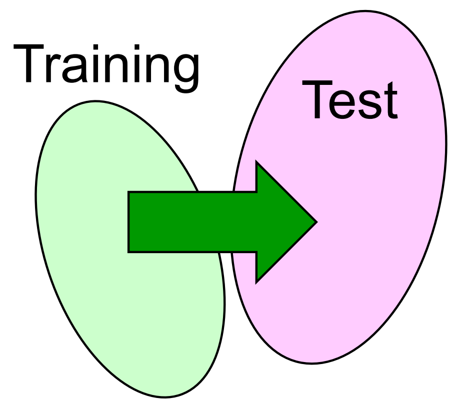
Slides→

Reliable Machine Learning

- Reliability of machine learning systems can be degraded by various factors:
  - Insufficient information: weak supervision.
  - Label noise: human error, sensor error.
  - Data bias: changing environments, privacy.
- Improving the reliability is an urgent challenge!







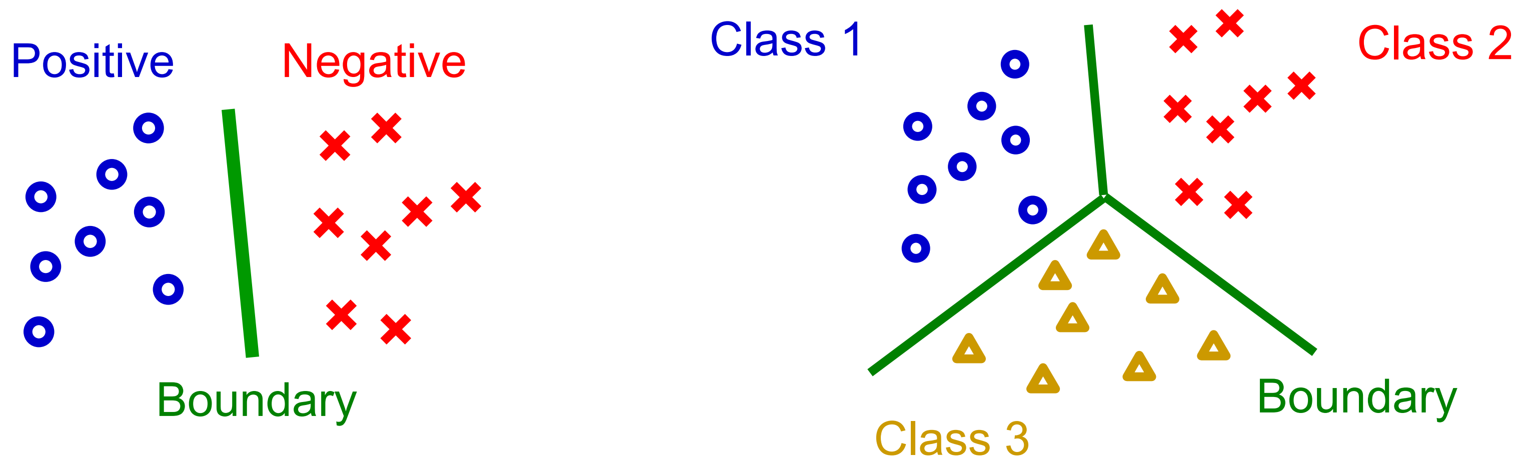
Contents

1. Weakly Supervised Learning
   A) Positive-Unlabeled Classification
   B) Various Extensions
2. Noisy-Label Learning
3. Transfer Learning
4. Towards More Reliable Learning

Slides→

Weakly Supervised Classification

- Supervised classification from big labeled data is successful: speech, image, language, …



- However, there are many applications where big labeled data is not available:
  - Medicine, disaster, robot, brain, …

- We want to utilize "weak" supervision that can be collected easily!

Contents

1. Weakly Supervised Learning
   A) Positive-Unlabeled Classification
   B) Various Extensions
2. Noisy-Label Learning
3. Transfer Learning
4. Towards More Reliable Learning

Slides→

Positive-Unlabeled (PU) Classification

Li+ (IJCAI2003)

- **Given:** PU samples (no N samples).

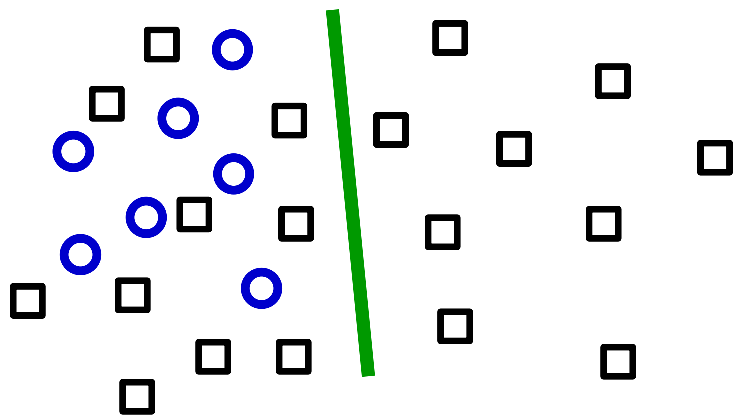
$$\{\boldsymbol{x}_i^{\mathrm{P}}\}_{i=1}^{n_{\mathrm{P}}} \overset{\mathrm{i.i.d.}}{\sim} p(\boldsymbol{x}|y=+1) \qquad \{\boldsymbol{x}_j^{\mathrm{U}}\}_{j=1}^{n_{\mathrm{U}}} \overset{\mathrm{i.i.d.}}{\sim} p(\boldsymbol{x})$$

- **Goal:** Obtain a classifier minimizing the PN risk.

$$\min_f R(f) \qquad R(f) = \mathbb{E}_{p(\boldsymbol{x},y)}\left[\ell\Big(y, f(\boldsymbol{x})\Big)\right]$$

$\mathbb{E}$: expectation $\quad$ ℓ : loss $\quad$ $y = \{+1, -1\}$

Positive [Negative]



Unlabeled (mixture of positives and negatives)

Example: Ad click prediction

- Clicked ad: User likes it → P
- Unclicked ad: User dislikes it or User likes it but doesn't have time to click it → U (=P or N)

PU Unbiased Risk Estimation

du Plessis+ (NeurIPS2014, ICML2015)

- Decompose the risk:

$$R(f) = \underbrace{\pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)}\Big[\ell\Big(+1, f(\boldsymbol{x})\Big)\Big]}_{\text{Risk for P data}} + \underbrace{(1-\pi)\mathbb{E}_{p(\boldsymbol{x}|y=-1)}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big]}_{\text{Risk for N data } R^{-}(f)}$$

$\pi = p(y=+1)$: Class prior (assumed known) →

Scott+ (AISTATS2009)
Ramaswamy+ (ICML2016)
du Plessis+ (MLJ2017)

- Without N data, $R^{-}(f)$ can not be estimated directly:
  - Eliminate the expectation over N data as

$$R^{-}(f) = \mathbb{E}_{p(\boldsymbol{x})}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big] - \pi \mathbb{E}_{p(\boldsymbol{x}|y=+1)}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big]$$

$$p(\boldsymbol{x}) = \pi p(\boldsymbol{x}|y=+1) + (1-\pi)p(\boldsymbol{x}|y=-1)$$

- Unbiased risk estimator:

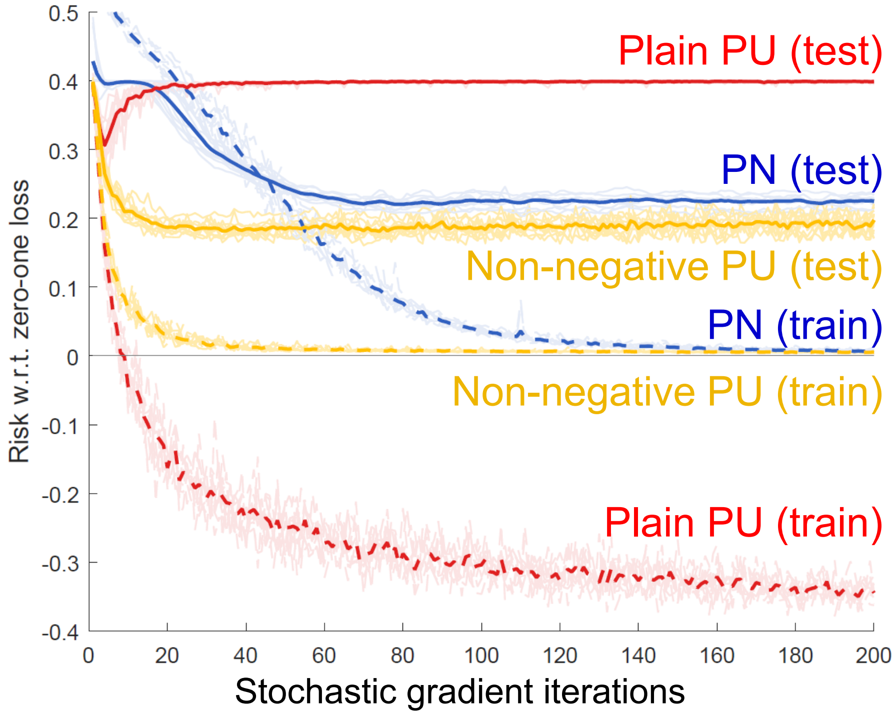
$$\widehat{R}_{\mathrm{PU}}(f) = \frac{\pi}{n_{\mathrm{P}}}\sum_{i=1}^{n_{\mathrm{P}}}\ell\Big(+1, f(\boldsymbol{x}_i^{\mathrm{P}})\Big) + \frac{1}{n_{\mathrm{U}}}\sum_{j=1}^{n_{\mathrm{U}}}\ell\Big(-1, f(\boldsymbol{x}_j^{\mathrm{U}})\Big) - \frac{\pi}{n_{\mathrm{P}}}\sum_{i=1}^{n_{\mathrm{P}}}\ell\Big(-1, f(\boldsymbol{x}_i^{\mathrm{P}})\Big)$$

Non-Negative Risk Correction

Kiryo+ (NeurIPS2017) , Lu+ (AISTATS2020)

$$R(f) = \underbrace{\pi\mathbb{E}_{p(\boldsymbol{x}|y=+1)}\Big[\ell\Big(+1, f(\boldsymbol{x})\Big)\Big]}_{\text{Risk for P data}} + \underbrace{(1-\pi)\mathbb{E}_{p(\boldsymbol{x}|y=-1)}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big]}_{\text{Risk for N data } R^-(f)}$$

- Risk for N data: $R^-(f) = \mathbb{E}_{p(\boldsymbol{x})}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big] - \pi\mathbb{E}_{p(\boldsymbol{x}|y=+1)}\Big[\ell\Big(-1, f(\boldsymbol{x})\Big)\Big]$
- Empirical estimate: $\widehat{R}^-_{\mathrm{PU}}(f) = \frac{1}{n_\mathrm{U}}\sum_{i=1}^{n_\mathrm{U}}\ell\Big(-1, f(\boldsymbol{x}_i^\mathrm{U})\Big) - \frac{\pi}{n_\mathrm{P}}\sum_{i=1}^{n_\mathrm{P}}\ell\Big(-1, f(\boldsymbol{x}_i^\mathrm{P})\Big)$
- When loss is non-negative:
  - True $R^-(f)$ is non-negative.
  - But empirical estimate can be negative!



- Non-negative correction:

$$\widetilde{R}_{\mathrm{PU}}(f) = \frac{\pi}{n_\mathrm{P}}\sum_{i=1}^{n_\mathrm{P}}\ell\Big(f(\boldsymbol{x}_i^\mathrm{P})\Big) + \max\left\{0,\ \widehat{R}^-_{\mathrm{PU}}(f)\right\}$$

Contents

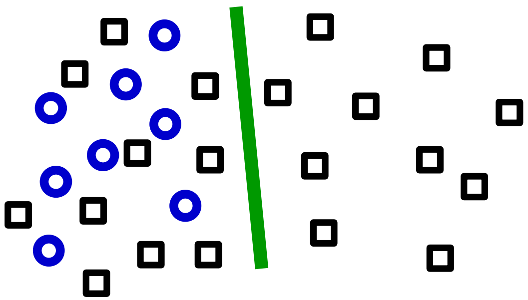
1. Weakly Supervised Learning
   A) Positive-Unlabeled Classification
   B) Various Extensions
2. Noisy-Label Learning
3. Transfer Learning
4. Towards More Reliable Learning

Slides→

Various Extensions (Binary)

- Similar unbiased risk estimation is possible!

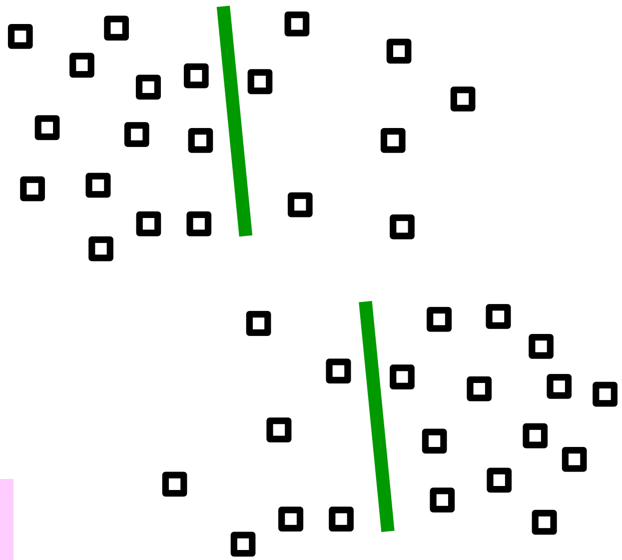
Positive-Unlabeled (PU)



du Plessis+ (NeurIPS2014, ICML2015, MLJ2017), Niu+ (NeurIPS2016), Kiryo+ (NeurIPS2017), Hsieh+ (ICML2019)

Click prediction

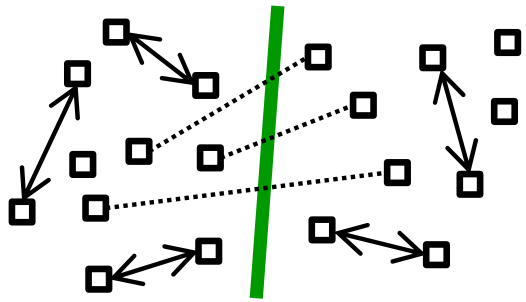
Unlabeled-Unlabeled (UU)



du Plessis+ (TAAI2013), Lu+ (ICLR2019, AISTATS2020), Charoenphakdee+ (ICML2019), Lei+ (ICML2021)

Different populations

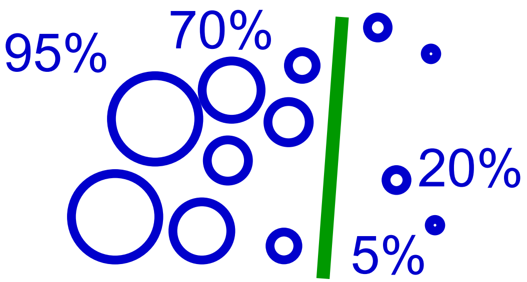
Similar-Dissimilar (SD)



Bao+ (ICML2018), Shimada+ (NeCo2021), Dan+ (ECMLPKDD2021), Cao+ (ICML2021), Feng+ (ICML2021)

Sensitive prediction

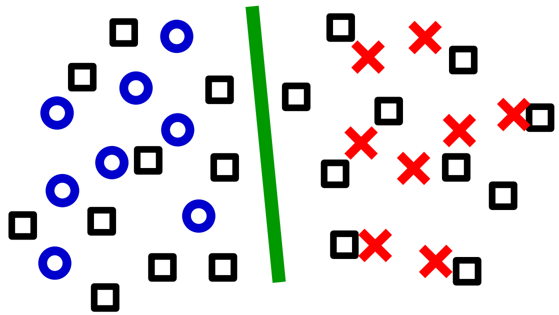
Positive-confidence (Pconf)



Ishida+ (NeurIPS2018), Shinoda+ (IJCAI2021)

Purchase prediction

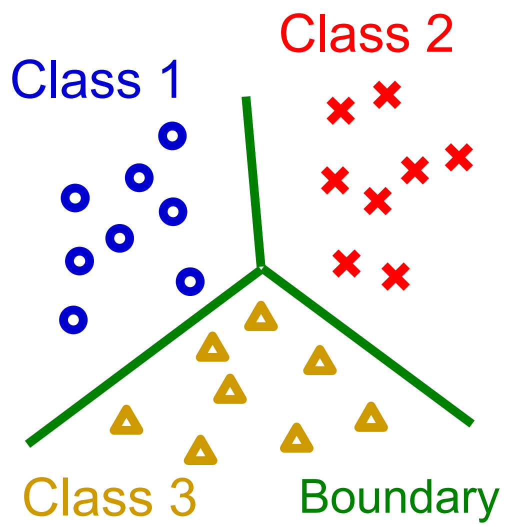
Positive-Negative-Unlabeled (PNU)



Sakai+ (ICML2017, ML2018)

Semi-supervised classification without manifold/clusters →

Various Extensions (Multiclass)



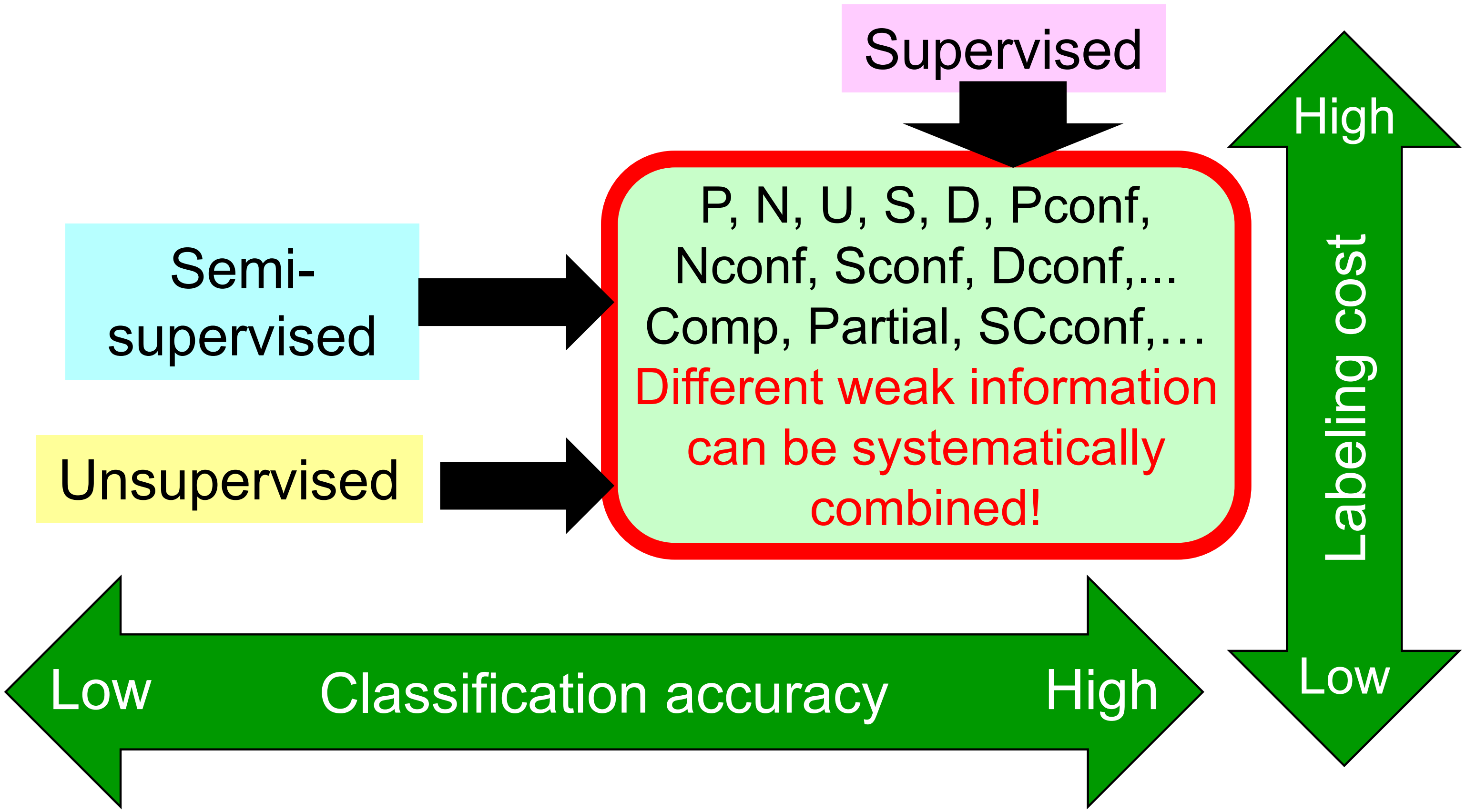
- Labeling patterns in multi-class problems is even more painful.

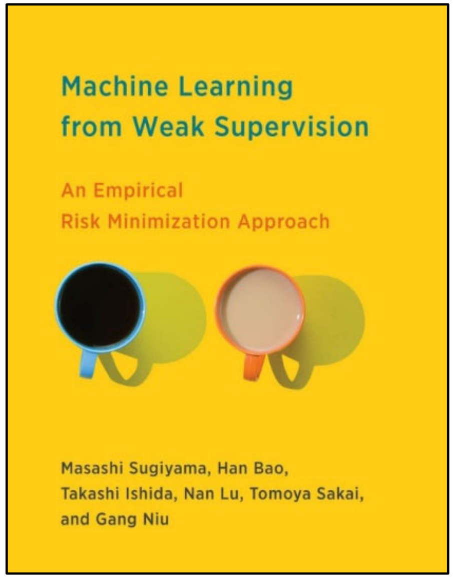
- Multi-class weak-labels:
  - Complementary label: Specifies a class that a pattern does not belong to ("not 1"). Ishida+ (NeurIPS2017, ICML2019), Chou+ (ICML2020)
  - Partial label: Specifies a subset of classes that contains the correct one ("1 or 2"). Feng+ (ICML2020, NeurIPS2020), Lv+ (ICML2020)
  - Single-class confidence: Cao+ (arXiv2021) One-class data with full confidence ("1 with 60%, 2 with 30%, and 3 with 10%")

- Similar unbiased risk estimation is possible!

Summary: Weakly Supervised Learning

- Empirical risk minimization framework for weakly supervised learning:
  - Any loss, classifier, and optimizer can be used.





Sugiyama, Bao, Ishida,
Lu, Sakai & Niu,
MIT Press, 2022.

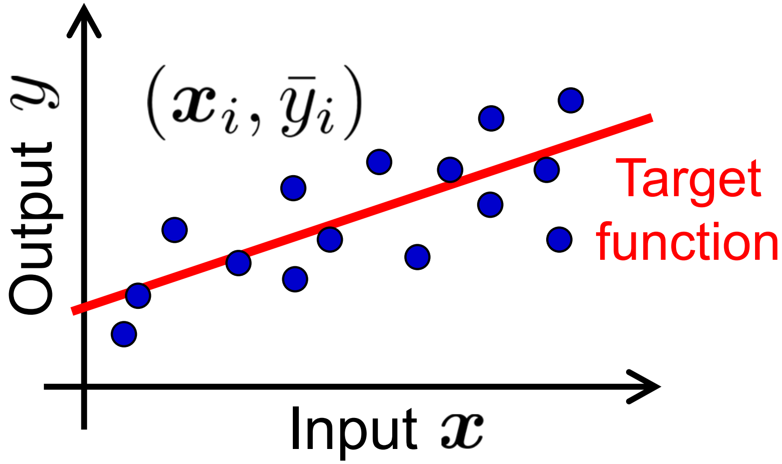
Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
   A) Noise Transition
   B) Algorithms
3. Transfer Learning
4. Towards More Reliable Learning

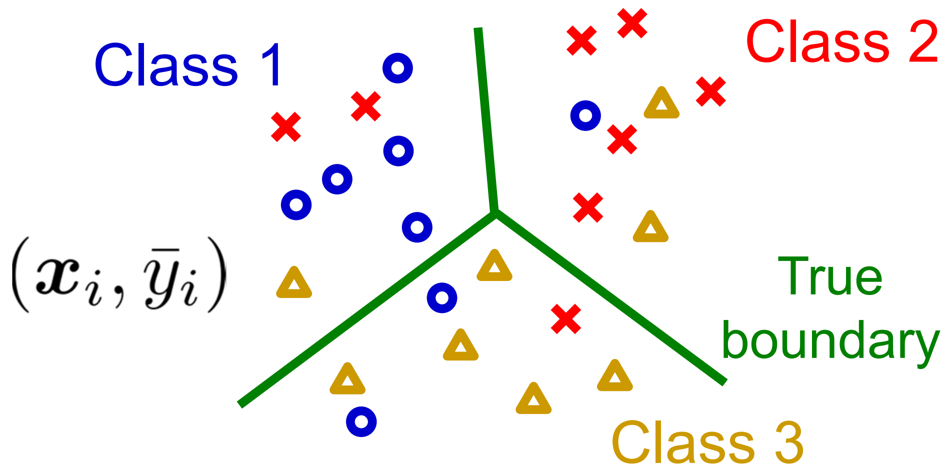
Slides→

Supervised Learning with Noisy Output

Regression (additive noise)



Classification (label flipping noise)



$$\min_{\boldsymbol{g}} \sum_{i=1}^{n} \ell\Big(\bar{y}_i, \boldsymbol{g}(\boldsymbol{x}_i)\Big)$$

ℓ: loss

$\bar{y}$: noisy output

$\boldsymbol{g}$: probabilistic classifier

- Hasn't such a classic problem been solved?
  - Regression: Yes, noisy big data yield consistency.
  - Classification: Specific noise reduction mechanism is needed to achieve consistency!

Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
   A) Noise Transition
   B) Algorithms
3. Transfer Learning
4. Towards More Reliable Learning

Slides→

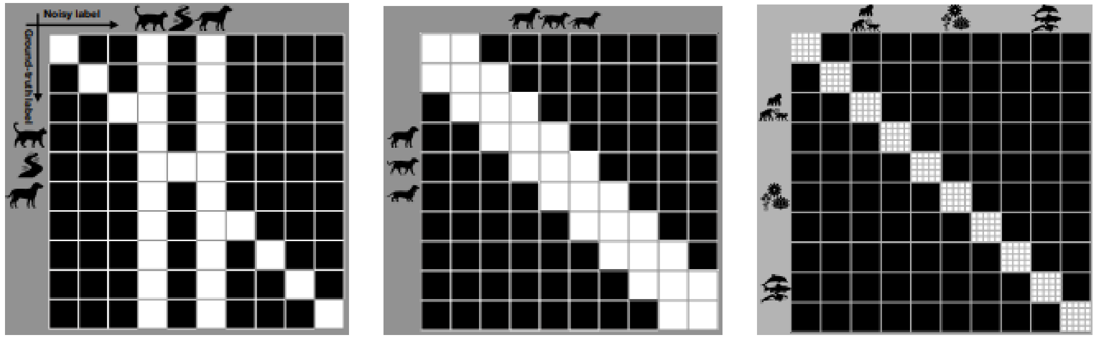
Modeling Input-Independent Noise

- Noise transition matrix: $T_{y,\bar{y}} = \bar{p}(\bar{y}|y)$
  - Probability of flipping y to $\bar{y}$.

$$\boldsymbol{T} = \begin{array}{c} \bar{y} \\ \begin{bmatrix} 1 & 0 & 0 \\ 0.1 & 0.8 & 0.1 \\ 0.5 & 0.5 & 0 \end{bmatrix} \end{array} \, y$$

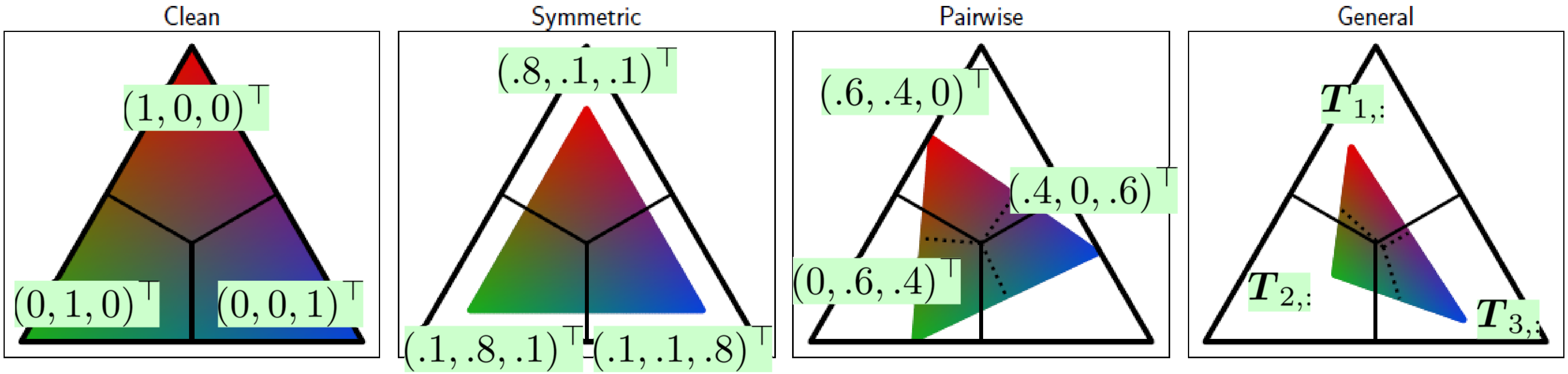
- Human-cognitive bias can be encoded in $\boldsymbol{T}$.

Han+ (NeurIPS2018)



(a) Column-diagonal (b) Tri-diagonal (c) Block-diagonal

- $\boldsymbol{T}$ can be visualized in a simplex.



Loss Correction with Noise Transition

Patrini+ (CVPR2017)

$\boldsymbol{\ell}$: vectorized loss

$\ell_y(\boldsymbol{g}(\boldsymbol{x})) = \ell(y, \boldsymbol{g}(\boldsymbol{x}))$

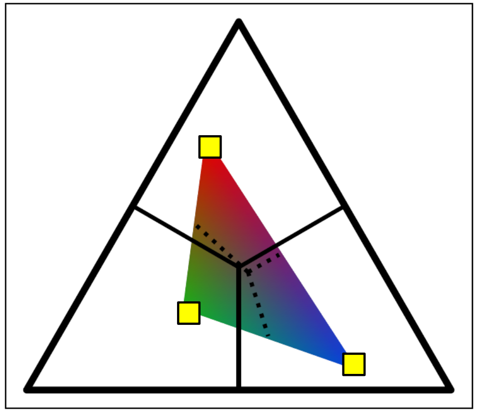
- Forward correction: $\boldsymbol{\ell}(\boldsymbol{T}^\top \boldsymbol{g}(\boldsymbol{x}))$
  - Add noise by $\boldsymbol{T}^\top$.
- Backward correction: $\boldsymbol{T}^{-1}\boldsymbol{\ell}(\boldsymbol{g}(\boldsymbol{x}))$
  - Remove noise by $\boldsymbol{T}^{-1}$.
- If $\boldsymbol{T}$ is given, consistency can be guaranteed!
- If $\boldsymbol{T}$ is unknown, how is it estimated?

Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
   A) Noise Transition
   B) Algorithms
3. Transfer Learning
4. Towards More Reliable Learning

Slides→

Basic Approach



- With noiseless labels, $\boldsymbol{T}$ can be obtained naively:
  - We know the vertices of the triangle.
- Can we estimate $\boldsymbol{T}$ from noisy labels?
  - Generally, $\boldsymbol{T}$ is non-identifiable:

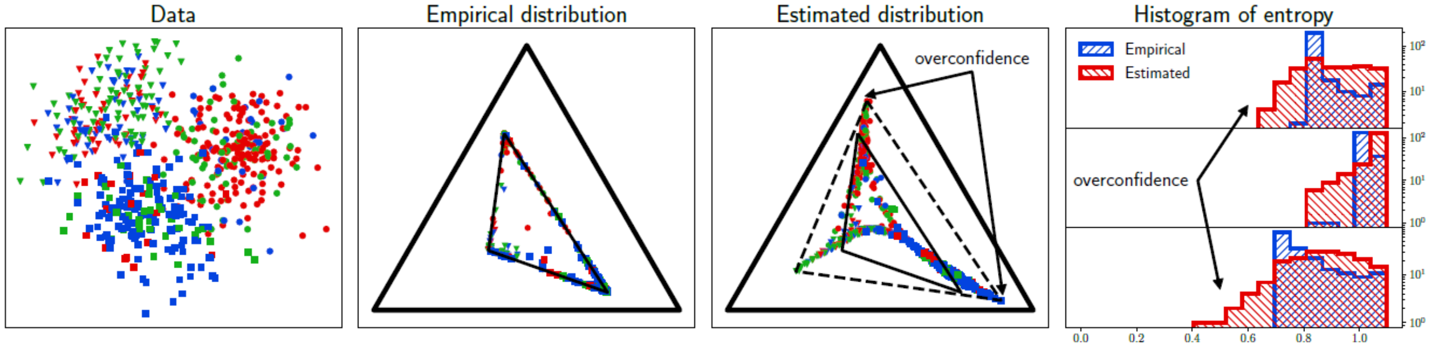
$$\boldsymbol{T}^\top \boldsymbol{p} = \boldsymbol{T}_2^\top (\boldsymbol{T}_1^\top \boldsymbol{p}) \qquad \boldsymbol{T} = \boldsymbol{T}_1 \boldsymbol{T}_2$$

- Assume noiseless labels exist in the training set:
  - Select the most confident data as noiseless ones.

$$\boldsymbol{x}^y \leftarrow \boldsymbol{x}_i \text{ s.t. } \widehat{g}_y(\boldsymbol{x}_i) \approx 1 \qquad \widehat{\boldsymbol{g}} = \operatorname*{argmin}_{\boldsymbol{g}} \sum_{i=1}^{n} \ell(\bar{y}_i, \boldsymbol{g}(\boldsymbol{x}_i))$$

Limitations

- Over-confidence of neural networks is harmful.



Zhang+ (ICML2021)

- The two-step nature magnifies the estimation error:
  1. Noise transition estimation: $\widehat{\boldsymbol{T}}$
  2. Classifier training with estimated $\widehat{\boldsymbol{T}}$:

$$\min_{\boldsymbol{g}} \sum_{i=1}^{n} \ell(\bar{y}_i, \widehat{\boldsymbol{T}}^\top \boldsymbol{g}(\boldsymbol{x}_i))$$

  - Naïve simultaneous estimation suffers non-identifiability.

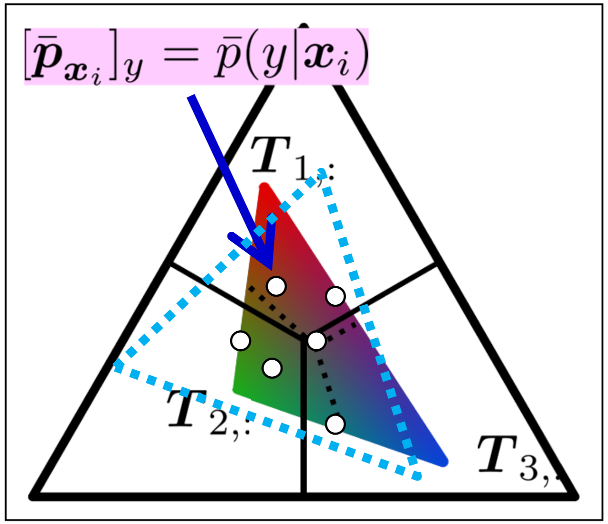
$$\min_{\boldsymbol{T}', \boldsymbol{g}} \sum_{i=1}^{n} \ell(\bar{y}_i, \boldsymbol{T}'^\top \boldsymbol{g}(\boldsymbol{x}_i))$$

- Assumption of having noiseless labels is too strong.

Volume Minimization

Li+ (ICML2021)

- Noisy training data $\{(\boldsymbol{x}_i, \bar{y}_i)\}_{i=1}^{n}$ can be mapped in the triangle formed by noise transition matrix $\boldsymbol{T}$.

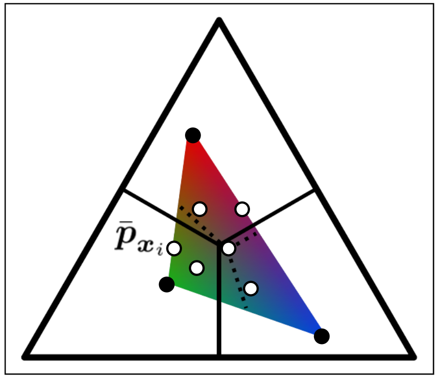


- Minimizing the volume of the triangle can give a solution:

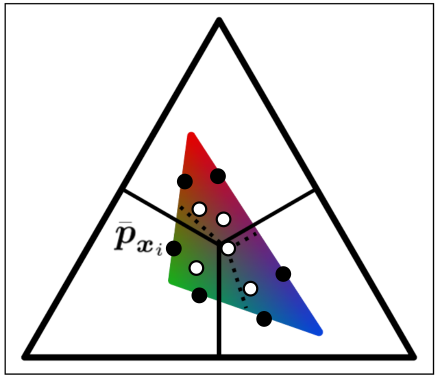
$$\min_{\boldsymbol{T}', \boldsymbol{g}} \sum_{i=1}^{n} \ell(\bar{y}_i, \boldsymbol{T}'^{\top} \boldsymbol{g}(\boldsymbol{x}_i)) + \lambda \log \det(\boldsymbol{T}')$$

$\lambda > 0$

  - With noiseless labels, we can find the true $\boldsymbol{T}$.

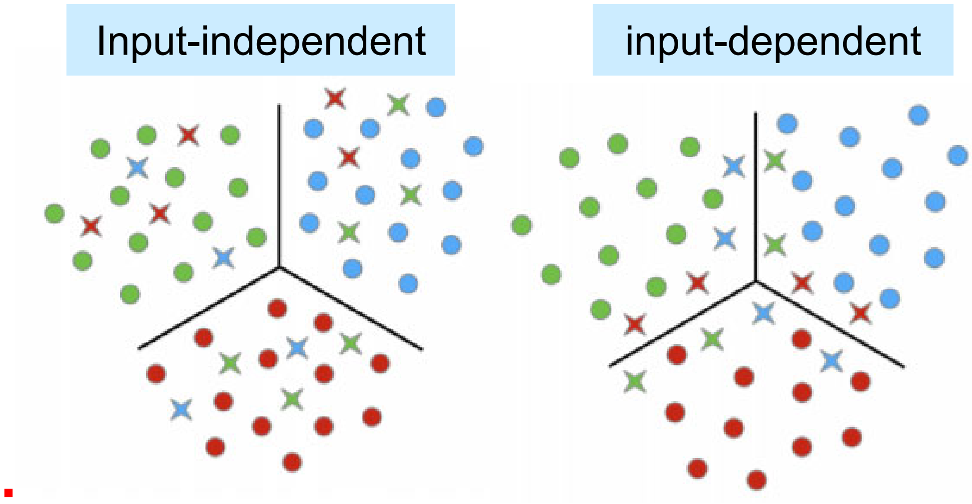


  - Even without noiseless labels, "sufficiently scattered" training data allow identification of the true $\boldsymbol{T}$!



Input-Dependent Noise

- Real-world noise is often input-dependent.
  - E.g., more noise near the boundary.



- Noise transition function:

$$T_{y,\bar{y}}(\boldsymbol{x}) = \bar{p}(\bar{y} | y, \boldsymbol{x})$$

  - Extremely challenging to estimate it!

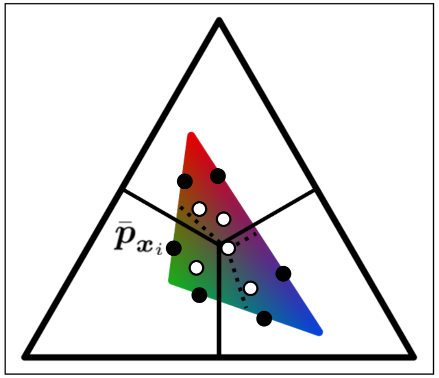
- Heuristics:
  - Parts-based estimation. Xia+ (NeurIPS2020)
  - Use of additional confidence scores. Berthon+ (ICML2021)
  - Manifold regularization. Cheng+ (CVPR2022)

Summary: Noisy-Label Learning

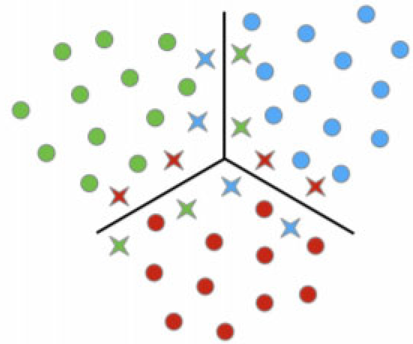
- Explicit treatment of label noise is necessary:
  - Loss correction by noise transition is promising.

$$T_{y,\bar{y}} = \bar{p}(\bar{y}|y)$$

- However, noise transition is generally non-identifiable:
  - Recent development allows consistent estimation under mild assumptions.



- Real-world noise is often input-dependent:
  - Heuristic solutions have been developed.
  - Further theoretical development is needed.



Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
3. Transfer Learning
   - A) Importance Weighting
   - B) Continuous Distribution Shift
4. Towards More Reliable Learning

Slides→

Learning under Distribution Shift

Given:

- Training data $\{(\boldsymbol{x}_i^{\mathrm{tr}}, y_i^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y)$

$\boldsymbol{x}$: Input

y : Output

Goal:

- Learn predictor $y = f(\boldsymbol{x})$ minimizing the test risk (with some additional data from the test domain).

$$\min_f R(f) \qquad R(f) = \mathbb{E}_{p_{\mathrm{te}}(\boldsymbol{x},y)}[\ell(f(\boldsymbol{x}), y)]$$

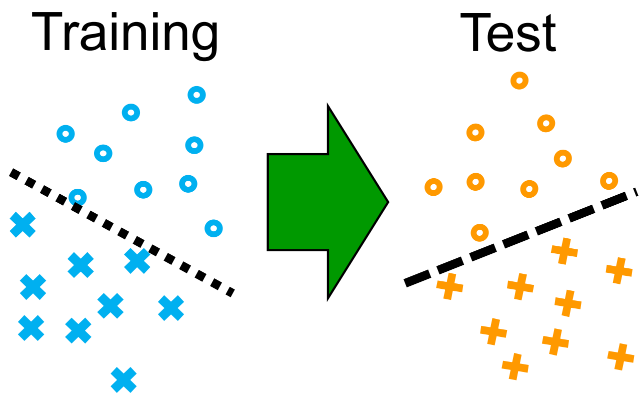
ℓ : loss

Challenge:

- Overcome changing distributions!

$$p_{\mathrm{tr}}(\boldsymbol{x}, y) \neq p_{\mathrm{te}}(\boldsymbol{x}, y)$$

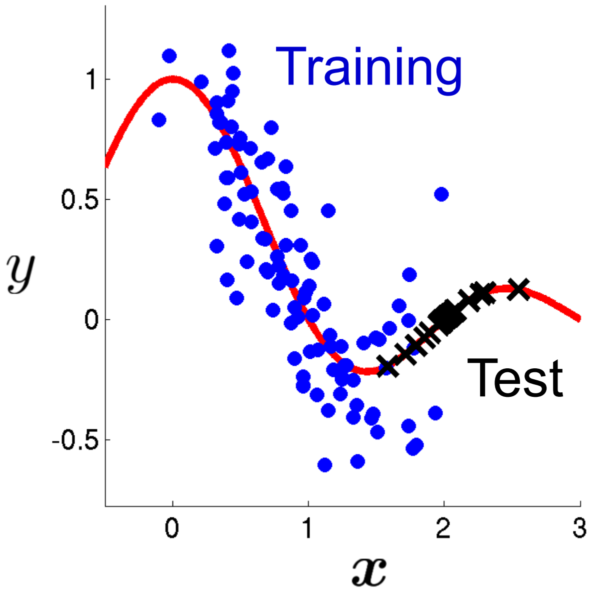
  - Non-stationary of the environments.
  - Sample selection bias due to privacy concerns.

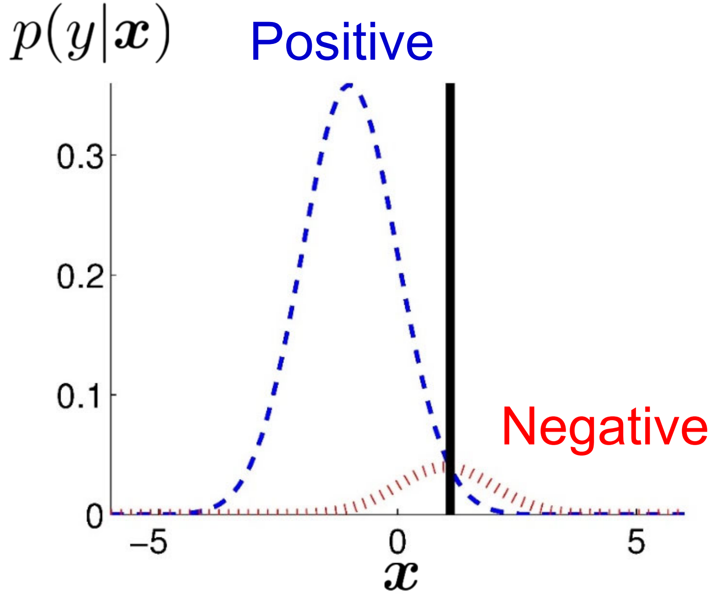


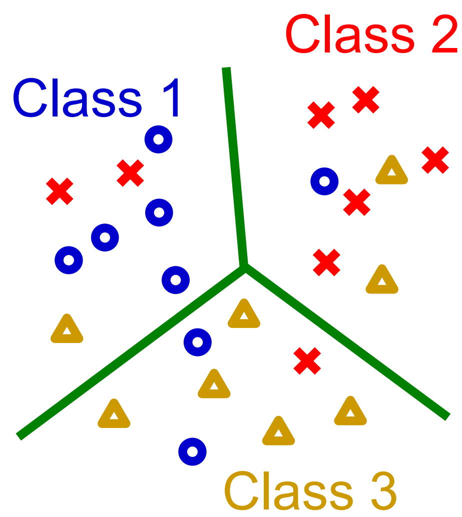
Types of Distribution Shift

$\boldsymbol{x}$: Input y : Output

- Joint shift: $p_{\mathrm{tr}}(\boldsymbol{x}, y) \neq p_{\mathrm{te}}(\boldsymbol{x}, y)$
- Covariate shift: $p_{\mathrm{tr}}(\boldsymbol{x}) \neq p_{\mathrm{te}}(\boldsymbol{x})$
- Class-prior shift: $p_{\mathrm{tr}}(y) \neq p_{\mathrm{te}}(y)$
- Output noise: $p_{\mathrm{tr}}(y|\boldsymbol{x}) \neq p_{\mathrm{te}}(y|\boldsymbol{x})$
- Class-conditional shift: $p_{\mathrm{tr}}(\boldsymbol{x}|y) \neq p_{\mathrm{te}}(\boldsymbol{x}|y)$







Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
3. Transfer Learning
    - A) Importance Weighting
    - B) Continuous Distribution Shift
4. Towards More Reliable Learning

Slides→

Covariate Shift

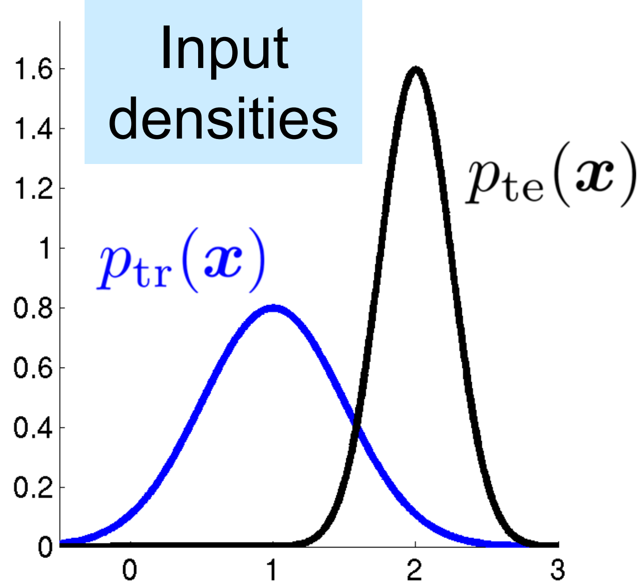
Shimodaira (JSPI2000)

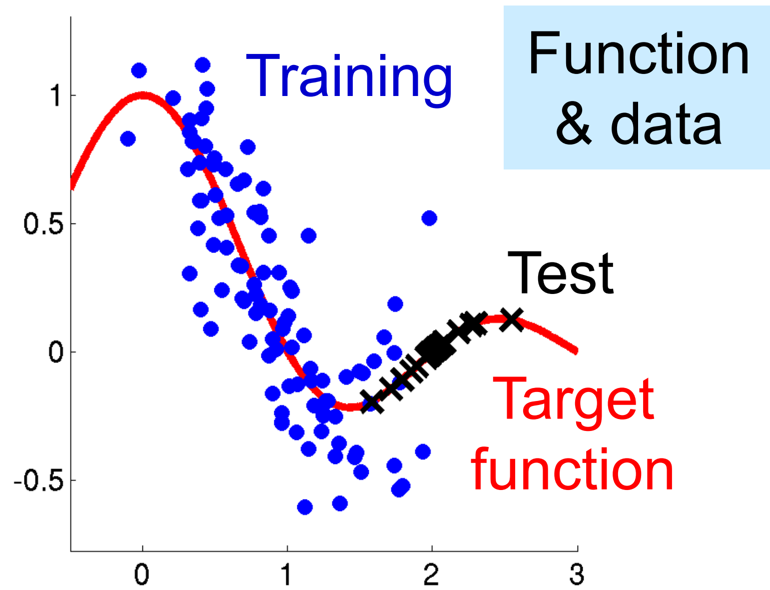
- Training and test input distributions are different,

$$p_{\mathrm{tr}}(\boldsymbol{x}) \neq p_{\mathrm{te}}(\boldsymbol{x})$$

  but the output-given-input distribution is unchanged:

$$p_{\mathrm{tr}}(y|\boldsymbol{x}) = p_{\mathrm{te}}(y|\boldsymbol{x}) = p(y|\boldsymbol{x})$$





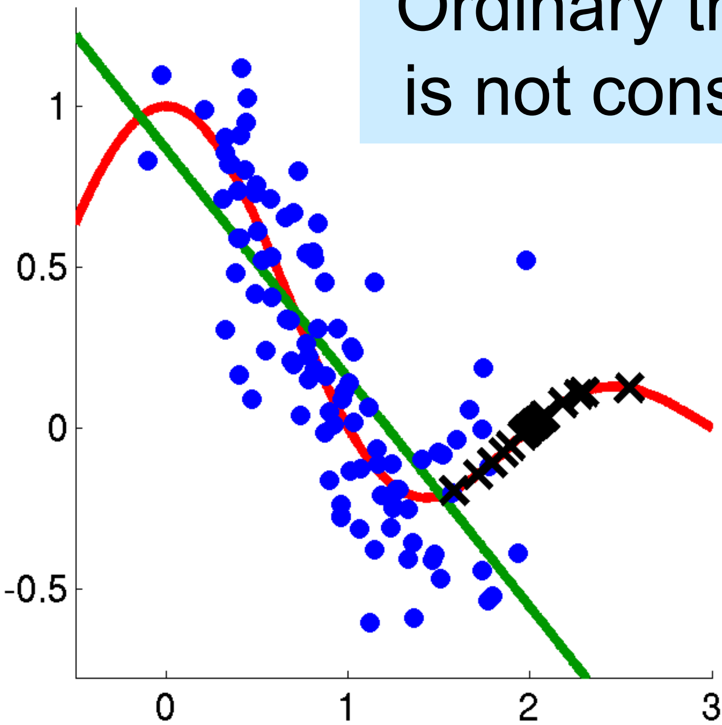
- Given:
  - Labeled training data: $\{(\boldsymbol{x}_i^{\mathrm{tr}}, y_i^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y)$
  - Unlabeled test data: $\{\boldsymbol{x}_j^{\mathrm{te}}\}_{j=1}^{n_{\mathrm{te}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{te}}(\boldsymbol{x})$

Importance-Weighted Training

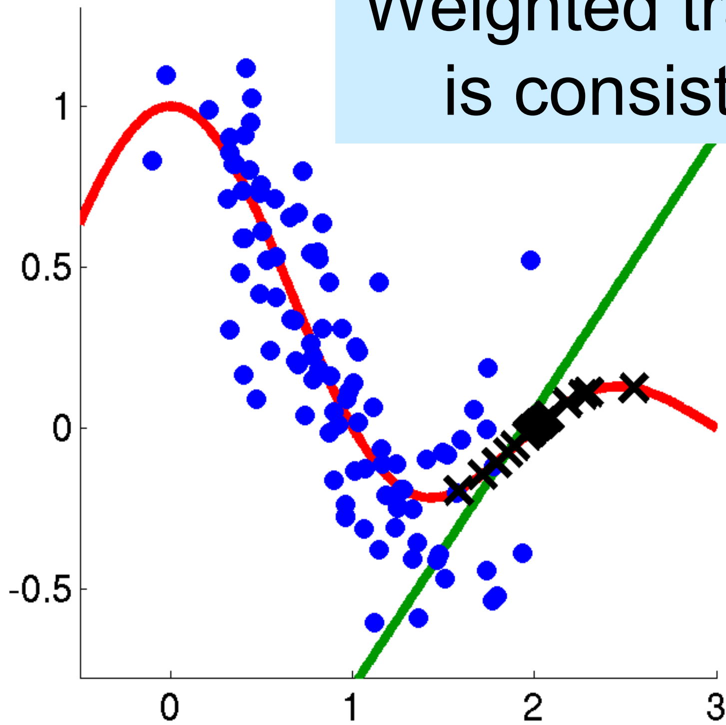
$$\underset{f}{\operatorname{argmin}}\left[\sum_{i=1}^{n_{\mathrm{tr}}}\ell(f(\boldsymbol{x}_i^{\mathrm{tr}}),y_i^{\mathrm{tr}})\right]$$

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

$$\underset{f}{\operatorname{argmin}}\left[\sum_{i=1}^{n_{\mathrm{tr}}}\underbrace{\frac{p_{\mathrm{te}}(\boldsymbol{x}_i^{\mathrm{tr}})}{p_{\mathrm{tr}}(\boldsymbol{x}_i^{\mathrm{tr}})}}_{\text{Importance}}\ell(f(\boldsymbol{x}_i^{\mathrm{tr}}),y_i^{\mathrm{tr}})\right]$$



Ordinary training is not consistent



Weighted training is consistent

- How do we estimate the importance?

Direct Importance Estimation

- Given: training and test input data

$$\{\boldsymbol{x}_i^{\mathrm{tr}}\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}) \qquad \{\boldsymbol{x}_j^{\mathrm{te}}\}_{j=1}^{n_{\mathrm{te}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{te}}(\boldsymbol{x})$$

- Kernel mean matching: Huang+ (NeurIPS2006)
  - Match the means of $r(\boldsymbol{x})p_{\mathrm{tr}}(\boldsymbol{x})$ and $p_{\mathrm{te}}(\boldsymbol{x})$ in RKHS $\mathcal{H}$.

$$\min_{r\in\mathcal{H}} \left\| \int K(\boldsymbol{x},\cdot)p_{\mathrm{te}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x} - \int K(\boldsymbol{x},\cdot)r(\boldsymbol{x})p_{\mathrm{tr}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x} \right\|_{\mathcal{H}}^2$$

$K(\boldsymbol{x},\cdot)$: kernel

- Least-squares importance fitting (LSIF): Kanamori+ (NeurIPS2008)
  - Fit a model $r(\boldsymbol{x})$ to $\frac{p_{\mathrm{te}}(\boldsymbol{x})}{p_{\mathrm{tr}}(\boldsymbol{x})}$ by least squares:

$$\operatorname*{argmin}_r \left[\int \left(r(\boldsymbol{x}) - \frac{p_{\mathrm{te}}(\boldsymbol{x})}{p_{\mathrm{tr}}(\boldsymbol{x})}\right)^2 p_{\mathrm{tr}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}\right]$$

$$= \operatorname*{argmin}_r \left[\int r(\boldsymbol{x})^2 p_{\mathrm{tr}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x} - 2\int r(\boldsymbol{x})p_{\mathrm{te}}(\boldsymbol{x})\mathrm{d}\boldsymbol{x}\right]$$

- They do not estimate $p_{\mathrm{tr}}(\boldsymbol{x}), p_{\mathrm{te}}(\boldsymbol{x})$, but $\frac{p_{\mathrm{te}}(\boldsymbol{x})}{p_{\mathrm{tr}}(\boldsymbol{x})}$ directly!

Joint Importance-Predictor Estimation

Zhang+ (ACML2020, SNCS2021)

- The classical approaches are two steps:
  1. Importance weight estimation (e.g., LSIF):

$$\widehat{r} = \operatorname*{argmin}_{r} J_1(r) \qquad J_1(r) = \mathbb{E}_{p_{\mathrm{tr}}(\boldsymbol{x})}\left[\left(r(\boldsymbol{x}) - \frac{p_{\mathrm{te}}(\boldsymbol{x})}{p_{\mathrm{tr}}(\boldsymbol{x})}\right)^2\right]$$

  2. Importance-weighted predictor training:

$$\widehat{f} = \operatorname*{argmin}_{f} J_2(f, \widehat{r}) \qquad J_2(f, r) = \mathbb{E}_{p_{\mathrm{tr}}(\boldsymbol{x}, y)}\left[r(\boldsymbol{x})\ell(f(\boldsymbol{x}), y)\right]$$

- For $\ell_{\mathrm{te}} \leq 1, \ell_{\mathrm{tr}} \geq \ell_{\mathrm{te}}, r \geq 0$, the test risk $R_\ell(f) = \mathbb{E}_{p_{\mathrm{te}}(\boldsymbol{x}, y)}[\ell(f(\boldsymbol{x}), y)]$ can be bounded as

$$\frac{1}{2} R_{\ell_{\mathrm{te}}}(f)^2 \leq J_{\ell_{\mathrm{tr}}}(f, r) \qquad J_\ell(f, r) = J_1(r) + J_2(f, r)$$

- Joint upper-bound minimization: $\widehat{f} = \operatorname*{argmin}_{f} \min_{r \geq 0} \widehat{J}_{\ell_{\mathrm{tr}}}(f, r)$

Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
3. Transfer Learning
   - A) Importance Weighting
   - B) Continuous Distribution Shift
4. Towards More Reliable Learning

Slides→

Continuous Class-Prior Shift

Bai+ (NeurIPS2022)

- Class-priors $p_t(y)$ change arbitrarily over time, but class-conditional is unchanged: $p_{\mathrm{tr}}(\boldsymbol{x}|y) = p_t(\boldsymbol{x}|y)$

- Given: $t = 1, \ldots, T$
  - (Large) labeled training data: $\{(\boldsymbol{x}_i^{\mathrm{tr}}, y_i^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y)$
  - (Small) unlabeled test data: $\{\boldsymbol{x}_i^{(t)}\}_{i=1}^{n_t} \overset{\mathrm{i.i.d.}}{\sim} p_t(\boldsymbol{x})$

- We use online convex optimization: Hazan (2016)
  - convex loss ℓ (e.g., logistic),
  - linear model $f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x}, \quad \boldsymbol{w} \in \mathcal{W}$.
  - $p_{t-1}(y)$ is estimated by black box shift estimation. Lipton+ (ICML2018)

$$\boldsymbol{w}_t = \Pi_{\mathcal{W}}\left[\boldsymbol{w}_{t-1} - \eta \nabla \widehat{R}_{t-1}(\boldsymbol{w}_{t-1})\right]$$

$\Pi_{\mathcal{W}}$: projection

$$\widehat{R}_{t-1}(f) = \frac{1}{n_{\mathrm{tr}}} \sum_{i=1}^{n_{\mathrm{tr}}} \frac{\widehat{p}_{t-1}(y_i^{\mathrm{tr}})}{\widehat{p}_{\mathrm{tr}}(y_i^{\mathrm{tr}})} \ell(f(\boldsymbol{x}_i^{\mathrm{tr}}), y_i^{\mathrm{tr}})$$

$\eta > 0$: step size

Choice of Step Size η

$$\boldsymbol{w}_t = \Pi_{\mathcal{W}}\left[\boldsymbol{w}_{t-1} - \eta\nabla\widehat{R}_{t-1}(\boldsymbol{w}_{t-1})\right]$$

- If the speed of distribution shift is
  - slow, η should be small to keep the previous classifier.
  - fast, η should be large to quickly update the classifier.
- How do we choose η in practice?
  - Ensemble learning! Zhao+ (NeurIPS2020)
- For $0 < \eta_1 < \cdots < \eta_M$, we run M learners:

$$\boldsymbol{w}_t^{(m)} = \Pi_{\mathcal{W}}\left[\boldsymbol{w}_{t-1}^{(m)} - \eta_m\nabla\widehat{R}_{t-1}(\boldsymbol{w}_{t-1}^{(m)})\right]$$

- Final output is the weighted average (cf. Hedge):

Freund+ (JCSS1997)

$$\boldsymbol{w}_t = \sum_{m=1}^{M} p_t^{(m)}\boldsymbol{w}_t^{(m)}$$

$$p_t^{(m)} \propto \exp\left(-\varepsilon\sum_{s=1}^{t-1}\widehat{R}_s(\boldsymbol{w}_s^{(m)})\right)$$

$$\varepsilon = \Theta\left(\sqrt{\frac{\ln M}{T}}\right)$$

Theoretical Analysis

- Shift intensity: $V_T = \sum_{t=2}^{T} \sum_{y=1}^{c} |p_t(y) - p_{t-1}(y)| \geq \Theta(T^{-\frac{1}{2}})$
- When V_T is known:
  - Online learning with step size $\eta = \Theta(V_T^{\frac{1}{3}} T^{-\frac{1}{3}})$ achieves the optimal dynamic regret:

$$\mathbb{E}\left[\underbrace{\sum_{t=1}^{T} R_t(\boldsymbol{w}_t)}_{\text{Risk of our model}} - \underbrace{\sum_{t=1}^{T} \min_{\boldsymbol{w} \in \mathcal{W}} R_t(\boldsymbol{w})}_{\text{Risk of the best model at each iteration}}\right] = \mathcal{O}(V_T^{\frac{1}{3}} T^{\frac{2}{3}})$$

- Even when V_T is unknown:
  - Our method still achieves the optimal dynamic regret!
    - Number of learners: $M = 1 + \lceil \frac{1}{2} \log_2(1 + 2T) \rceil$
    - Step size: $\eta_m = 2^{m-1} Z / \sqrt{T}, \quad m = 1, \ldots, M$

Continuous Covariate Shift

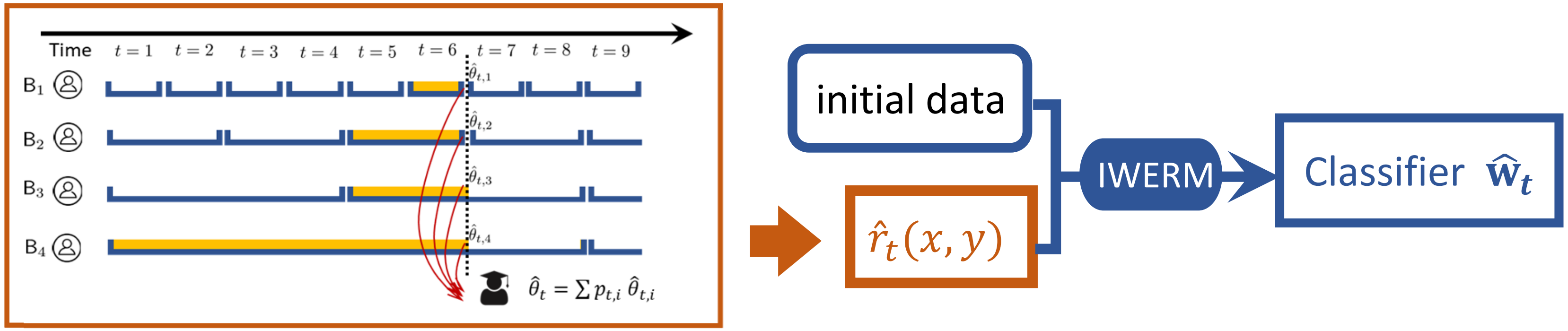
Zhang+ (arXiv2023)

- **Input density** $p_t(\boldsymbol{x})$ **change** arbitrarily over time, but **output-given-input** is unchanged: $p_{\mathrm{tr}}(y|\boldsymbol{x}) = p_t(y|\boldsymbol{x})$

$t = 1, \ldots, T$

- **Given**:
  - (Large) labeled training data: $\{(\boldsymbol{x}_i^{\mathrm{tr}}, y_i^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y)$
  - (Small) unlabeled test data: $\{\boldsymbol{x}_i^{(t)}\}_{i=1}^{n_t} \overset{\mathrm{i.i.d.}}{\sim} p_t(\boldsymbol{x})$

- We use **online density ratio estimation**:



Stay tuned!

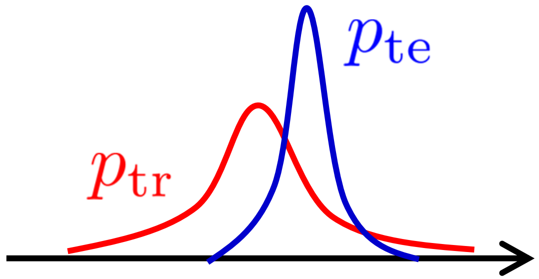
Contents

1. Weakly Supervised Learning
2. Noisy-Label Learning
3. Transfer Learning
4. Towards More Reliable Learning

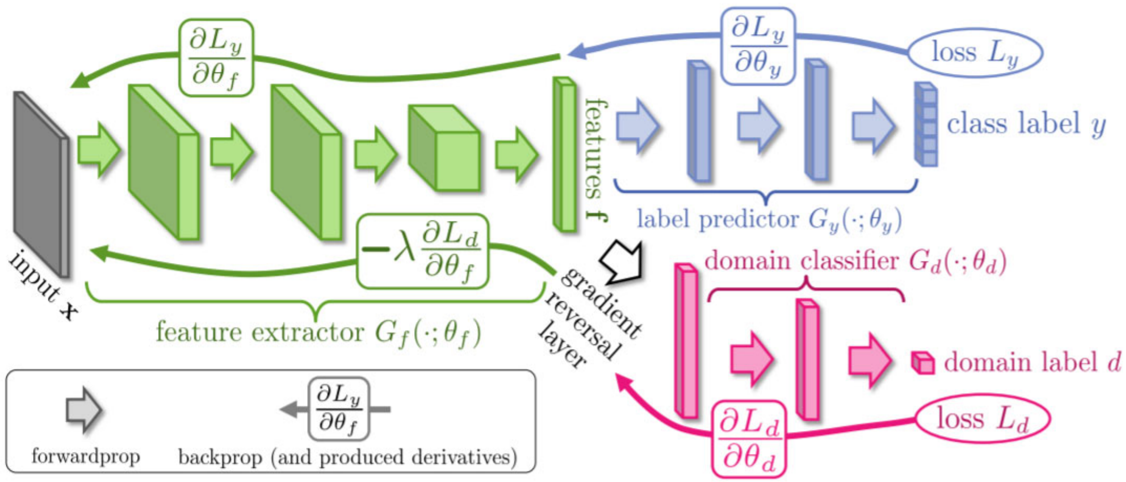
Slides→

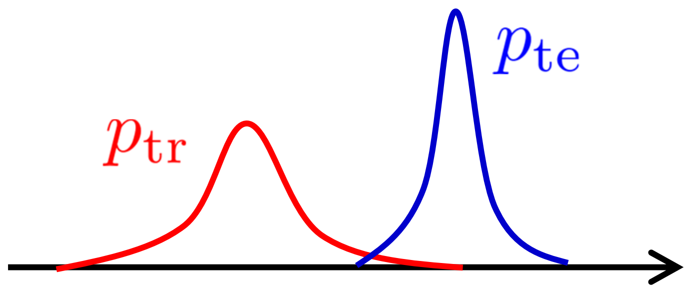
Beyond Importance Weighting?

- Limitation of importance weighting:
  - The training domain must cover the test domain. $\dfrac{p_{\mathrm{te}}(\boldsymbol{x}, y)}{p_{\mathrm{tr}}(\boldsymbol{x}, y)} < \infty$



- What if the test domain sticks out from the training domain?
  - Feature matching





Ben-David+ (NeurIPS2006), Ganin+ (ICML2015)

- However, considering covariate shift is still essential.

Joint Shift

- Many distribution shift works focus on a particular shift type (e.g., covariate shift):

$$p_{\mathrm{tr}}(\boldsymbol{x}) \neq p_{\mathrm{te}}(\boldsymbol{x}) \qquad p_{\mathrm{tr}}(y|\boldsymbol{x}) = p_{\mathrm{te}}(y|\boldsymbol{x})$$

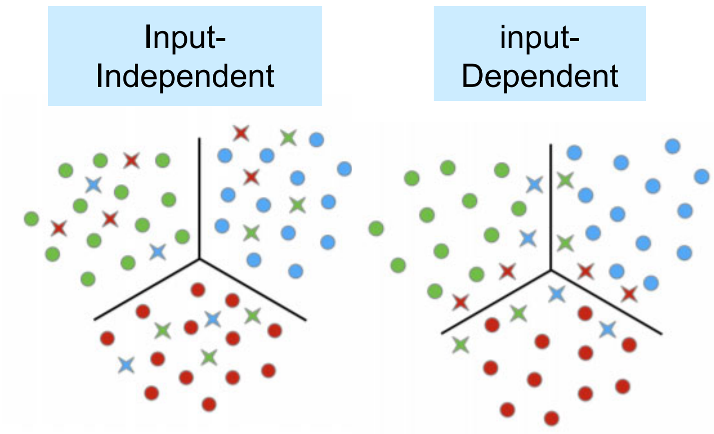
  - However, identification of the shift type is challenging.

- Label noise is also a type of distribution shift:

$$p_{\mathrm{tr}}(\bar{y}|\boldsymbol{x}) = \sum_{y} \underbrace{p(\bar{y}|y,\boldsymbol{x})}_{\text{Noise transition}} p_{\mathrm{te}}(y|\boldsymbol{x})$$

$\bar{y}$: Noisy class label

  - Nice theory for input-independent noise.
  - But input-dependent noise is hard.



- Let's consider joint shift:

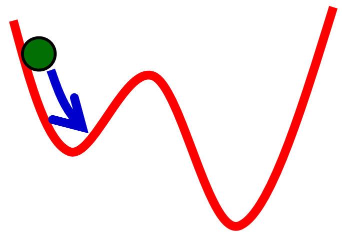
$$p_{\mathrm{tr}}(\boldsymbol{x}, y) \neq p_{\mathrm{te}}(\boldsymbol{x}, y)$$

Mini-Batch-Wise Loss Matching

Fang+ (NeurIPS2020)

- **Given**:
  - (Large) labeled training data: $\{(\boldsymbol{x}_i^{\mathrm{tr}}, y_i^{\mathrm{tr}})\}_{i=1}^{n_{\mathrm{tr}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y)$
  - (Small) labeled test data: $\{(\boldsymbol{x}_j^{\mathrm{te}}, y_j^{\mathrm{te}})\}_{j=1}^{n_{\mathrm{te}}} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{te}}(\boldsymbol{x}, y)$

- We try to learn the importance weight dynamically in the mini-batch-wise manner.



$$f \leftarrow f - \eta \nabla \widehat{R}(f)$$

$\eta > 0$: step size

- For each mini-batch $\{(\tilde{\boldsymbol{x}}_i^{\mathrm{tr}}, \tilde{y}_i^{\mathrm{tr}})\}_{i=1}^{\tilde{n}_{\mathrm{tr}}}, \{(\tilde{\boldsymbol{x}}_j^{\mathrm{te}}, \tilde{y}_j^{\mathrm{te}})\}_{j=1}^{\tilde{n}_{\mathrm{te}}}$, importance weights are estimated by kernel mean matching for loss values:

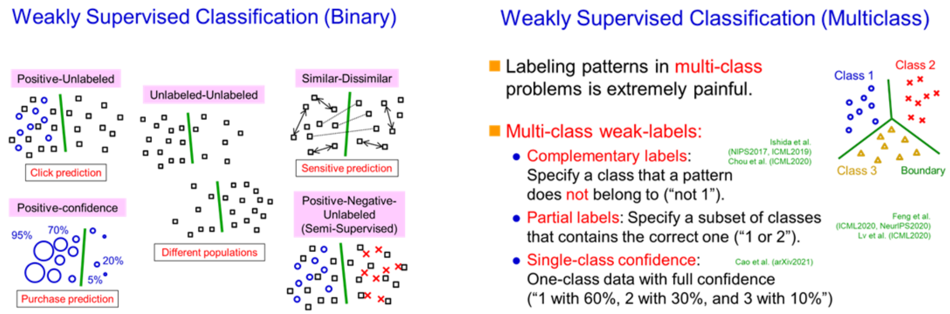
Huang+ (NeurIPS2006)

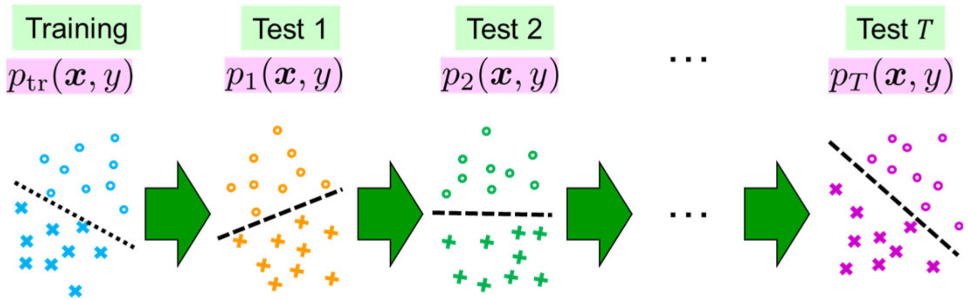
$$\frac{1}{\tilde{n}_{\mathrm{tr}}} \sum_{i=1}^{\tilde{n}_{\mathrm{tr}}} r_i \ell(f(\tilde{\boldsymbol{x}}_i^{\mathrm{tr}}), \tilde{y}_i^{\mathrm{tr}}) \approx \frac{1}{\tilde{n}_{\mathrm{te}}} \sum_{j=1}^{\tilde{n}_{\mathrm{te}}} \ell(f(\tilde{\boldsymbol{x}}_j^{\mathrm{te}}), \tilde{y}_j^{\mathrm{te}})$$

$$r_i \approx \frac{p_{\mathrm{tr}}(\tilde{\boldsymbol{x}}_i^{\mathrm{tr}}, \tilde{y}_i^{\mathrm{tr}})}{p_{\mathrm{tr}}(\tilde{\boldsymbol{x}}_i^{\mathrm{tr}}, \tilde{y}_i^{\mathrm{te}})}$$

Future Challenges

- For joint shift, requiring labeled test data is too strong.
  - Can we perform joint shift adaptation from weak supervision?
  - Can we extend it to continuous joint shift?
  - Can we extend it to a limited-memory setting?





- In real-world application, updating the system online is dangerous because new data can be malicious:
  - Updating the system periodically (daily, etc.) is practical.
  - But we want the system to reflect the latest data.
  - Can we systematically use a buffer for temporary update?

Grateful to Collaborators!

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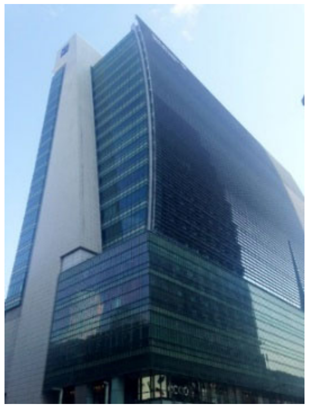

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