

Rethinking Importance Weighting for Transfer Learning

Masashi Sugiyama

RIKEN Center for Advanced Intelligence Project/
The University of Tokyo



<http://www.ms.k.u-tokyo.ac.jp/sugi/>



Problem of Transfer Learning

2

- **Given:** Training data

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

\mathbf{x} : Input

y : Output

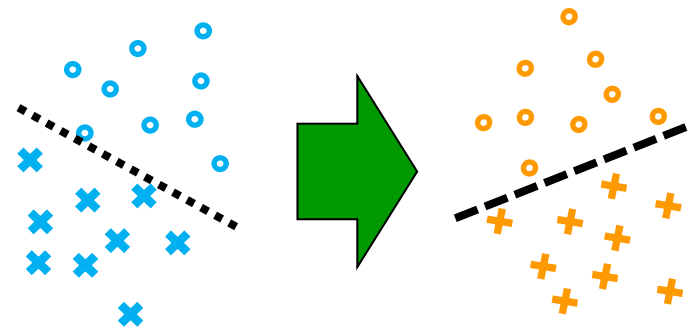
- **Goal:** Train a predictor $y = f(\mathbf{x})$
that works well in the test domain.

$$\min_f R(f) \quad R(f) = \mathbb{E}_{p_{\text{te}}(\mathbf{x}, y)} [\ell(f(\mathbf{x}), y)]$$

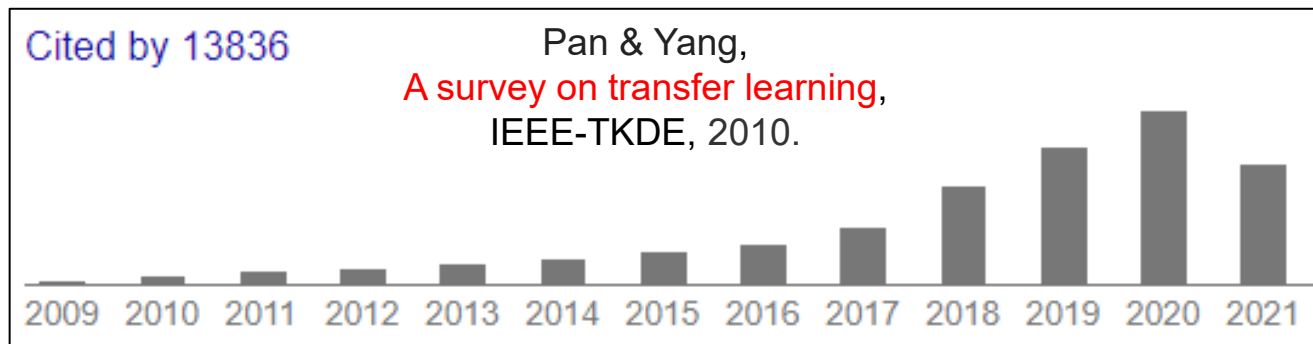
ℓ : loss function

- **Challenge:** Overcome changing distributions!

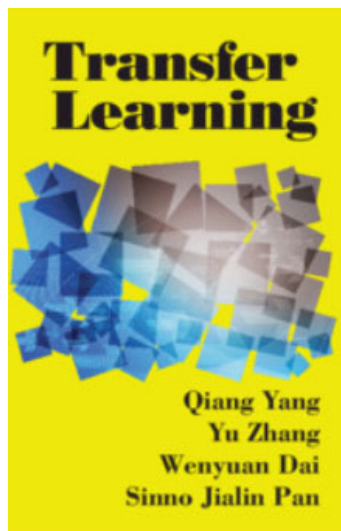
$$p_{\text{tr}}(\mathbf{x}, y) \neq p_{\text{te}}(\mathbf{x}, y)$$



Transfer Learning Has been a Hot Topic for Many Years!

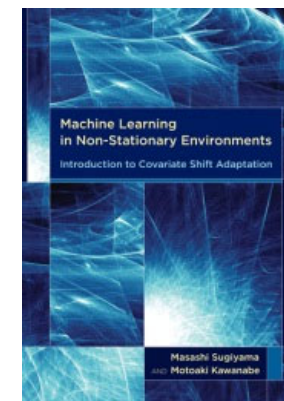


Quiñonero-Candela, Sugiyama,
Schwaighofe & Lawrence (Eds.),
Dataset Shift in Machine Learning,
MIT Press, 2009.



Yang, Zhang, Dai & Pan,
Transfer Learning,
Cambridge University Press, 2020

Sugiyama & Kawanabe,
**Machine Learning
in Non-Stationary Environments**,
MIT Press, 2012



Various Scenarios

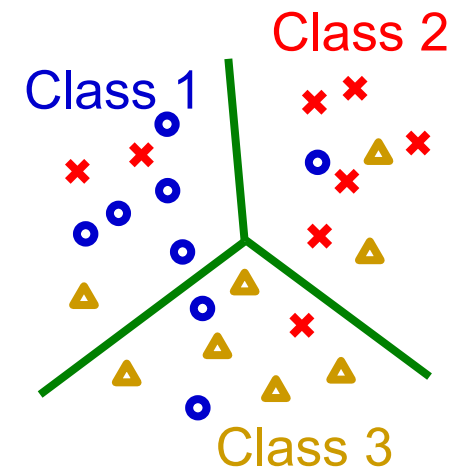
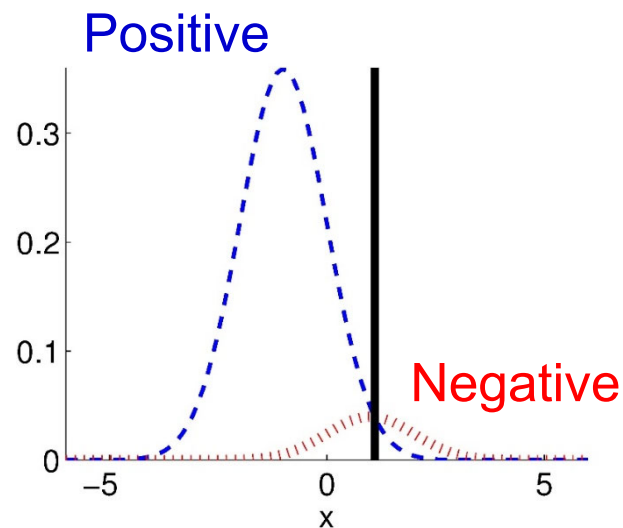
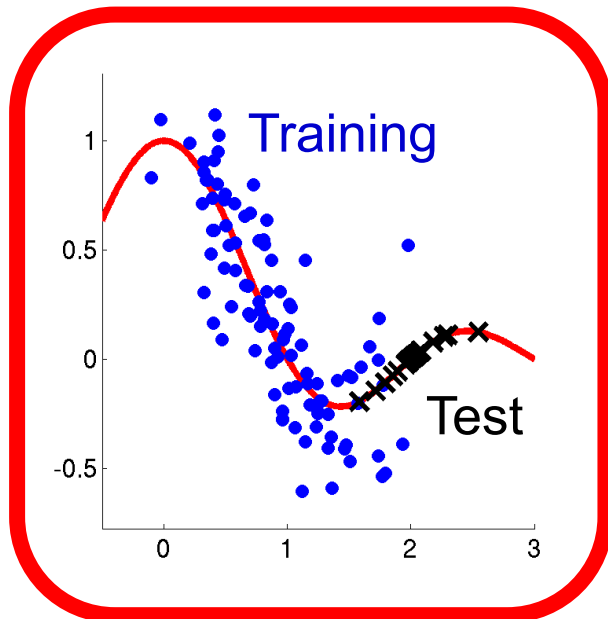
■ Full-distribution shift: $p_{\text{tr}}(\mathbf{x}, y) \neq p_{\text{te}}(\mathbf{x}, y)$

■ Covariate shift: $p_{\text{tr}}(\mathbf{x}) \neq p_{\text{te}}(\mathbf{x})$

■ Class-prior/target shift: $p_{\text{tr}}(y) \neq p_{\text{te}}(y)$

■ Output noise: $p_{\text{tr}}(y|\mathbf{x}) \neq p_{\text{te}}(y|\mathbf{x})$

■ Class-conditional shift: $p_{\text{tr}}(\mathbf{x}|y) \neq p_{\text{te}}(\mathbf{x}|y)$





Organization of My Talk

5

1. Introduction

2. **Classical results**

A) Importance weighting

B) Adaptive importance weighting

3. Recent results

A) Joint upper-bound minimization

B) Dynamic importance weighting

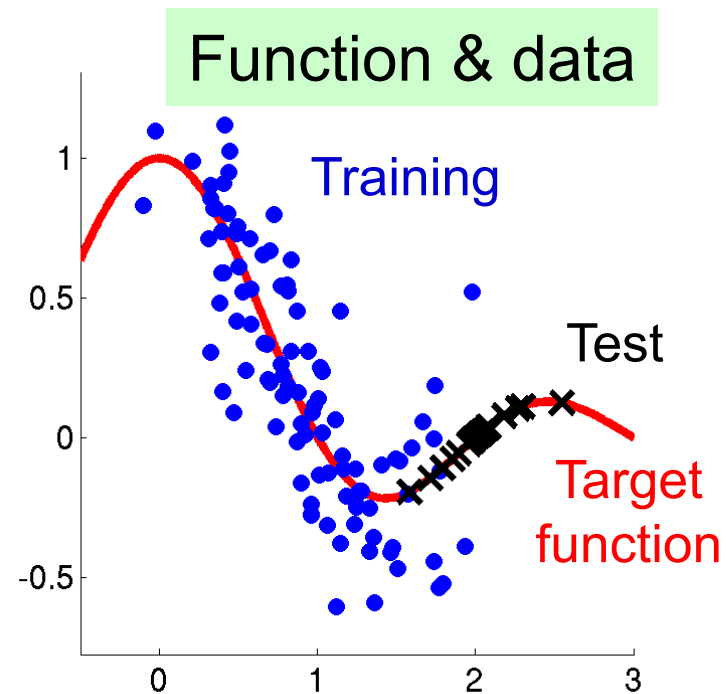
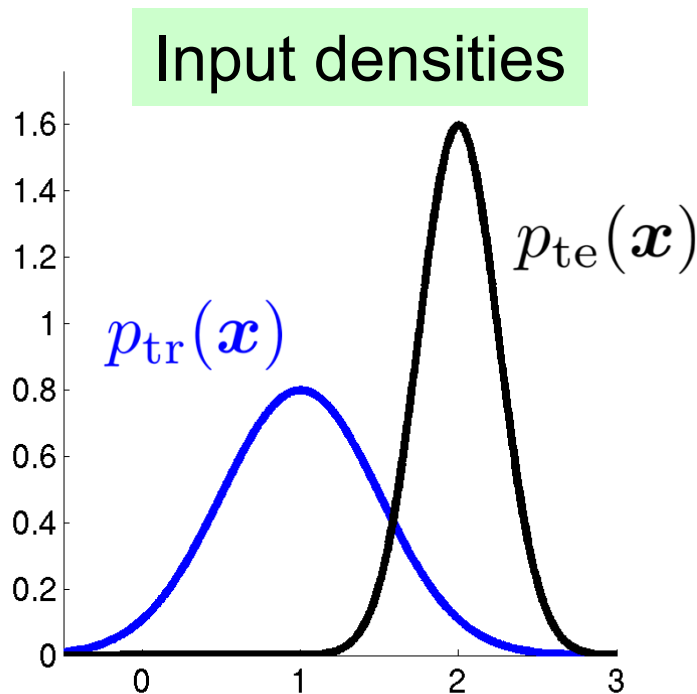
Regression under Covariate Shift ⁶

■ Covariate shift: Shimodaira (JSPI2000)

- Training and test input distributions are different:

$$p_{\text{tr}}(\mathbf{x}) \neq p_{\text{te}}(\mathbf{x})$$

- But the output-given-input distribution remains unchanged: $p_{\text{tr}}(y|\mathbf{x}) = p_{\text{te}}(y|\mathbf{x}) = p(y|\mathbf{x})$



Empirical Risk Minimization (ERM) ⁷

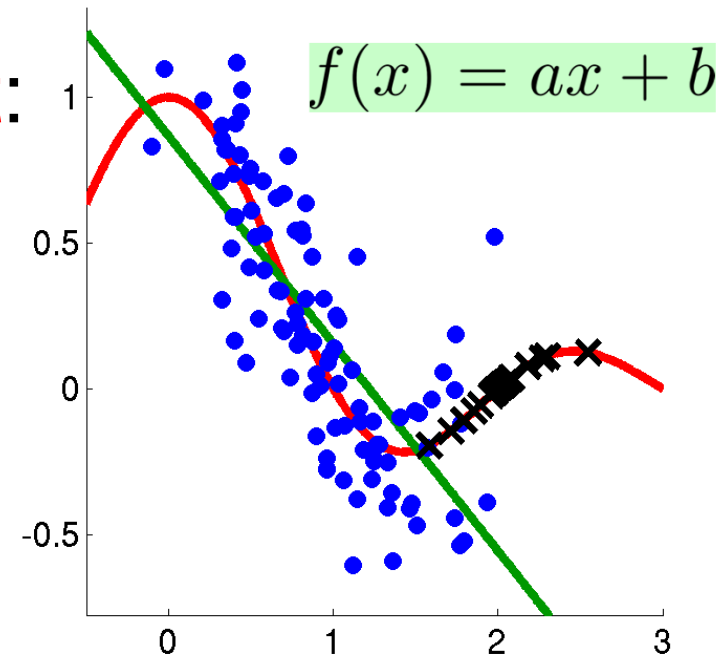
$$\min_f \left[\sum_{i=1}^{n_{\text{tr}}} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \right]$$

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

■ Generally, ERM is **consistent**:

- Learned function converges to the optimal solution when $n_{\text{tr}} \rightarrow \infty$.

■ However, covariate shift makes ERM **inconsistent**:



$$\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \xrightarrow{n_{\text{tr}} \rightarrow \infty} \mathbb{E}_{p_{\text{tr}}(\mathbf{x}, y)} [\ell(f(\mathbf{x}), y)] \neq R(f)$$

$p_{\text{tr}}(\mathbf{x}) \neq p_{\text{te}}(\mathbf{x})$



Organization of My Talk

8

1. Introduction

2. **Classical results**

A) **Importance weighting**

B) Adaptive importance weighting

3. Recent results

A) Joint upper-bound minimization

B) Dynamic importance weighting

Importance-Weighted ERM (IWERM) ⁹

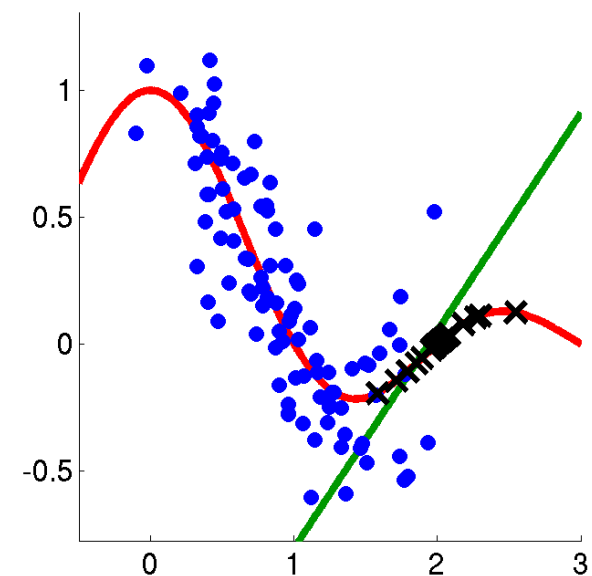
$$\min_f \left[\sum_{i=1}^{n_{\text{tr}}} \underbrace{\frac{p_{\text{te}}(\mathbf{x}_i^{\text{tr}})}{p_{\text{tr}}(\mathbf{x}_i^{\text{tr}})}}_{\text{Importance}} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \right]$$

- IWERM is **consistent** even under covariate shift.

$$\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} \frac{p_{\text{te}}(\mathbf{x}_i^{\text{tr}})}{p_{\text{tr}}(\mathbf{x}_i^{\text{tr}})} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}})$$

$$\begin{aligned} & \xrightarrow[n_{\text{tr}} \rightarrow \infty]{} \mathbb{E}_{p_{\text{tr}}(\mathbf{x}, y)} \left[\frac{p_{\text{te}}(\mathbf{x})}{p_{\text{tr}}(\mathbf{x})} \ell(f(\mathbf{x}), y) \right] \\ & = \mathbb{E}_{p_{\text{te}}(\mathbf{x}, y)} [\ell(f(\mathbf{x}), y)] = R(f) \end{aligned}$$

$$f(x) = ax + b$$



- How can we know the importance weight?

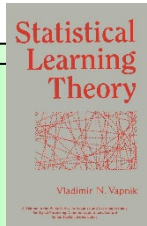
Importance Weight Estimation

10



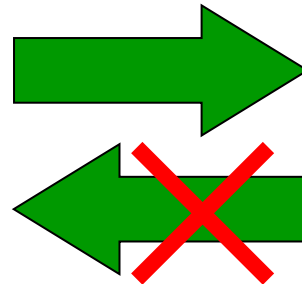
Vapnik's principle: Vapnik (Wiley, 1998)

When solving a problem of interest,
one should not solve a more general problem
as an intermediate step



Knowing densities

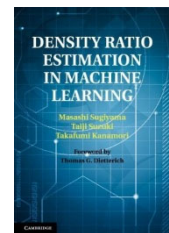
$$p_{\text{te}}(\mathbf{x}), p_{\text{tr}}(\mathbf{x})$$



Knowing ratio

$$r^*(\mathbf{x}) = \frac{p_{\text{te}}(\mathbf{x})}{p_{\text{tr}}(\mathbf{x})}$$

- Estimating the density ratio is substantially easier than estimating both the densities!
- Various direct density-ratio estimators were developed.



Sugiyama, Suzuki & Kanamori,
Density Ratio Estimation
in Machine Learning
(Cambridge University Press, 2012)

Least-Squares Importance Fitting (LSIF) 11

Kanamori, Hido & Sugiyama (JMLR2009)

- Given training and test input data:

$$\{\mathbf{x}_i^{\text{tr}}\}_{i=1}^{n_{\text{tr}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{tr}}(\mathbf{x}) \quad \{\mathbf{x}_j^{\text{te}}\}_{j=1}^{n_{\text{te}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{te}}(\mathbf{x})$$

- Directly fit a model r to $r^*(\mathbf{x}) = \frac{p_{\text{te}}(\mathbf{x})}{p_{\text{tr}}(\mathbf{x})}$ by LS:

$$\min_r Q(r) \quad Q(r) = \int \left(r(\mathbf{x}) - r^*(\mathbf{x}) \right)^2 p_{\text{tr}}(\mathbf{x}) d\mathbf{x}$$

- Empirical approximation:

$$Q(r) = \int r(\mathbf{x})^2 p_{\text{tr}}(\mathbf{x}) d\mathbf{x} - 2 \int r(\mathbf{x}) p_{\text{te}}(\mathbf{x}) d\mathbf{x} + C$$

$$\approx \frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} r(\mathbf{x}_i^{\text{tr}})^2 - \frac{2}{n_{\text{te}}} \sum_{j=1}^{n_{\text{te}}} r(\mathbf{x}_j^{\text{te}}) + C$$



Organization of My Talk

12

1. Introduction

2. Classical results

A) Importance weighting

B) Adaptive importance weighting

3. Recent results

A) Joint upper-bound minimization

B) Dynamic importance weighting

Bias-Variance Trade-Off

13

- Importance-weighted empirical risk estimator

$$\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} \frac{p_{\text{te}}(\mathbf{x}_i^{\text{tr}})}{p_{\text{tr}}(\mathbf{x}_i^{\text{tr}})} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}})$$

has **no bias, but has large variance.**

- The ordinary empirical risk estimator

$$\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}})$$

has **small variance (statistically efficient), but has large bias.**

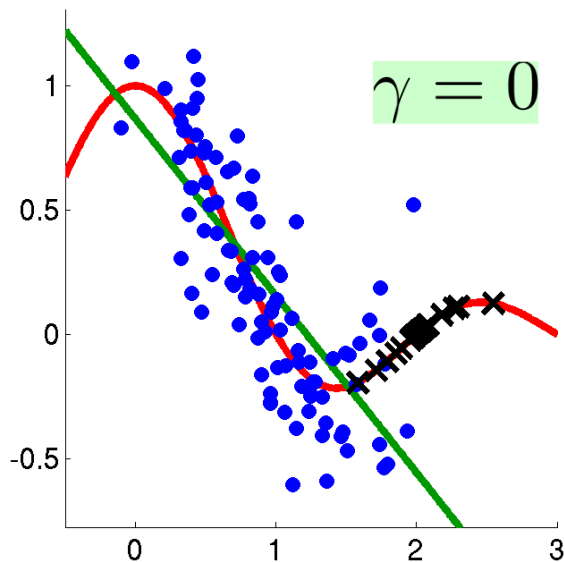
- How can we control the **bias-variance trade-off?**

Flattened Importance Weighting ¹⁴

$$\min_f \left[\sum_{i=1}^{n_{\text{tr}}} \left(\frac{p_{\text{te}}(\mathbf{x}_i^{\text{tr}})}{p_{\text{tr}}(\mathbf{x}_i^{\text{tr}})} \right)^\gamma \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \right]$$

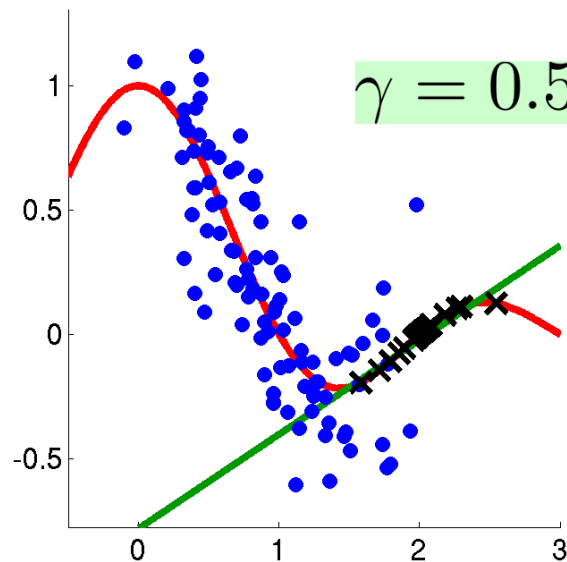
Shimodaira
(JSPI2000)

$$0 \leq \gamma \leq 1$$



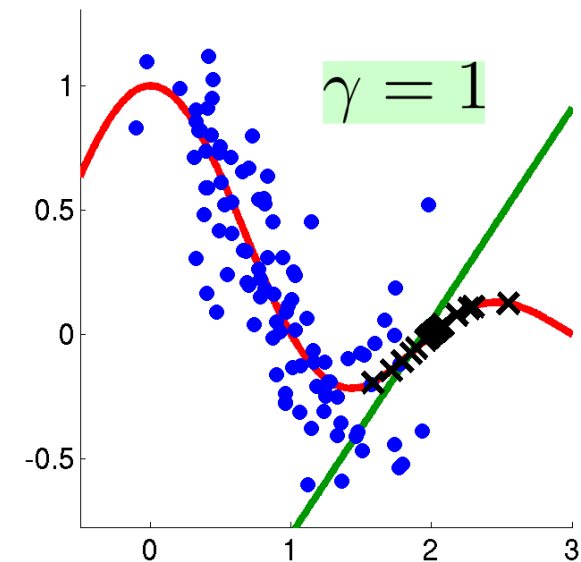
$\gamma = 0$

Large bias, small variance



$\gamma = 0.5$

(Intermediate)



$\gamma = 1$

Small bias, large variance

■ **Flattening factor** γ may be chosen by

Shimodaira
(JSPI2000)

- Importance-weighted Akaike information criterion
- Importance-weighted cross-validation

Sugiyama, Krauledat
& Müller (JMLR2007)

Relative Importance Weighting

15

- Even with direct methods, reliably estimating the importance weight is hard:

- $r^*(\mathbf{x})$ could be highly fluctuated.

$$r^*(\mathbf{x}) = \frac{p_{\text{te}}(\mathbf{x})}{p_{\text{tr}}(\mathbf{x})}$$

- Thus, flattening unreliable importance estimator $\hat{r}(\mathbf{x})$ by power factor γ is also unreliable.

$$\min_f \left[\sum_{i=1}^{n_{\text{tr}}} \hat{r}(\mathbf{x}_i^{\text{tr}})^\gamma \ell(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \right]$$

- Let's use **relative importance weight**:

Yamada, Suzuki, Kanamori, Hachiya & Sugiyama (NIPS2011, NeCo2013)

$$r_\beta(\mathbf{x}) = \frac{p_{\text{te}}(\mathbf{x})}{\beta p_{\text{tr}}(\mathbf{x}) + (1 - \beta) p_{\text{te}}(\mathbf{x})} \quad 0 \leq \beta \leq 1$$

- Directly estimable for each β by relative LSIF.



Organization of My Talk

16

1. Introduction
2. Classical results
 - A) Importance weighting
 - B) Adaptive importance weighting
3. **Recent results**
 - A) Joint upper-bound minimization
 - B) Dynamic importance weighting

One-Step Adaptation

■ The classical approaches are **two steps**:

1. Weight estimation (e.g., LSIF):

$$\hat{r} = \operatorname{argmin}_r \mathbb{E}_{p_{\text{tr}}(\mathbf{x})} [(r(\mathbf{x}) - r^*(\mathbf{x}))^2]$$

2. Weighted predictor training (e.g., IWERM):

$$\hat{f} = \operatorname{argmin}_f \mathbb{E}_{p_{\text{tr}}(\mathbf{x}, y)} [\hat{r}(\mathbf{x}) \ell(f(\mathbf{x}), y)]$$

■ Can we integrate these two steps?



Organization of My Talk

18

1. Introduction
2. Classical results
 - A) Importance weighting
 - B) Adaptive importance weighting
3. **Recent results**
 - A) **Joint upper-bound minimization**
 - B) Dynamic importance weighting

Risk Upper-Bounding

19

Zhang, Yamane,
Lu & Sugiyama
(ACML2020,
SNCS2021)

- For $\ell \leq 1, \ell' \geq \ell, r \geq 0, \frac{1}{2}R_\ell(f)^2 \leq J_{\ell'}(r, f)$:

$$R_\ell(f) = \mathbb{E}_{p_{\text{te}}(\mathbf{x}, y)}[\ell(f(\mathbf{x}), y)]$$

$$J_{\ell'}(r, f) = (\mathbb{E}_{p_{\text{tr}}(\mathbf{x}, y)}[r(\mathbf{x})\ell'(f(\mathbf{x}), y)])^2 \leftarrow \text{IWERM}$$
$$+ \mathbb{E}_{p_{\text{tr}}(\mathbf{x})}[(r(\mathbf{x}) - r^*(\mathbf{x}))^2] \leftarrow \text{LSIF}$$

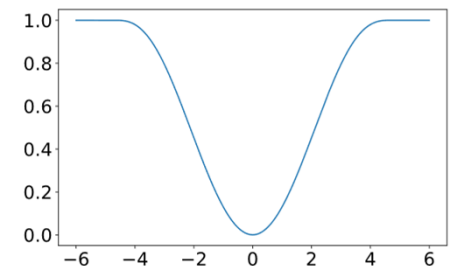
- In terms of this upper-bound minimization, LSIF followed by IWERM is sub-optimal:

- Let's directly minimize the upper bound w.r.t. r, f !

- $\ell \leq 1, \ell' \geq \ell$ is satisfied by

- ℓ : 0/1, ℓ' : hinge/softmax cross-entropy (classification)
- ℓ : Tukey, ℓ' : squared (regression)

Tukey loss



Theoretical Analysis

20

- Let $\hat{f} = \operatorname{argmin}_f \min_r \hat{J}_{\ell'}(r, f)$ be an empirical solution.

$$\hat{J}_{\ell'}(r, f) = \left(\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} r(\mathbf{x}_i^{\text{tr}}) \ell'(f(\mathbf{x}_i^{\text{tr}}), y_i^{\text{tr}}) \right)^2 + \left(\frac{1}{n_{\text{tr}}} \sum_{i=1}^{n_{\text{tr}}} r(\mathbf{x}_i^{\text{tr}})^2 - \frac{2}{n_{\text{te}}} \sum_{j=1}^{n_{\text{te}}} r(\mathbf{x}_j^{\text{tr}}) + C \right)$$

$$\{(\mathbf{x}_i^{\text{tr}}, y_i^{\text{tr}})\}_{i=1}^{n_{\text{tr}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{tr}}(\mathbf{x}, y) \quad \{\mathbf{x}_j^{\text{te}}\}_{j=1}^{n_{\text{te}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{te}}(\mathbf{x})$$

- Under some mild conditions, the risk of the empirical solution is upper-bounded as

$$R_{\ell}(\hat{f}) \leq \sqrt{2} \min_f R_{\ell'}(f) + \mathcal{O}_p(n_{\text{tr}}^{-1/4} + n_{\text{te}}^{-1/4})$$

$$R_{\ell}(\hat{f}) = \mathbb{E}_{p_{\text{te}}(\mathbf{x}, y)}[\ell(\hat{f}(\mathbf{x}), y)]$$

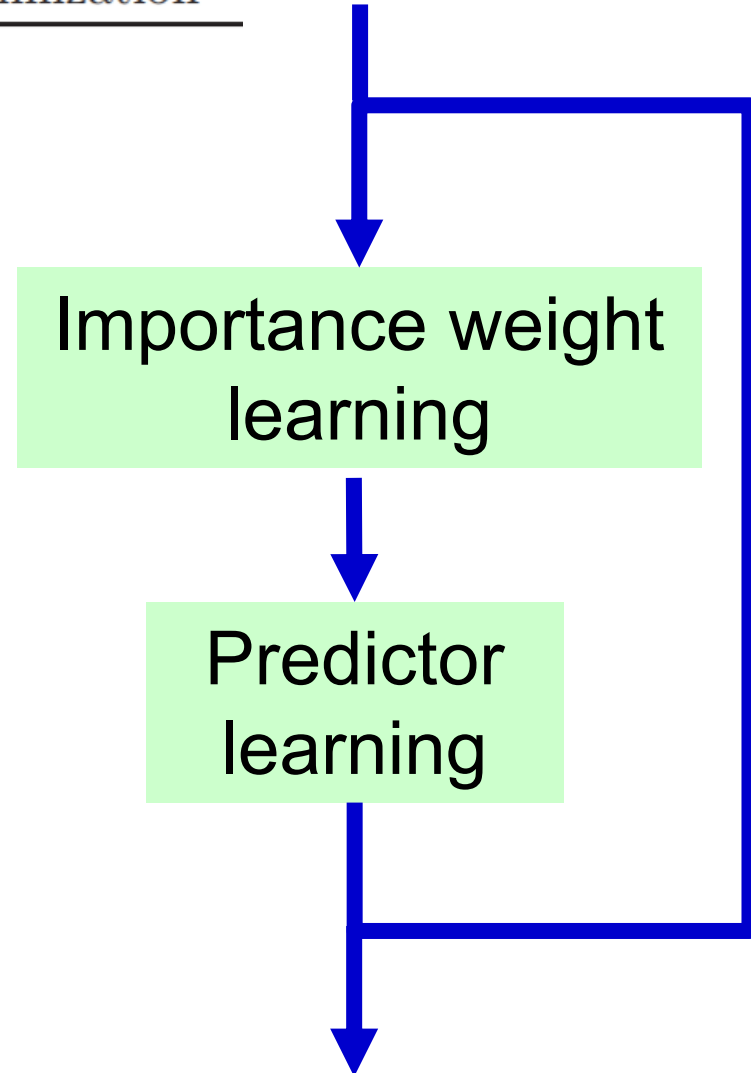
$$R_{\ell'}(f) = \mathbb{E}_{p_{\text{te}}(\mathbf{x}, y)}[\ell'(f(\mathbf{x}), y)]$$

Practical Implementation

21

Algorithm 2 Gradient-based Alternating Minimization

```
1:  $\mathcal{Z}^{\text{tr}}, \mathcal{X}^{\text{te}} \leftarrow \{(\mathbf{x}_i^{\text{tr}}, y_i^{\text{tr}})\}_{i=1}^{n_{\text{tr}}}, \{\mathbf{x}_i^{\text{te}}\}_{i=1}^{n_{\text{te}}}$ 
2:  $\mathcal{A} \leftarrow$  a gradient-based optimizer
3:  $f \leftarrow$  an arbitrary classifier
4: for round = 0, 1, ..., numOfRounds - 1 do
5:   for epoch = 0, 1, ..., numOfEpochsForG - 1 do
6:     for  $i = 0, 1, \dots, \text{numOfMiniBatches} - 1$  do
7:        $\mathcal{Z}_i^{\text{tr}}, \mathcal{X}_i^{\text{te}} \leftarrow \text{sampleMiniBatch}(\mathcal{Z}^{\text{tr}}, \mathcal{X}^{\text{te}})$ 
8:        $g \leftarrow \mathcal{A}(g, \nabla_g \hat{J}_{\text{UB}}(f, g; \mathcal{Z}_i^{\text{tr}} \cup \mathcal{X}_i^{\text{te}}))$ 
9:     end for
10:  end for
11:  for epoch = 0, 1, ..., numOfEpochsForF - 1 do
12:    for  $i = 0, 1, \dots, \text{numOfMiniBatches} - 1$  do
13:       $\mathcal{Z}_i^{\text{tr}} \leftarrow \text{sampleMiniBatch}(\mathcal{Z}^{\text{tr}})$ 
14:       $w_j \leftarrow \max(g(\mathbf{x}_j), 0), \forall (\mathbf{x}_j, \cdot) \in \mathcal{Z}_i^{\text{tr}}$ 
15:       $w_j \leftarrow w_j / \sum_j w_j, \forall j$ 
16:       $L_i \leftarrow \sum_{(\mathbf{x}_j, y_j) \in \mathcal{Z}_i^{\text{tr}}} w_j \ell_{\text{UB}}(f(\mathbf{x}_j), y_j)$ 
17:       $f \leftarrow \mathcal{A}(f, \nabla_f L_i)$ 
18:    end for
19:  end for
20: end for
```



Experimental Evaluation

22

Table 3 Mean test classification accuracy averaged over 5 trials on image datasets with neural networks. The numbers in the brackets are the standard deviations. For each dataset, the best method and comparable ones based on the *paired t-test* at the significance level 5% are described in bold face.

Dataset	Shift Level (a, b)	ERM	EIWERM	RIWERM	one-step
Fashion-MNIST	(2, 4)	81.71(0.17)	84.02(0.18)	84.12(0.06)	85.07(0.08)
	(2, 5)	72.52(0.54)	76.68(0.27)	77.43(0.29)	78.83(0.20)
	(2, 6)	60.10(0.34)	65.73(0.34)	66.73(0.55)	69.23(0.25)
Kuzushiji-MNIST	(2, 4)	77.09(0.18)	80.92(0.32)	81.17(0.24)	82.45(0.12)
	(2, 5)	65.06(0.26)	71.02(0.50)	72.16(0.19)	74.03(0.16)
	(2, 6)	51.24(0.30)	58.78(0.38)	60.14(0.93)	62.70(0.55)

Shimodaira (JSPI2000)

Yamada, Suzuki, Kanamori, Hachiya
& Sugiyama (NIPS2011, NeCo2013)



Organization of My Talk

23

1. Introduction
2. Classical results
 - A) Importance weighting
 - B) Adaptive importance weighting
3. **Recent results**
 - A) Joint upper-bound minimization
 - B) **Dynamic importance weighting**

Dynamic Importance Weighting ²⁴

Fang, Lu, Niu & Sugiyama (NeurIPS2020)

- Deep learning adopts **iterative optimization**.

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

$\eta > 0$: Learning rate

- Let's learn

- Importance weight r
- predictor f

dynamically in the **mini-batch-wise** manner.

Mini-Batch-Wise Loss Matching 25

■ Suppose we are given

- (Large) training data: $\{(\mathbf{x}_i^{\text{tr}}, y_i^{\text{tr}})\}_{i=1}^{n_{\text{tr}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{tr}}(\mathbf{x}, y)$
- (Small) test data: $\{(\mathbf{x}_i^{\text{te}}, y_i^{\text{te}})\}_{i=1}^{n_{\text{te}}} \stackrel{\text{i.i.d.}}{\sim} p_{\text{te}}(\mathbf{x}, y)$

■ For **each mini-batch** $\{(\bar{\mathbf{x}}_i^{\text{tr}}, \bar{y}_i^{\text{tr}})\}_{i=1}^{\bar{n}_{\text{tr}}}, \{(\bar{\mathbf{x}}_i^{\text{te}}, \bar{y}_i^{\text{te}})\}_{i=1}^{\bar{n}_{\text{te}}}$, importance weights are estimated by matching **loss values by kernel mean matching:**

Huang, Gretton, Borgwardt, Schölkopf & Smola (NeurIPS2007)

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

■ **No covariate shift assumption is needed!**

Practical Implementation

Algorithm 1 Dynamic importance weighting (in a mini-batch).

Require: a training mini-batch \mathcal{S}^{tr} , a validation mini-batch \mathcal{S}^{v} , the current model f_{θ_t}

- 1: forward the input parts of \mathcal{S}^{tr} & \mathcal{S}^{v}
 - 2: compute the loss values as \mathcal{L}^{tr} & \mathcal{L}^{v}
 - 3: match \mathcal{L}^{tr} & \mathcal{L}^{v} to obtain \mathcal{W}
 - 4: weight the empirical risk $\widehat{R}(f_{\theta})$ by \mathcal{W}
 - 5: backward $\widehat{R}(f_{\theta})$ and update θ
-

Experimental Evaluation

Table 4: Mean accuracy (standard deviation) in percentage on Fashion-MNIST (F-MNIST for short), CIFAR-10/100 under label noise (5 trials). Best and comparable methods (paired t -test at significance level 5%) are highlighted in bold. p/s is short for pair/symmetric flip.

	Noise	Clean	Uniform	Random	IW	Reweight	DIW
F-MNIST	0.3 p	71.05 (1.03)	76.89 (1.06)	84.62 (0.68)	82.69 (0.38)	88.74 (0.19)	88.19 (0.43)
	0.4 s	73.55 (0.80)	77.13 (2.21)	84.58 (0.76)	80.54 (0.66)	85.94 (0.51)	88.29 (0.18)
	0.5 s	73.55 (0.80)	73.70 (1.83)	82.49 (1.29)	78.90 (0.97)	84.05 (0.51)	87.67 (0.57)
CIFAR-10	0.3 p	45.62 (1.66)	77.75 (3.27)	83.20 (0.62)	45.02 (2.25)	82.44 (1.00)	84.44 (0.70)
	0.4 s	45.61 (1.89)	69.59 (1.83)	76.90 (0.43)	44.31 (2.14)	76.69 (0.57)	80.40 (0.69)
	0.5 s	46.35 (1.24)	65.23 (1.11)	71.56 (1.31)	42.84 (2.35)	72.62 (0.74)	76.26 (0.73)
CIFAR-100	0.3 p	10.82 (0.44)	50.20 (0.53)	48.65 (1.16)	10.85 (0.59)	48.48 (1.52)	53.94 (0.29)
	0.4 s	10.82 (0.44)	46.34 (0.88)	42.17 (1.05)	10.61 (0.53)	42.15 (0.96)	53.66 (0.28)
	0.5 s	10.82 (0.44)	41.35 (0.59)	34.99 (1.19)	10.58 (0.17)	36.17 (1.74)	49.13 (0.98)



Organization of My Talk

27

1. Introduction
2. Classical results
 - A) Importance weighting
 - B) Adaptive importance weighting
3. Recent results
 - A) Joint upper-bound minimization
 - B) Dynamic importance weighting

Conclusions

- In transfer learning, combining **importance estimation** and **predictor training** is promising.
- What should we do if the training and test distributions are very different?
 - **Mechanism transfer!**

Teshima, Sato & Sugiyama (ICML2020)

