Direct Importance Estimation with Model Selection and Its Application to Covariate Shift Adaptation

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Abstract

When training and test samples follow different input distributions (i.e., the situation called \textit{covariate shift}), the maximum likelihood estimator is known to lose its consistency. For regaining consistency, the log-likelihood terms need to be weighted according to the \textit{importance} (i.e., the ratio of test and training input densities). Thus, accurately estimating the importance is one of the key tasks in covariate shift adaptation. A naive approach is to first estimate training and test input densities and then estimate the importance by the ratio of the density estimates. However, since density estimation is a hard problem, this approach tends to perform poorly especially in high dimensional cases. In this paper, we propose a direct importance estimation method that does not require the input density estimates. Our method is equipped with a natural model selection procedure so tuning parameters such as the kernel width can be objectively optimized. This is an advantage over a recently developed method of direct importance estimation. Simulations illustrate the usefulness of our approach.
In supervised learning, we always assume

Training and test samples are drawn from the same distribution

\[ P_{\text{train}}(\mathbf{x}, y) = P_{\text{test}}(\mathbf{x}, y) \]

Is this assumption really true?

Not Always True!
Face Recognition

- We tend to collect easy-to-gather samples for training.
  - Training: less women in research labs
  - Test: almost 50-50 in general

The Yale Face Database B
Those who have strong opinions tend to reply to questionnaires.

- Training: extreme opinions
- Test: most people are neutral
Brain-Computer Interface

- Sample generation mechanism varies.
  - Input: EEG signals
  - Output: “left” or “right” commands
  - Different mental conditions between training (sleepy…) and test (exciting!) phases may change the EEG signals.

Figure provided by Fraunhofer FIRST, Berlin, Germany
Robot Control by Reinforcement Learning

Updating a robot’s behavior causes a distribution change.

Khepera Robot
Covariate Shift

- However, no chance for generalization if training and test samples have nothing in common.

\[ P_{\text{train}}(x, y) \neq P_{\text{test}}(x, y) \]

We need a (reasonable) constraint

Covariate shift

- Input distribution changes:
  \[ P_{\text{train}}(x) \neq P_{\text{test}}(x) \]

- Functional relation remains unchanged:
  \[ P_{\text{train}}(y|x) = P_{\text{test}}(y|x) \]
Illustration of Covariate Shift

(Weak) extrapolation:
Predict output values outside training region

Input Density
Generalization error (expected test error):

\[ \mathbb{E} \int \left( \hat{f}(\mathbf{x}) - f(\mathbf{x}) \right)^2 p_{test}(\mathbf{x}) d\mathbf{x} \]

\[ = \int \left( \mathbb{E}\hat{f}(\mathbf{x}) - f(\mathbf{x}) \right)^2 p_{test}(\mathbf{x}) d\mathbf{x} \]

\[ + \mathbb{E} \int \left( \mathbb{E}\hat{f}(\mathbf{x}) - \hat{f}(\mathbf{x}) \right)^2 p_{test}(\mathbf{x}) d\mathbf{x} \]

\(\mathbb{E}: \text{expectation over samples}\)
Model Specification

- Model is said to be correctly specified if

\[ \exists \alpha^*, \hat{f}(x; \alpha^*) = f(x) \]

- In practice, our model may not be correct.
- Therefore, we need to explicitly deal with misspecified models!
**Ordinary Least-Squares (OLS)**

\[
\min_{\alpha} \left[ \sum_{i=1}^{n_{\text{train}}} \left( \hat{f}(x_i^{\text{train}}) - y_i^{\text{train}} \right)^2 \right]
\]

- **If model is correct:**
  - OLS minimizes bias asymptotically

- **If model is misspecified:**
  - OLS does not minimize bias even asymptotically.

We want to reduce bias!
Importance-Weighted LS (IWLS)\(^3\)

\[
\min_{\alpha} \left[ \sum_{i=1}^{n_{\text{train}}} w(x_i^{\text{train}}) \left( \hat{f}(x_i^{\text{train}}) - y_i^{\text{train}} \right)^2 \right]
\]

\[ w(x) = \frac{p_{\text{test}}(x)}{p_{\text{train}}(x)} \quad : \text{Importance} \]

\[ p_{\text{train}}(x) \quad : \text{Assumed strictly positive} \]

- Even for misspecified models, IWLS minimizes bias asymptotically.
- We need to estimate the importance in practice.
Importance Estimation

- **Setting:** training and test inputs are given

\[
\{ \mathbf{x}_{i \text{train}} \}_{i=1}^{n_{\text{train}}} \overset{i.i.d.}{\sim} p_{\text{train}}(\mathbf{x}) \\
\{ \mathbf{x}_{j \text{test}} \}_{j=1}^{n_{\text{test}}} \overset{i.i.d.}{\sim} p_{\text{test}}(\mathbf{x})
\]

- Naïve approach: estimate \( p_{\text{train}}(\mathbf{x}) \) and \( p_{\text{test}}(\mathbf{x}) \) separately, and take the ratio of the density estimates

- Naïve approach does not work well since density estimation is hard in high dimensions.
We use a linear model:

\[
\hat{w}(x) = \sum_{\ell=1}^{t} \theta_{\ell} \phi_{\ell}(x) \quad \theta_{\ell}, \phi_{\ell}(x) \geq 0
\]

Test density is approximated by

\[
\hat{p}_{\text{test}}(x) = \hat{w}(x)p_{\text{train}}(x)
\]

Learn \(\{\theta_{\ell}\}_{\ell=1}^{t}\) so that \(\hat{p}_{\text{test}}(x)\) approximates \(p_{\text{test}}(x)\) well.
Kullback-Leibler Divergence

\[ \min_{\{\theta_i\}_{i=1}^t} KL[p_{\text{test}}(x) \| \hat{p}_{\text{test}}(x)] \]

\[ \hat{p}_{\text{test}}(x) = \hat{w}(x)p_{\text{train}}(x) \]

- \[ KL[p_{\text{test}}(x) \| \hat{w}(x)p_{\text{train}}(x)] = \int p_{\text{test}}(x) \log \frac{p_{\text{test}}(x)}{\hat{w}(x)p_{\text{train}}(x)} \, dx \]

- \[ = \int p_{\text{test}}(x) \log \frac{p_{\text{test}}(x)}{p_{\text{train}}(x)} \, dx \text{ (constant)} \]

- \[ - \int p_{\text{test}}(x) \log \hat{w}(x) \, dx \text{ (relevant)} \]
Thus

$$\min_{\{\theta_\ell\}_{\ell=1}^t} KL[\hat{w}(x)p_{\text{train}}(x) \| p_{\text{test}}(x)]$$

$$\max_{\{\theta_\ell\}_{\ell=1}^t} \int p_{\text{test}}(x) \log \hat{w}(x) dx$$

(objective function)

Since $\hat{p}_{\text{test}}(x) = \hat{w}(x)p_{\text{train}}(x)$ is density,

$$\int \hat{w}(x)p_{\text{train}}(x) dx = 1$$

(constraint)
KLIEP (Kullback-Leibler Importance Estimation Procedure)

$$\max_{\{\theta_\ell\}_{\ell=1}^t} \left[ \sum_{j=1}^{n_{\text{test}}} \log \hat{w}(x_j^{\text{test}}) \right]$$

subject to \( \sum_{i=1}^{n_{\text{train}}} \hat{w}(x_i^{\text{train}}) = n_{\text{train}} \)

\( \theta_1, \theta_2, \ldots, \theta_t \geq 0 \)

- **Convexity:** unique global solution is available
- **Sparse solution:** prediction is fast!
\[ \hat{w}(\mathbf{x}) = \sum_{\ell=1}^{n_{\text{test}}} \theta_{\ell} K(\mathbf{x}, \mathbf{x}_{\ell}^{\text{test}}) \]

\[ K(\mathbf{x}, \mathbf{x}') = \exp \left( -\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\sigma^2} \right) \]
How to choose tuning parameters (such as Gaussian width)?

Likelihood cross-validation:
- Divide test samples $\{x_j^{\text{test}}\}_{j=1}^{n_{\text{test}}}$ into $\mathcal{X}$ and $\mathcal{X}'$.
- Learn importance from $\mathcal{X}$.
- Estimate the likelihood using $\mathcal{X}'$.

$$\frac{1}{|\mathcal{X}'|} \sum_{x' \in \mathcal{X}'} \log \hat{w}_x(x')$$

This gives an unbiased estimate of KL (up to an irrelevant constant).
Illustrative Experiments: Setup

Kernel density estimator (KDE):
- Separately estimate training and test input densities.
- Gaussian kernel width is chosen by likelihood cross-validation.

Kernel mean matching (KMM): (Huang et al., NIPS2006)
- Direct importance estimation method using universal reproducing kernel Hilbert spaces
- There is no model selection method for kernel width; we test several different widths.

Input distributions: standard Gaussian with
- Training: mean (0,0,…,0)
- Test: mean (1,0,…,0)
KDE: Suffers from the curse of dimensionality

KMM: Performance depends on kernel width

KLIEP: Model selection by LCV works well
Goal: given \( \{x_i^{\text{train}}, y_i^{\text{train}}\}_{i=1}^{n_{\text{train}}}, \{x_j^{\text{test}}\}_{j=1}^{n_{\text{test}}} \)
 predict \( \{y_j^{\text{test}}\}_{j=1}^{n_{\text{test}}} \).

Gaussian kernel model:

\[
\hat{f}(x) = \sum_{\ell=1}^{50} \alpha_\ell \exp \left( -\frac{\|x - m_\ell\|^2}{2h^2} \right)
\]

Regularized IWLS:

\[
\min_\alpha \left[ \sum_{i=1}^{n_{\text{train}}} \hat{w}(x_i^{\text{train}}) \left( \hat{f}(x_i^{\text{train}}) - y_i^{\text{train}} \right)^2 + \gamma \|\alpha\|^2 \right].
\]

Importance is estimated by KLIEP with LCV.

\( h, \gamma \) are chosen by importance-weighted cross-validation. (Sugiyama et al., JMLR2007)
## Results

Normalized test error
(mean and standard deviation over 100 trials)

<table>
<thead>
<tr>
<th>Data</th>
<th>Dim</th>
<th>Uniform</th>
<th>KLIEP(LCV)</th>
<th>KDE(LCV)</th>
<th>KMM(0.01)</th>
<th>KMM(0.3)</th>
<th>KMM(1)</th>
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</thead>
<tbody>
<tr>
<td>Kin-8fh</td>
<td>8</td>
<td>1.00(0.34)</td>
<td>0.95(0.31)</td>
<td>1.22(0.52)</td>
<td>1.00(0.34)</td>
<td>0.97(0.34)</td>
<td>1.47(0.24)</td>
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<td>Kin-8fm</td>
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<tr>
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<td>1.15(0.25)</td>
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<tr>
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<td>0.97(0.25)</td>
<td>1.14(0.26)</td>
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<td>1.19(0.22)</td>
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<td>Abalone</td>
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<td>1.02(0.41)</td>
<td>0.99(0.50)</td>
<td>1.03(0.74)</td>
<td>0.93(0.40)</td>
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<tr>
<td>Image</td>
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<td>1.00(0.50)</td>
<td>0.92(0.41)</td>
<td>0.98(0.44)</td>
<td>0.97(0.50)</td>
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<td>1.06(0.50)</td>
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<tr>
<td>Ringnorm</td>
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<td>0.99(0.06)</td>
<td>0.87(0.04)</td>
<td>1.00(0.04)</td>
<td>0.96(0.07)</td>
<td>0.88(0.06)</td>
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<tr>
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<td>1.05(0.47)</td>
<td>1.00(0.45)</td>
<td>0.94(0.34)</td>
<td>1.00(0.33)</td>
</tr>
</tbody>
</table>

**Red**: Best method and comparable ones by Wilcoxon signed rank test at significance level 5%