A new similarity measure for covariate shift with applications to nonparametric regression

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ICML 2022
Challenges with distribution shift
Recht, Roelofs, Schmidt, Shankar, 2019

ImageNet

New test accuracy (top-1, %)

Original test accuracy (top-1, %)
Regression under covariate shift

our work focuses on regression under covariate shift

**observational model**
we observe a dataset \( \{(X_i, Y_i)\}_{i=1}^n \), where

\[
Y_i = f^*(X_i) + \xi_i, \quad i = 1, \ldots, n,
\]

where \( f^* = \mathbb{E}[Y \mid X = \cdot] \)

**covariate distribution**
covariates are sampled from *source* distribution \( P \) and *target* distribution \( Q \):

- **source** covariates: \( X_1, \ldots, X_{np} \) i.i.d. \( P \), \( (n = np + n_Q) \)
- **target** covariates: \( X_{np+1}, \ldots, X_{np+n_Q} \) i.i.d. \( Q \),
we define a measure between two distributions $P, Q$ on metric space $(\mathcal{X}, d)$

**similarity measure**

for radius $h > 0$, we define

$$
\rho_h(P, Q) := \int_{\mathcal{X}} \frac{1}{P(B(x, h))} \, dQ(x) = E_{X \sim Q} \left[ \frac{1}{P(B(X, h))} \right]
$$

above, $B(x, h)$ is closed ball of radius $h$ centered at $x$

- at fixed $h > 0$, absolute continuity is not required for finite similarity measure
- measure generalizes existing notions of “similarity” for pair $(P, Q)$
- our results use scaling of mapping $h \mapsto \rho_h(P, Q)$ in limit $h \to 0^+$
Bounds on similarity measure

we bound the similarity measure using covering numbers

**covering number** \( N(h) := \text{minimal number of balls of radius } h \text{ required to cover } \mathcal{X} \)
Bounds on similarity measure

can bound similarity measure by approximating the integral over minimal covers

**Proposition**

*Suppose that for some \( h > 0 \) there is \( \lambda > 0 \) such that the mass comparison condition*

\[
\lambda \, P(B(x, h)) \geq Q(B(x, h))
\]

*holds for all \( x \in \mathcal{X} \). Then, the similarity measure satisfies*

\[
\rho_h(P, Q) \leq \lambda \, N(h/2).
\]

*(note \( \lambda \) can depend on \( h \) in claim above)*
Consequences of general bound

using previous claim, can bound similarity measure in some situations

examples

▶ **bounded likelihood ratio:** if $Q \ll P$ and $\frac{dQ}{dp}(x) \leq b$ for all $x$, have $\rho_h(P, Q) \leq b N\left(\frac{h}{2}\right)$

▶ **transfer exponent** (Kpotufe & Martinet, 2018; 2021):
  - pair $(P, Q)$ has $(\gamma, C_\gamma)$-transfer exponent if
    $$P(B(x, h)) \geq C_\gamma h^\gamma Q(B(x, h)) \quad \text{for all } x \in \mathcal{X}, \text{ all } h > 0. \quad (\gamma, C_\gamma) \in \mathbb{R}_+ \times (0, 1]$$
  - implies similarity measure bound, $\rho_h(P, Q) \leq (h^\gamma C_\gamma)^{-1} N(h/2)$,

(note that $N(h) \leq h^{-k}$ as $h \to 0^+$ for compact domains $\mathcal{X} \subset \mathbb{R}^k$)
Assumptions on regression setup

recall our regression setup,

\[ Y_i = f^*(X_i) + \xi_i, \quad \text{for } i = 1, \ldots, n \]

**smoothness condition**
assume \( \mathcal{X} = [0, 1] \) and assume that \( f^* \) is \( L \)-Lipschitz,

\[ f^* \in \mathcal{F}(L) := \left\{ f : [0, 1] \rightarrow \mathbb{R} \mid |f(x) - f(x')| \leq L|x - x'| \text{ for any } x, x' \in [0, 1] \right\} \]

**noise condition**
assume the noise variables satisfy (almost surely)

\[ \mathbb{E} \left[ \xi_i^2 \mid X_i \right] \leq \sigma^2, \quad \text{for } i = 1, \ldots, n \]
Classes of covariate shifts

below are families of covariate shift instances based on the map $h \mapsto \rho_h(P, Q)$

families of covariate shifts

▶ we consider pairs $(P, Q)$ for which (roughly) $\rho_h(P, Q) \lesssim h^{-\alpha}$ as $h \to 0^+$:

$$\mathcal{D}(\alpha, C) := \left\{(P, Q) \mid \sup_{0<h\leq 1} h^\alpha \rho_h(P, Q) \leq C\right\} \quad (\alpha \geq 1 \text{ and } C \geq 1)$$

▶ note that $\mathcal{D}(\alpha, C) \subset \mathcal{D}(\alpha', C')$ if $\alpha \leq \alpha'$ and $C \leq C'$

(some additional discussion and extensions in our full paper)
Main result: minimax upper and lower bounds

Our minimax results are stated for excess prediction error under $Q$,

$$\|\hat{f} - f^*\|^2_{L^2(Q)} = \mathbf{E}_{X' \sim Q} \left[ \left( \hat{f}(X') - f^*(X') \right)^2 \right].$$

**Theorem**

Suppose $\sigma \ge L$. Let $\alpha \ge 1, C \ge 1$. For a sufficiently large sample size, we have

$$\sup_{(P,Q) \in \mathcal{D}(\alpha, C)} \inf_{\hat{f}} \sup_{f^* \in \mathcal{F}(L)} \mathbf{E}\|\hat{f} - f^*\|^2_{L^2(Q)} \asymp \left( \frac{n_P}{\sigma^2} \right)^{\frac{3}{2+\alpha}} + \left( \frac{n_Q}{\sigma^2} \right)^{-\frac{2}{3}}.$$

- When $\alpha > 1$, the worst-case rate (with no access to samples under $Q$) is $n^{-\frac{2}{2+\alpha}} \gg n^{-\frac{2}{3}}$
- Upper bound is achieved by analyzing Nadaraya-Watson estimator under covariate shift
- Lower bound is achieved by pair $(P_{\alpha,C}, Q_{\alpha,C}) \in \mathcal{D}(\alpha, C)$ that we construct
Achievable result

achievable result based on classical Nadaraya-Watson estimator

**Nadaraya–Watson (NW) estimator**
derived pointwise by the local average,

\[
\hat{f}(x) := \frac{\sum_{i=1}^{n} Y_i \mathbb{1}\{X_i \in B(x, h_n)\}}{\sum_{i=1}^{n} \mathbb{1}\{X_i \in B(x, h_n)\}}
\]

(above, \(h_n > 0\) is a bandwidth parameter)

▶ the estimator is defined to be zero when denominator is zero
▶ we establish minimax upper bounds by selecting \(h_n\) as a function of \((n_p, n_Q, \sigma^2, L, \alpha, C)\)
This implies that

\( \subinterval \text{density of } r, z \) must scale as

assign probability

This implies that

The following proposition verifies that

error must scale as the righthand side of inequality (2).

We construct a hard pair \( (P, Q) \in \mathcal{D}(\alpha, C) \)

we construct a hard family of regression functions within \( \mathcal{F}(L) \)

we establish our minimax lower bound by combining these two pieces with Fano’s inequality and packing-based arguments
For some instances, transfer exponent is loose

Hardest instances coincide

our results have consequences for previously proposed notion of transfer exponent

- $(P, Q)$ have $(\gamma, C_\gamma)$-transfer exponent when for all $x, h$
  \[ P(B(x, h)) \geq C_\gamma h^\gamma Q(B(x, h)) \]

- can show if $(P, Q)$ have $(\gamma, C_\gamma)$-transfer exponent, then $(P, Q) \in \mathcal{D}(\gamma + 1, 2/C_\gamma)$

- consequently, can obtain upper bounds for instances with known transfer exponent
Conclusions

summary
▶ we introduce a similarity measure between two probability measures on the same space
▶ we show that this measure can be bounded easily under natural conditions
▶ we derive matching minimax upper and lower bounds for nonparametric regression under classes of covariate shifts that are parameterized by the scaling of this measure

additional results (not discussed)
▶ bounds under more general Hölder-smoothness conditions and additional classes of covariate shifts
▶ consequences of achievability results for bounded likelihood ratio and transfer exponent