Questions and tries

Jiaxin Hu

May 3, 2022

1 Q&A

1. Any relationship between W_1 and TV norm?

Let f, g be two probability measures on a one-dimensional measurable space Ω with corresponding CDFs F, G. Recall the definitions

$$TV(f,g) = \int_{\mathbb{R}} |f(t) - g(t)| dt, \quad W_1(F,G) = \int_{\mathbb{R}} |F(t) - G(t)| dt,$$

We have

$$d_{\min}TV(f,g) \le W_1(F,G) \le \operatorname{diam}(\Omega)TV(f,g),$$

where $d_{\min} = \inf_{x,y \in \Omega} |x-y|$ and $\dim(\Omega) = \sup_{x,y \in \Omega} |x-y|$. Hence, when Ω is a finite space, the distances TV(f,g) and $W_1(F,G)$ are equivalent up to constants.

Suppose f_n, g_n are empirical distributions with **given** observations x_1, \ldots, x_n and y_1, \ldots, y_n , respectively. The f_n, g_n are supported on spaces subset in the finite space $\Omega = \{x_1, \ldots, x_n, y_1, \ldots, y_n\}$. So, with given observations x_1, \ldots, x_n and y_1, \ldots, y_n , the $TV(f_n, g_n)$ and $W_1(F_n, G_n)$ are equivalent up to the constant.

Question: Is $TV(f_n, g_n)$ well-defined as f_n, g_n are sums of dirac functions? The integral of dirac function is equal to 0; i.e., $\int_{\mathbb{R}} \delta_{x_i}(t)dt = 0$.

2. Does the number of partition L in Ding's distance (L-distance) relate to biasvariance trade-off?

My answer is yes.

Notice that L-distance is a discretized version of empirical TV norm, which calculates the area difference under the density curves.

With given observations, we use a step function related to L to estimate the true (smooth/continuous) density. Specifically, for the true density f(t) with observations X_1, \ldots, X_n , we consider the estimator

$$\hat{f}_{n,L}(t) = \frac{1}{n} \sum_{i \in [n]} \mathbb{1}\{t - \frac{1}{2L} \le X_i \le t + \frac{1}{2L}\}. \tag{1}$$

The choice of L affects the estimation error; see Section 3 Waterman and Whiteman (1978) and specifically L is the analogy of $1/\lambda$ in the paper. The L can also be explained by the resolution of the step function to approximate the density, which is another kind of biasvariance trade-off. **Q4** also discusses the explanation of L.

One thing need to be noticed is that Waterman and Whiteman (1978) choose the optimal $L = n^{1/5}$ to minimize the difference between estimated density and the true density. In our case, with observations $X_1, \ldots, X_n \sim F, Y_1, \ldots, Y_n \sim G$ with true PDFs f, g, we consider the estimation of TV norm as

$$\hat{T}V(f,g|L) = \sum_{l \in [L]} |\hat{f}_{n,L}(t_l) - \hat{g}_{n,L}(t_l)| \cdot \frac{1}{L},\tag{2}$$

where $\hat{f}_{n,L}$ and $\hat{g}_{n,L}$ are defined as (1). We need to choose the series $\{t_l\}_{l\in[L]}$ and an optimal L to make the step function approximation accurate to reflect the correlation relation via $\hat{T}V(f,g|L)$. Our choice is $L=C\log n$ based on the proofs in Ding's paper and note 0403. This is a different than the choice in Waterman and Whiteman (1978).

3. What's the counterpart of L in W_1 distance?

The W_1 distance works on the CDF directly. Suppose we have observations $X_1, \ldots, X_n \sim F, Y_1, \ldots, Y_n \sim G$ with true CDFs F, G, and empirical distribution $F_n(t) = \frac{1}{n} \sum_{i \in [n]} \mathbb{1}\{X_i \leq t\}, G_n(t) = \frac{1}{n} \sum_{i \in [n]} \mathbb{1}\{Y_i \leq t\}.$

We may have different estimations for $W_1(F,G)$ using different series of $F_n(t)$ and $G_n(t)$ to approximate the trajectories of F,G.

One natural estimation is

$$\hat{W}_1(F,G) = \sum_{k=2}^{2n} |F_n(U_k) - G_n(U_k)| \cdot |U_k - U_{k-1}|, \tag{3}$$

where we sort and rename the random samples $X_1, \ldots, X_n, Y_1, \ldots, Y_n$ as $U_1 \leq U_2 \leq \cdots \leq U_{2n}$. Another estimation is to find a series of points $\{t_l\}_{l \in [L]}$ on the real line and calculate

$$\hat{W}_1(F,G|L) = \sum_{l=2}^{L} |F_n(t_l) - G_n(t_l)| \cdot |t_l - t_{l-1}|.$$
(4)

The error of estimation (4) relates to the choice of L and the series $\{t_l\}$.

Section 2 in the following note show that the estimator (4) also chooses $L = C \log n$, which agrees with the choice using (2). Though the choices of $\{t_l\}$ using for W_1 (4) and TV (2) are different. With the optimal choice of L, we can obtain the same matching algorithm guarantee using $\hat{W}_1(F, G|L)$ under the condition $\sigma < 1/\log n$ as shown in Ding's paper.

4. What's the fundamental principle for us to consider the discretization? Other statistical examples?

The discretization comes from the step function approximation to the true (smooth) distribution, and finding an optimal resolution, L, of the discretization is equal to handling the bias-variance trade-off in the approximation.

I believe L is also proposed with the same intuition of regularization parameter, like LASSO penalty. If we choose a large L, the step function approximation to the true PDF will overfit; if we choose a small L, the step function approximation surfers from the information loss.

5. How to explain the simulation results that empirical W_1 is much better than L-distance?

In simulation, the performance of distance $\hat{T}V(f,g|L)$ in (2) is way worse than the distance $\hat{W}_1(F,G)$ in (3). Particularly, we implement the estimated W_1 distance using its equivalent form $\hat{W}_1(F,G) = \frac{1}{n} \sum_{i \in [n]} |X_{(i)} - Y_{(i)}|$, where $X_{(i)}$ is the *i*-th smallest variables among X_1, \ldots, X_n and $Y_{(i)}$'s are also the order statistics of Y.

Question: We have not shown the rigorous algorithm guarantee using $\hat{W}_1(F,G)$. Though we show that using $\hat{W}_1(F,G)$ leads to exact recovery under the same condition $\sigma < 1/\log n$, current results can not explain the worse performance of $\hat{T}V(f,g|L)$. Because we do not show the error rates of different distances under the finite sample cases. We just know the errors with different distances will tend to 0 but know nothing about the speed.

2 Tail bounds for $\hat{W}_1(F,G|L)$

Suppose that we have i.i.d. samples $(X_1, Y_1), \ldots, (X_n, Y_n)$ following the multivariate zero-mean Gaussian distribution with variance 1 and correlation $\rho \in [0, 1)$; i.e,

$$(X_i, Y_i) \sim \mathcal{N}\left(\mathbf{0}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right), \text{ and } (X_i, Y_i) \perp (X_j, Y_j), \text{ for all } i \neq j.$$
 (5)

Consider an uniform partition $\{I_l\}_{l\in[L]}$ over the interval [-L,L], where $|I_l|=2$ and $\bigcup_{l\in[L]}I_l=[-L,L]$. Let t_l be the right boundary of I_l for all $l\in[L]$, and particularly $t_L=L$. We define the discretized empirical $\hat{W}_1(F,G|L)$ in (4) as

$$W_L = \sum_{l \in [L]} |F_n(t_l) - G_n(t_l)|.$$
 (6)

Lemma 1 (Tail bounds for W_L). Consider the i.i.d. samples (X_i, Y_i) for $i \in [n]$ from model (5).

When $\rho > 0$, we have

$$\mathbb{P}\left(W_L \gtrsim L\sqrt{\frac{2\sigma}{n}} + t\right) \lesssim \exp\left(-nt^2\right),\,$$

where $\sigma = \sqrt{1 - \rho^2}$ and for all t > 0.

When $\rho = 0$, we have

$$\mathbb{P}\left(W_L \lesssim \sqrt{\frac{L}{n}} - t\right) \lesssim \exp\left(-nt^2\right),\,$$

for all t > 0.

Remark 1 (Success of W_L). In Lemma 1, we need to choose $t = \sqrt{\frac{\log n}{n}}$ to make the tail bounds decay to 0. Let $\xi_{\text{true}} = L\sqrt{\frac{2\sigma}{n}}$ and $\xi_{\text{fake}} = \sqrt{\frac{L}{n}}$. Now, we need to choose the optimal L to make the the differences of W_L under true/fake cases dominate the t; i.e.,

$$\xi_{\text{fake}} - \xi_{\text{true}} = \sqrt{\frac{L}{n}} - L\sqrt{\frac{2\sigma}{n}} \gtrsim \sqrt{\frac{\log n}{n}}.$$

The optimal choice of L is $C \log n$ for some positive constant C with $\sigma \leq 1/L$. If $L = o(\log n)$, the difference $\xi_{\text{fake}} - \xi_{\text{true}}$ does not dominate t; if $L > \mathcal{O}(\log n)$, we need a stricter condition on $\sigma \leq 1/L$.

Remark 2 (Comparison with Ding's distance). The distance W_L share the same spirit with Ding's distance. Though optimal numbers of uniform partition, L, are equal to $\log n$ in both distances, the W_L considers a partition in a larger range from [-L, L].

Remark 3 (Comparison with empirical W_1). Compared with the empirical W_1 in (3), W_L and $\hat{W}_1(F,G)$ have similar formula. The difficulty to proof the tail bound for $\hat{W}_1(F,G)$ comes from the randomness of U_k 's while the partition boundaries t_l 's in W_L are fixed.

Proof of Lemma 1. By Proposition 1, we apply the Berstein-type McDiarmid's inequality to W_L , and we have

$$\mathbb{P}(|W_L - \mathbb{E}[W_L]| \ge t) \lesssim \exp(-nt^2),$$

for all t > 0. Now, we only need to show

when
$$\rho > 0$$
, $L\sqrt{\frac{2\sigma}{n}} \gtrsim \mathbb{E}[W_L]$, and when $\rho = 0$, $\sqrt{\frac{L}{n}} \lesssim \mathbb{E}[W_L]$.

When $\rho > 0$, we have

$$\begin{split} \mathbb{E}[W_L] &\leq L \max_{t \in \mathbb{R}} \mathbb{E}[|F_n(t) - G_n(t)|] \\ &\leq \frac{L}{n} \max_{t \in \mathbb{R}} \sqrt{\mathbb{E}[\sum_{i \in [n]} |\mathbb{1}\{X_i \leq t\} - \mathbb{1}\{Y_i \leq t\}|^2]} \\ &\leq \frac{L}{\sqrt{n}} \max_{t \in \mathbb{R}} \sqrt{\mathbb{P}(X_i \leq t, Y_i > t) + \mathbb{P}(X_i \geq t, Y_i < t)} \\ &\leq L\sqrt{\frac{2\sigma}{n}}, \end{split}$$

where the second inequality follows the Jensen's inequality and the last inequality follows by the Proposition 2.

When $\rho = 0$, we have

$$\begin{split} \mathbb{E}[W_L] &\geq L \min_{l \in [L]:t_l} \mathbb{E}[|F_n(t_l) - G_n(t_l)|] \\ &\geq \frac{L}{n} \min_{l \in [L]:t_l} \mathbb{E}\left[|\sum_{i \in [n]} \mathbb{1}\{X_i \leq t_l\} - m_l|\right] \\ &\geq \frac{L}{\sqrt{n}} \min_{l \in [L]:t_l} \sqrt{\mathbb{P}(X_1 \leq t_l)\mathbb{P}(X_1 \geq t_l)} \\ &\geq \frac{L}{\sqrt{n}} \sqrt{\mathbb{P}(X_1 \leq L)\mathbb{P}(X_1 \geq L)} \\ &\geq \sqrt{\frac{L}{n}}, \end{split}$$

where m_l is the median of $Bin(0, \mathbb{P}(X_1 \leq t_l))$, and the third inequality follows by the mean absolute deviation of binomial distribution, and the last inequality follows by the fact that $\mathbb{P}(X_1 \geq L) \lesssim \frac{1}{L}$ and $\mathbb{P}(X_1 \leq L)$ close to 1 with large L.

Proposition 1 (Difference bounded proposition of W_L). The distance (6) satisfies the $(c/n^2, \ldots, c/n^2)$ -bounded difference property for some positive constant c.

Proof of Proposition 1. Let $f(X_1, \ldots, X_n, Y_1, \ldots, Y_n) := W_L$. Without loss of generality, we consider two independent variables X_i, X_i' for an arbitrary $i \in [n]$, and define the difference

$$D := f(X_1, \dots, X_i, \dots, Y_n) - f(X_1, \dots, X_i', \dots, Y_n).$$

By the definition of W_L , we have

$$D = \frac{1}{n} \lceil |X_i - X_i'| \rceil.$$

Note that $X_i - X_i' \sim N(0, 2)$. We have

$$\mathbb{E}[|D|^k|X_j, j \neq i, Y_1, \dots, Y_n] \le C \frac{1}{n^k} = C \frac{1}{n^2} M^{k-2},$$

for some positive constant C and M = 1/n.

Lemma 2 (Berstein-type McDiarmid's inequality). Let X_1, \ldots, X_n be independent random variables, where X_i has range $X_i \in \mathbb{R}$. Let $f: X_1 \times \cdots \times X_n \mapsto \mathbb{R}$ by any function satisfies the $(\sigma_1^2, \ldots, \sigma_n^2)$ -bounded differences property; i.e., for any $i \in [n]$, $X_i, X_i' \in X_i$, and $X_j \in X_j$ for all $j \neq i$, we define

$$D_i = f(X_1, \dots, X_i, \dots, X_n) - f(X_1, \dots, X_i', \dots, X_n),$$

and

$$\mathbb{E}[|D_i|^k|X_j, j \neq i] \le \frac{1}{2}\sigma_i^2 M^{k-2} k!$$

Then, for any t > 0, we have

$$\mathbb{P}\left(|f(X_1,\ldots,X_n) - \mathbb{E}[f(X_1,\ldots,X_n)]| \ge t\right) \le 2\exp\left(-\frac{t^2}{2\sum_{i\in[n]}\sigma_i^2 + 2Mt}\right).$$

Proposition 2. Suppose that we have samples $(X_1, Y_1), \ldots, (X_n, Y_n)$ from (5); i.e., (X_i, Y_i) i.i.d. follow the multivariate zero-mean Gaussian distribution with variance 1 and correlation $\rho \in (0, 1)$. Then, for all $t \in \mathbb{R}$, we have

$$p(t) := \mathbb{P}(X_1 \le t, Y_1 > t) \le \sqrt{1 - \rho^2}$$

Proof of Proposition 2. See note 0403.

References

Waterman, M. and Whiteman, D. (1978). Estimation of probability densities by empirical density functions. *International Journal of Mathematical Education in Science and Technology*, 9(2):127–137.