TIGHT BOUNDS FOR AUGMENTED KL DIVERGENCE IN TERMS OF AUGMENTED TOTAL VARIATION DISTANCE

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ABSTRACT. We provide optimal variational upper and lower bounds for the augmented Kullback-Leibler divergence in terms of the augmented total variation distance between two probability measures defined on two Euclidean spaces having different dimensions.

1. Introduction

In this note we are concerned with finding the optimal upper and lower bounds for the augmented Kullback-Leibler (KL) divergence between probability measures defined on two Euclidean spaces having different dimensions in terms of their augmented total variation (TV) distance. Bounding the KL divergence in terms of the TV metric is a well studied problem, of paramount importance in statistics and machine learning. Notorious lower bounds are given by Pinsker’s inequality [5] and Vajda’s lower bound [10], while a famous upper bound is given by reverse Pinsker’s inequality [3, 9]. These results are particularly useful in the optimal quantization of probability measures [3] and in Bayesian nonparametrics [2]. In the present work, we generalize results from [1, 6] on tight upper and lower bounds to the case in which $P$ and $Q$ are defined on different spaces. To do so we use the framework developed in [4].

The note is divided as follows. Section 2 gives the needed background, and section 3 presents our main result. Section 4 is a discussion.

2. Preliminaries

Recall that given two probability measures $P, Q$ defined on the same measurable space $(\Omega, \mathcal{F})$ and such that $P \ll Q$, the KL divergence and the TV distance between them are defined as

$$D_{KL}(P||Q) := \int_{\Omega} \log \left( \frac{dP}{dQ} \right) dP$$
and
$$d_{TV}(P, Q) := \sup_{A \in \mathcal{F}} \left| P(A) - Q(A) \right|,$$

respectively.¹

Fix now $\delta, m \geq 0$, $M < \infty$, and consider the set $\mathcal{A}(\delta, m, M)$ of all probability measures pairs $(P, Q)$ defined on a common measurable space $(\Omega, \mathcal{F})$ satisfying

(1) $P \ll Q$.

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¹We do not need the absolute continuity assumption to hold for the TV metric.
Then, consider the function
\[ \delta \mapsto L(\delta) := \inf_{d_{TV}(P,Q)=\delta} D_{KL}(P\| Q). \]
Curve \( \gamma : \delta \mapsto (\delta, L(\delta)) \) is a differentiable curve in the \((d_{TV}, D_{KL})\)-plane, symmetric around the \( D_{KL} \)-axes. With \( t = \frac{d L}{d \delta} \), the relationship \( t \leftrightarrow \delta \) is a diffeomorphism between \( \mathbb{R} \) and \((-2, 2)\). Using \( t \in \mathbb{R} \) as a parameter, by [6, Theorem 1] \( \gamma \) is parametrized by
\[
\delta(t) = t \left( 1 - \left( \coth(t) - \frac{1}{t} \right)^2 \right)
\]
\[
L(\delta(t)) = \log \left( \frac{t}{\sinh(t)} \right) + t \coth(t) + \frac{t^2}{\sinh^2(t)}.
\]
We have the following important result.

**Theorem 1.** If \( \mathcal{A}(\delta, m, M) \neq \emptyset \), the following are tight bounds
\[
L(\delta) \leq D_{KL}(P\| Q) \leq \delta \left( \frac{\log(M^{-1})}{M^{-1} - 1} + \frac{\log(m^{-1})}{m^{-1} - 1} \right).
\]

*Proof.** The tight upper bound for \( D_{KL}(P\| Q) \) comes from [1, Equation (9)], while the tight lower bound comes from [6, Theorem 1]. \(\square\)

We can find a lower bound for \( L(\delta) \) that makes computing a lower bound for the KL divergence in terms of the TV metric easier.

**Theorem 2.** The following is true
\[
L(\delta) \geq \frac{1}{2} \delta^2 + \frac{1}{36} \delta^4 + \frac{1}{270} \delta^6 + \frac{221}{340200} \delta^8.
\]

*Proof.** Immediate from [6, Theorem 7]. \(\square\)

In this paper, we adopt the framework of [4] to prove a version of Theorems 1 and 2 for probability measures pairs \((P, Q)\) belonging to \( \Delta(\mathbb{R}^d, B(\mathbb{R}^d)) \times \Delta(\mathbb{R}^n, B(\mathbb{R}^n)) \), where \( \Delta(\mathbb{R}^*, B(\mathbb{R}^*)) \) denotes the space of probability measures on measurable space \((\mathbb{R}^*, B(\mathbb{R}^*))\), and \( B(\mathbb{R}^*) \) is the Borel sigma-algebra on \( \mathbb{R}^* \). Let \( M(\Omega) \) denote the set of all Borel probability measures on \( \Omega \subset \mathbb{R}^n \) and let \( M^p(\Omega) \subset M(\Omega) \) denote those with finite \( p \)-th moments, \( p \in \mathbb{N} \). For convenience, we restrict our attention to probability measures with densities so that we do not have to keep track of which measure is absolutely continuous to which other measure [4, Section III]. Let \( \lambda^n \) be the Lebesgue measure restricted to \( \Omega \subset \mathbb{R}^n \). With respect to \( \lambda^n \) we define
\[
M_{dens}(\Omega) := \{ \mu \in M(\Omega) : \mu \text{ has density} \}
\]
\[
M_{pd}(\Omega) := \{ \mu \in M_{dens}(\Omega) : \mu \text{ has strictly positive density} \}.
\]
Notice that \( \mu \in M_{dens}(\Omega) \) if and only if it is absolutely continuous with respect to \( \lambda^n \).
For any \(d, n \in \mathbb{N}, d \leq n\), let
\[
O(d, n) := \{V \in \mathbb{R}^{d \times n} : VV^{	op} = I_d\},
\]
that is, the Stiefel manifold on \(d \times n\) matrices with orthonormal rows. For any \(V \in O(d, n)\) and \(b \in \mathbb{R}^d\), let
\[
\varphi_{V,b} : \mathbb{R}^n \to \mathbb{R}^d, \quad x \mapsto \varphi_{V,b}(x) := Vx + b,
\]
and for any \(\mu \in M(\mathbb{R}^n)\), let \(\varphi_{V,b}(\mu) := \mu \circ \varphi_{V,b}^{-1}\) be the pushforward measure.

**Definition 3.** Let \(d, n \in \mathbb{N}, d \leq n\). For any \(P \in M(\mathbb{R}^d)\) and \(Q \in M(\mathbb{R}^n)\), the embeddings of \(P\) into \(\mathbb{R}^n\) are the set
\[
\Phi^+(P, n) := \{\alpha \in M(\mathbb{R}^n) : \varphi_{V,b}(\alpha) = P, \text{ for some } V \in O(d, n), b \in \mathbb{R}^d\}
\]
and the projections of \(Q\) onto \(\mathbb{R}^d\) are the set
\[
\Phi^-(Q, d) := \{\beta \in M(\mathbb{R}^d) : \varphi_{V,b}(\beta) = Q, \text{ for some } V \in O(d, n), b \in \mathbb{R}^d\}.
\]
The following is an important subset of \(\Phi^+(P, n)\)
\[
\Phi_{dens}^+(P, n) := \{\alpha \in M_{d\text{dens}}(\mathbb{R}^n) : \varphi_{V,b}(\alpha) = P, \text{ for some } V \in O(d, n), b \in \mathbb{R}^d\}.
\]
Then, we have a crucial result.

**Theorem 4.** Let \(d, n \in \mathbb{N}, d \leq n\). For any \(P \in M(\mathbb{R}^d)\) and \(Q \in M(\mathbb{R}^n)\), let
\[
D_{KL}^{-}(P\|Q) := \inf_{\beta \in \Phi^-(Q, d)} D_{KL}(P\|\beta), \quad D_{KL}^{+}(P\|Q) := \inf_{\alpha \in \Phi_{d\text{dens}}^+(P, n)} D_{KL}(\alpha\|Q),
\]
\[
d_{TV}^{-}(P, Q) := \inf_{\beta \in \Phi^-(Q, d)} d_{TV}(P, \beta), \quad d_{TV}^{+}(P, Q) := \inf_{\alpha \in \Phi_{d\text{dens}}^+(P, n)} d_{TV}(\alpha, Q).
\]
Then,
\[
D_{KL}^{-}(P\|Q) = D_{KL}^{+}(P\|Q) = \hat{D}_{KL}(P\|Q)
\]
and
\[
d_{TV}^{-}(P, Q) = d_{TV}^{+}(P, Q) = \hat{d}_{TV}(P, Q).
\]

**Proof.** Immediate from [4, Theorem III.4]. \(\Box\)

We call \(\hat{D}_{KL}(P\|Q)\) the augmented KL divergence, while \(\hat{d}_{TV}(P, Q)\) the augmented TV distance. Notice that [4, Lemma III.2] guarantees the existence of \(D_{KL}(P\|Q), D_{KL}^{+}(P\|Q), d_{TV}^{-}(P, Q), \) and \(d_{TV}^{+}(P, Q)\).

### 3. Main Result

Consider function
\[
\delta \mapsto \hat{L}(\delta) := \inf_{d_{TV}(P, Q) = \delta \geq 0} \hat{D}_{KL}(P\|Q).
\]
Denote by \(\alpha \in \Phi_{d\text{dens}}^+(P, n)\) and \(\beta \in \Phi^-(Q, d)\) the probability measures such that \(\hat{d}_{TV}(P, Q) = d_{TV}(P, \beta) = d_{TV}(\alpha, Q)\), and let
\[
\text{ess inf } \frac{d\alpha}{dQ} = m_1, \quad \text{ess inf } \frac{dP}{d\beta} = m_2, \quad \text{ess sup } \frac{d\alpha}{dQ} = M_1, \quad \text{ess sup } \frac{dP}{d\beta} = M_2.
\]
The following is the main result of the note.
Theorem 5. Pick \( d, n \in \mathbb{N} \) such that \( d \leq n \) and consider any \( P \in M_{dens}(\mathbb{R}^d) \) and \( Q \in M_{pd}(\mathbb{R}^n) \). Let
\[
\text{pol}_{d_{TV}} := \frac{1}{2} \hat{d}_{TV}(P, Q)^2 + \frac{1}{36} \hat{d}_{TV}(P, Q)^4 + \frac{1}{270} \hat{d}_{TV}(P, Q)^6 + \frac{221}{340200} \hat{d}_{TV}(P, Q)^8
\]
and
\[
\mathfrak{m} := \min \left\{ \hat{d}_{TV}(P, Q) \left( \frac{\log(M_1^{-1})}{M_1^{-1} - 1} + \frac{\log(m_1^{-1})}{m_1^{-1} - 1} \right), \hat{d}_{TV}(P, Q) \left( \frac{\log(M_2^{-1})}{M_2^{-1} - 1} + \frac{\log(m_2^{-1})}{m_2^{-1} - 1} \right) \right\}.
\]

If \( m_1, m_2 \geq 0, M_1, M_2 < \infty \), and \( \hat{d}_{TV}(P, Q) \geq 0 \), then
\[
\text{pol}_{d_{TV}} \leq \hat{L}(\delta) \leq \hat{D}_{KL}(P\|Q) \leq \mathfrak{m}.
\]

Proof. The proof has four steps.

1. We first show that \( \text{pol}_{d_{TV}} \leq \hat{D}_{KL}(P\|Q) \). We have that
\[
\hat{D}_{KL}(P\|Q) := \inf_{\beta \in \Phi^-(Q, d)} D_{KL}(P\|\beta) \geq \inf_{\beta \in \Phi^-(Q, d)} \left[ \frac{1}{2} d_{TV}(P, \beta)^2 + \frac{1}{36} d_{TV}(P, \beta)^4 \right. \\
+ \left. \frac{1}{270} d_{TV}(P, \beta)^6 + \frac{221}{340200} d_{TV}(P, \beta)^8 \right],
\]
where the inequality is a consequence of the properties of the infimum operator and of Theorems 1 and 2. The statement follows.

2. The fact that \( \hat{D}_{KL}(P\|Q) \geq \hat{L}(\delta) \) comes from equation (3). In addition, since the infimum operator preserves convexity, using \( t = \frac{dL}{d\delta} \) as a parameter and following the steps in the proof of [6, Theorem 1], we obtain that curve \( \gamma : \delta \mapsto (\delta, \hat{L}(\delta)) \) is parametrized as in (1).

3. We now find the upper bound for \( \hat{D}_{KL}(P\|Q) \). We have that
\[
\hat{D}_{KL}(P\|Q) = \inf_{\beta \in \Phi^-(Q, d)} D_{KL}(P\|\beta) \leq \inf_{\beta \in \Phi^-(Q, d)} d_{TV}(P, \beta) \left( \frac{\log(M_2^{-1})}{M_2^{-1} - 1} + \frac{\log(m_2^{-1})}{m_2^{-1} - 1} \right) =: U_2,
\]
where the inequality is a consequence of the properties of the infimum operator and of Theorem 1. But we also have that
\[
\hat{D}_{KL}(P\|Q) = \inf_{\alpha \in \Phi_{dens}^+(P, n)} D_{KL}(\alpha\|Q) \leq \inf_{\alpha \in \Phi_{dens}^+(P, n)} d_{TV}(\alpha, Q) \left( \frac{\log(M_1^{-1})}{M_1^{-1} - 1} + \frac{\log(m_1^{-1})}{m_1^{-1} - 1} \right) =: U_1,
\]
where again the inequality is a consequence of the properties of the infimum operator and of Theorem 1. Hence, by selecting the smallest between \( U_1 \) and \( U_2 \) we find the desired upper bound for \( \hat{D}_{KL}(P\|Q) \).

4. Finally, we show that \( \text{pol}_{d_{TV}} \leq \hat{L}(\delta) \). We have that
\[
\hat{L}(\delta) = \inf_{\beta \in \Phi^-(Q, d)} \inf_{d_{TV}(P, \beta) = \delta \geq 0} D_{KL}(P\|\beta) \geq \inf_{\beta \in \Phi^-(Q, d)} \left[ \frac{1}{2} d_{TV}(P, \beta)^2 + \frac{1}{36} d_{TV}(P, \beta)^4 \right. \\
\left. + \frac{1}{270} d_{TV}(P, \beta)^6 + \frac{221}{340200} d_{TV}(P, \beta)^8 \right],
\]
where the inequality is a consequence of the properties of the infimum operator and of Theorem 2. The statement follows.

\[ \square \]

4. Conclusion

In this note we presented tight upper and lower bounds for the augmented KL divergence in terms of the augmented TV distance. In the future, we plan to find tight bounds for more augmented divergences in terms of augmented metrics and vice versa, in the spirit of [7]. An encouraging result of this kind is presented in [4, Corollary III.6]: the authors give a bound for the augmented TV metric in terms of the augmented Hellinger squared divergence.

It is worth to notice that in [8, Corollary 1] the authors give an explicit value for \( L(\delta) \), in contrast with (1) where the value is implicit. In particular, they show that given two probability measures \( P, Q \) on the same Euclidean space such that \( d_{TV}(P, Q) = \delta \geq 0 \), then

\[
L(\delta) = \min_{\gamma \in [\delta - 2, 2 - \delta]} \left[ \left( \frac{\delta + 2 - \gamma}{4} \right) \log \left( \frac{\gamma - 2 - \delta}{\gamma - 2 + \delta} \right) + \left( \frac{\gamma + 2 - \delta}{4} \right) \log \left( \frac{\gamma + 2 - \delta}{\gamma + 2 + \delta} \right) \right].
\]

We will generalize this value to the augmented counterpart in future work.

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