On The Chain Rule Optimal Transport Distance

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Abstract

We define a novel class of distances between statistical multivariate distributions by solving an optimal transportation problem on their marginal densities with respect to a ground distance defined on their conditional densities. By using the chain rule factorization of probabilities, we show how to perform optimal transport on a ground space being an information-geometric manifold of conditional probabilities. We prove that this new distance is a metric whenever the chosen ground distance is a metric. Our distance generalizes both the Wasserstein distances between point sets and a recently introduced metric distance between statistical mixtures. As a first application of this Chain Rule Optimal Transport (CROT) distance, we show that the ground distance between statistical mixtures is upper bounded by this optimal transport distance and its fast relaxed Sinkhorn distance, whenever the ground distance is joint convex. We report on our experiments which quantify the tightness of the CROT distance for the total variation distance, the square root generalization of the Jensen-Shannon divergence, the Wasserstein $W_p$ metric and the Rényi divergence between mixtures.

Keywords: Optimal transport, Wasserstein distances, Information geometry, $f$-divergences, Total Variation, Jensen-Shannon divergence, Bregman divergence, Rényi divergence, Statistical mixtures, Joint convexity.

1 Introduction

Calculating (dis)similarities between statistical mixtures is a core primitive often met in statistics, machine learning, signal processing, and information fusion [4] among others. However, the usual information-theoretic Kullback-Leibler (KL) divergence (also known as relative entropy) or the $f$-divergences between statistical mixtures [42] do not admit closed-form formula, and is in practice approximated by costly Monte Carlo stochastic integration [42].

To tackle this computational tractability problem, two research directions have been considered in the literature:
• The first line of research consists in proposing some new distances between mixtures that yield closed-form formula \([33, 35]\) (e.g., the Cauchy-Schwarz divergence, the Jensen quadratic Rényi divergence, the statistical Minkowski distances).

• The second line of research consists in lower and upper bounding the \(f\)-divergences between mixtures \([12]\). This is tricky when considering bounded divergences like the Total Variation (TV) distance or the Jensen-Shannon (JS) divergence that are upper bounded by 1 and \(\log 2\), respectively. See also Appendix A.

When dealing with probability densities, two main classes of statistical distances have been widely studied in the literature:

1. The Information-Geometric (IG) invariant \(f\)-divergences \([1]\) (characterized as the class of separable distances which are information monotone), and

2. The Optimal Transport (OT)/Wasserstein distances \([31, 52]\) which can be computationally accelerated using entropy regularization \([6, 14]\) (i.e., the Sinkhorn divergence).

In general, computing closed-form formula for the OT between parametric distributions is difficult. A closed-form formula is known for elliptical distributions \([11]\) for the 2-Wasserstein metric (including the multivariate Gaussian distributions), and the OT of multivariate continuous distributions can be calculated from the OT of their copulas \([19]\).

Let us briefly mention that the geometry induced by the distance is different in these two OT/IG cases. For example, consider univariate location-scale families (or multivariate elliptical distributions):

1. For OT, the 2-Wasserstein distance between any two members admit the same closed-form formula \([11, 18]\) (depending only on the mean and variance parameters, not on the type of location-scale family). The OT geometry of Gaussian distributions has positive curvature \([17, 56]\).

2. For any \(f\)-divergence, the information-geometric manifold has negative curvature \([27]\) (hyperbolic geometry).

It is known that for the Kullback-Leibler divergence, the manifold of mixtures with prescribed components (called a mixture family in information geometry) is dually flat, and therefore admits an equivalent Bregman divergence \([37]\) for the strictly convex Shannon negative entropy (negentropy).

In this paper, we build on the seminal work of Liu and Huang \([30]\) that proposed a novel family of statistical distances for statistical mixtures by solving linear programs between \([30]\) component weights of mixtures where the elementary distance between any two mixtures is prescribed. They proved that their distance between mixtures (that we term MCOT distance for Mixture Component Optimal Transport) is a metric whenever the elementary distance between mixture components is a metric. See \([5]\) for another recent work further pushing that research direction and discussing displacement interpolation and barycenter calculations for Gaussian Mixture Models. We note that this framework also applies to semi-parametric mixtures obtained from Kernel Density Estimators \([53]\) (KDEs).

We describe our main contributions as follows:
We define the Chain Rule Optimal Transport (CROT) distance in Definition 1, and prove that the CROT distance is a metric whenever the distance between conditional distributions is a metric in \(\S 2.2\) (Theorem 3). The CROT distance extends the Wasserstein/EMD distances and the MCOT distance between statistical mixtures. We further sketch how to build recursively hierarchical families of CROT distances.

We report a novel generic upper bound for statistical distances between mixtures \[43\] using CROT distances in \(\S 3\) (Theorem 5) whenever the ground distance is joint convex, and introduce its relaxed Sinkhorn distance.

In \(\S 4\), numerical experiments highlight quantitatively the upper bound performance of the CROT distance for bounding the total variation distance, a generalization of the square root of the Jensen-Shannon distance, the Wasserstein \(W_p\) metric, and the Rényi \(\alpha\)-divergences.

2 The Chain Rule Optimal Transport (CROT) distance

2.1 Definition

We define a novel class of distances between statistical multivariate distributions. Recall the basic chain rule factorization of a joint probability distribution \(p(x, y)\):

\[ p(x, y) = p(y)p(x|y), \]

where probability \(p(y)\) is called the marginal probability, and probability \(p(x|y)\) is termed the conditional probability. Let \(\mathcal{Y} = \{p(y)\}\) and \(\mathcal{C} = \{p(x|y)\}\) denote the manifolds of marginal probability densities and conditional probability densities, respectively.

For example, for latent models like statistical mixtures or hidden Markov models \([60, 54]\), \(x\) plays the role of the observed variable while \(y\) denotes the hidden variable \([13]\) (unobserved so that inference has to tackle incomplete data, say, using the EM algorithm \([9]\)).

First, we state the generic definition of the Chain Rule Optimal Transport distance between joint distributions \(p\) and \(q\) (with \(q(x, y) = q(y)q(x|y)\)) as follows:

**Definition 1** (CROT distance). Given two multivariate distributions \(p\) and \(q\), we define the Chain Rule Optimal Transport (CROT) as follows:

\[
H_\delta(p, q) := \inf_r E_{r(y, z)} \left[ \delta \left( p(x|y), q(x|z) \right) \right], \\
= \inf_r \int r(y, z)\delta \left( p(x|y), q(x|z) \right) dydz,
\]

where \(\delta(\cdot, \cdot)\) is a ground distance defined on conditional density manifold \(\mathcal{C} = \{p(x|y)\}\) (e.g., the Total Variation — TV), and \(r \in \Gamma(p, q)\) (set of all probability measures on \(\mathcal{Y}^2\) with marginals \(p\) and \(q\)) satisfying the following constraint:

\[
\int r(y, z)dz = p(y), \quad \int r(y, z)dy = q(z),
\]

When the ground distance \(\delta\) is clear from the context, we write \(H(p, q)\) for a shortcut of \(H_\delta(p, q)\). Since \(\int r(y, z)dydz = 1\) and since \(r(y, z) = p(y)q(z)\) is a feasible transport solution, we get the following upper bounds:
Property 2 (Upper bounds). The CROT is upper bounded by

\[ H_\delta(p, q) \leq \int_y \int_z p(y)q(z)\delta(p(x|y), q(x|z))\,dy\,dz \leq \max_{y,z} \delta(p(x|y), q(x|z)). \]

Figure 1 illustrates the principle of the CROT distance. Another complementary motivation when dealing with statistical mixtures is presented in §3.

Let us notice that the CROT distance generalizes two distances met in the literature:

Remark 2.1 (CROT generalizes Wasserstein/EMD). In the case that \( p(x|y) = \delta(y) \) (Dirac distributions), we recover the Wasserstein distance \([56]\) between point sets (or Earth Mover Distance \([51]\)), where \( \delta(\cdot, \cdot) \) is the ground metric distance.

The Wasserstein distance \( W_p \) (for \( p \geq 1 \), with \( W_1 \) introduced in \([58]\)) follows from the Kantorovich’s relaxation framework \([23, 24]\) of Monge’s original optimal mass transport formulation \([31]\).

Remark 2.2 (CROT generalizes MCOT). When both \( p(y) \) and \( q(z) \) are both (finite) categorical distributions, we recover the distance formerly defined in \([30]\) that we term the MCOT distance in the remainder (for Mixture Component Optimal Transport).

2.2 CROT is a metric when the ground distance is a metric

We state the main theorem:

Theorem 3 (CROT metric). \( H_\delta(p, q) \) is a metric whenever \( \delta(\cdot, \cdot) \) is a metric.

Proof. We prove that \( H(p, q) \) satisfies the following axioms of metric distances:

Non-negativity. As \( \delta(\cdot, \cdot) \geq 0 \), we have \( H_\delta(p, q) \geq 0 \).

Law of indiscernibles. If \( H_\delta(p, q) = 0 \), as \( \delta(\cdot, \cdot) \) is a metric, then the density \( r(y, z) \) is concentrated on the region \( p(x|y) = q(x|z) \) in \( C^2 \). We therefore have

\[ p(y)p(x|y) = \int r(y, z)\,dzp(x|y) = \int r(y, z)p(x|y)\,dz = \int r(y, z)q(x|z)\,dy = q(z)q(x|z). \]
Symmetry.

\[ H_\delta(p, q) = \inf_r \int r(y, z) \delta \left( p(x|y), q(x|z) \right) \, dy \, dz = \inf_r \int R(z, y) \delta \left( q(x|z), p(x|y) \right) \, dy \, dz \tag{5} \]

where \( R(z, y) = r(y, z) \) s.t. \( \int R(z, y) \, dy = q(z) \) and \( \int R(z, y) \, dz = p(y) \).

Triangle inequality. The proof of the triangle inequality is not straightforward.

\[ H_\delta(p_1, p_2) + H_\delta(p_2, p_3) = \inf_{r_1, r_2} E_{r_1(y, z)} \delta(p_1(x|y), p_2(x|z)) + \inf_{r_2} E_{r_2(y, z)} \delta(p_2(x|y), p_3(x|z)) \]

\[ = \inf_r E_{s(y_1, y_2, z)} (\delta(p_1(x|y_1), p_2(x|z)) + \delta(p_2(x|y_2), p_3(x|z))) \]

\[ \geq \inf_r E_{s(y_1, y_2, z)} \delta(p_1(x|y_1), p_3(x|z)) \]

\[ \geq \inf_r E_{r(y, z)} \delta(p_1(x|y), p_3(x|z)), \tag{7} \]

where \( s(p, q, r) \) denotes the set of all probability measures on \( \mathcal{X}^3 \) with marginals \( p, q \) and \( r \).

\section{CROT for finite statistical mixtures and relaxed fast Sinkhorn CROT}

Consider two finite statistical mixtures \( m_1(x) = \sum_{i=1}^{k_1} \alpha_i p_i(x) \) and \( m_2(x) = \sum_{i=1}^{k_2} \beta_i q_i(x) \), not necessarily homogeneous nor of the same type. Let \([k] := \{1, \ldots, k\}\). The Mixture Component Optimal Transport (MCOT) distance proposed in \cite{30} amounts to solve a Linear Program (LP) with the following objective function to minimize:

\[ H_\delta(p, q) = \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{ij} \delta(p_i, q_j), \tag{8} \]

satisfying the following constraints:

\[ w_{ij} \geq 0, \quad \forall i \in [k_1], j \in [k_2] \tag{9} \]

\[ \sum_{i=1}^{k_2} w_{il} = \alpha_i, \quad \forall i \in [k_1] \tag{10} \]

\[ \sum_{l=1}^{k_1} w_{lj} = \beta_j, \quad \forall j \in [k_2]. \tag{11} \]

By defining \( U(\alpha, \beta) \) to be set of non-negative matrices \( W = [w_{ij}] \) with \( \sum_{l=1}^{k_2} w_{il} = \alpha_i \) and \( \sum_{l=1}^{k_1} w_{lj} = \beta_j \) (transport polytope \cite{27}), we get the equivalent compact definition of MCOT/CROT:

\[ H_\delta(m_1 : m_2) = \min_{W \in U(\alpha, \beta)} \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{ij} \delta(p_i, q_j). \tag{12} \]
When the ground distance $\delta$ is asymmetric, we shall use the ‘:’ notation instead of the ‘,’ notation for separating arguments.

In general, the LP problem (with $k_1 \times k_2$ variables and inequalities, $k_1 + k_2$ equalities whom $k_1 + k_2 - 1$ are independent) delivers an optimal soft assignment of mixture components with exactly $k_1 + k_2 - 1$ nonzero coefficients in matrix $W = [w_{ij}]$. The complexity of linear programming in $n$ variables with $b$ bits using Karmarkar’s interior point methods is polynomial, in $O(n^{7/2}b^2)$ [28].

Observe that we necessarily have:

$$\max_{j \in [k_2]} w_{ij} \geq \frac{\alpha_i}{k_2},$$

and similarly that:

$$\max_{i \in [k_1]} w_{ij} \geq \frac{\beta_j}{k_1}.$$ 

Note that $H(m, m) = 0$ since $w_{ij} = \delta_{ij}$ where $\delta_{ij}$ denotes the Kronecker symbol: $\delta_{ij} = 1$ iff $i = j$, and 0 otherwise.

We can interpret MCOT as a *Discrete Optimal Transport* (DOT) between (non-embedded) histograms. When $k_1 = k_2 = d$, the transport polytope is the polyhedral set of non-negative $d \times d$ matrices:

$$U(\alpha, \beta) = \{P \in \mathbb{R}_{+}^{d \times d} : P1_d = \alpha, P^\top1_d = \beta\},$$

and

$$H_\delta(m_1 : m_2) = \min_{P \in U(\alpha, \beta)} \langle P, W \rangle,$$

where $\langle A, B \rangle = \text{tr}(A^\top B)$ is the Fröbenius inner product of matrices, and $\text{tr}(A)$ the matrix trace. This OT can be calculated using the network simplex in $O(d^3 \log d)$ time.

Cuturi [7] showed how to relax the objective function in order to get fast calculation using the Sinkhorn divergence:

$$S_\delta(m_1 : m_2) = \min_{P \in U(\alpha, \beta)} \langle P, W \rangle,$$

where $U(\alpha, \beta):=\{P \in U(\alpha, \beta) : \text{KL}(P : \alpha\beta^\top) \leq \lambda\}$. The KL divergence between two $k \times k$ matrices $M = [m_{i,j}]$ and $M' = [m'_{i,j}]$ is defined by

$$\text{KL}(M : M') := \sum_{i,j} m_{i,j} \log \frac{m_{i,j}}{m'_{i,j}},$$

with the convention that $0 \log \frac{0}{0} = 0$. The Sinkhorn divergence is calculated using the equivalent dual Sinkhorn divergence by using matrix scaling algorithms (e.g., the Sinkhorn-Knopp algorithm).

Because the minimization is performed on $U_\lambda(\alpha, \beta) \subset U(\alpha, \beta)$, we have

$$H_\delta(m_1 : m_2) \leq S_\delta(m_1 : m_2).$$

(14)

Notice that the smooth (dual) Sinkhorn divergence has also been shown experimentally to improve over the EMD in applications [7] (MNIST classification).

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1 A LP in $d$-dimensions has its solution located at a vertex of a polytope, described by the intersection of $d + 1$ hyperplanes (linear constraints).
3.1 Upper bounding statistical distances between mixtures with CROT

First, let us report the basic upper bounds for MCOT mentioned earlier in Property 2. The objective function is upper bounded by:

\[
H(m_1, m_2) \leq \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} \alpha_i \beta_j \delta(p_i, q_j) \leq \max_{\pi \in [k_1], j \in [k_2]} \delta(p_i, q_j).
\]

(15)

Now, when the conditional density distance \( \delta \) is separate convex (i.e., meaning convex in both arguments), we get the following Separate Convexity Upper Bound (SCUB):

\[
(SCUB): \quad \delta(m_1 : m_2) \leq \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} \alpha_i \beta_j \delta(p_i : q_j).
\]

(16)

For example, norm-induced distances or \( f \)-divergences \([10]\) are separate convex distances.

For the particular case of the KL divergence, we have:

\[
KL(p : q):= \int p(x) \log \frac{p(x)}{q(x)} dx,
\]

and when \( k_1 = k_2 \), we get the following upper bound using the log-sum inequality \([10, 41]\):

\[
KL(m_1 : m_2) \leq KL(\alpha : \beta) + \sum_{i=1}^{k} \alpha_i KL(p_i : q_i).
\]

(17)

Since this holds for any permutation of \( \sigma \) of mixture components, we can tighten this upper bound by minimizing over all permutations:

\[
KL(m_1 : m_2) \leq \min_{\sigma} KL(\alpha : \sigma(\beta)) + \sum_{i=1}^{k} \alpha_i KL(p_i : \sigma(q_i)).
\]

(18)

The best permutation \( \sigma \) can be computed using the Hungarian algorithm \([55, 50, 21, 20]\) in cubic time (with cost matrix \( C = [c_{ij}] \), and \( c_{ij} = KL(\alpha_i : \beta_j) + \alpha_i KL(p_i : q_j) \) with \( KL(a : b) = a \log \frac{a}{b} \)).

Now, let us further rewrite \( m_1(x) = \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w'_{i,j} q_j(x) \) with \( \sum_{i=1}^{k_1} w'_{i,j} = \alpha_i \), and \( m_2(x) = \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w'_{i,j} q_i(x) \) as mixtures of \( k = k_1 \times k_2 \) (redundant) components \( \{p_i(x) = p_i(x)\} \) and \( \{q_i(x) = q_j(x)\} \), and apply the upper bound of Eq. \([17]\) for the “best split” of matching mixture components \( \sum_{j=1}^{k_2} w'_{i,j} q_j(x) \leftrightarrow \sum_{j=1}^{k_1} w'_{i,j} q_i(x) \):

\[
KL(m_1 : m_2) \leq \min_{w \in U(\alpha, \beta)} \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} \log \frac{w_{i,j}}{w'_{i,j}} + \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} KL(p_i : q_j),
\]

(19)

Let

\[
O(m_1 : m_2) = \min_{w \in U(\alpha, \beta)} \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} \log \frac{w_{i,j}}{w'_{i,j}} + \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} KL(p_i : q_j).
\]

(20)
Then it follows that
\[
\text{KL}(m_1 : m_2) \leq O(m_1 : m_2) \leq \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} \log \frac{w_{i,j}}{w_{j,i}} + H_{\text{KL}}(m_1, m_2). \tag{21}
\]

Thus CROT allows to upper bound the KL divergence between mixtures. The technique of rewriting mixtures as mixtures of \( k = k_1 \times k_2 \) redundant components bears some resemblance with the variational upper bound on the KL between mixtures proposed in \cite{22} that requires to iterate until convergence an update of the variational upper bound.

In fact, the CROT distance provides an upper bound on the distance between mixtures provided the base distance \( \delta \) is joint convex \cite{2,43}.

**Definition 4 (Joint convex distance).** A distance \( D(\cdot : \cdot) \) is joint convex if and only if
\[
D((1 - \alpha)p_1 + \alpha p_2 : (1 - \alpha)q_1 + \alpha q_2) \leq (1 - \alpha)D(p_1 : p_2) + \alpha D(p_2 : q_2), \quad \forall \alpha \in [0, 1].
\]

We write this joint convex inequality more compactly as:
\[
D((p_1p_2)_{\alpha} : (q_1q_2)_{\alpha}) \leq (D(p_1 : p_2)D(p_2 : q_2))_{\alpha}, \quad \forall \alpha \in [0, 1],
\]
where \((ab)_{\alpha} := (1 - \alpha)a + \alpha b.

**Theorem 5 (Upper Bound on Joint Convex Mixture Distance (UBJCMD)).** Let \( m_1(x) = \sum_{i=1}^{k_1} \alpha_i p_i(x) \) and \( m_2(x) = \sum_{i=1}^{k_2} \beta_i q_i(x) \) be two finite mixtures, and \( \delta(\cdot , \cdot) \) any joint convex statistical base distance. Then CROT \( H_{\delta}(m_1 : m_2) \) upper bounds the distance \( \delta(m_1, m_2) \) between mixtures:
\[
(JCUB) : \quad \delta(m_1 : m_2) \leq H_{\delta}(m_1 : m_2). \tag{22}
\]

**Proof.**

\[
\delta(m_1 : m_2) = \delta \left( \sum_{i=1}^{k_1} \alpha_i p_i, \sum_{j=1}^{k_2} \beta_j q_j \right) \\
= \delta \left( \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} p_{i,j} : \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} q_{i,j} \right) \\
\leq \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} \delta(p_{i,j} : q_{i,j}), \\
\leq \sum_{i=1}^{k_1} \sum_{j=1}^{k_2} w_{i,j} \delta(p_i : q_j) =: H_{\delta}(m_1, m_2).
\]

Notice that \( H_{\delta}(m_1, m_2) \neq H_{\delta}(m_2, m_1) \) for asymmetric base distance \( \delta \).

For mixtures with same weights but different component basis and a joint convex distance \( D \) (e.g., KL), we get \( D(\sum_{i=1}^{k} w_ip_i : \sum_{i=1}^{k} w_iq_i) \leq \sum_{i=1}^{k} \alpha_i D(p_i : q_i) \).

Let us give some examples of joint convex distances:

8
Figure 2: An interpretation of CROT by rewriting the mixtures $m_1 = \sum_{i=1}^{2} \alpha_i p_i$ and $m_2 = \sum_{i=1}^{3} \beta_i q_i$ with $p_{i,j} = p_i$ and $q_{i,j} = q_j$ and using the joint convexity of the base distance $\delta$.

- The $f$-divergences \cite{45} $I_f(p : q) = \int p(x)f(q(x)/p(x))dx$ (for a convex generator $f(u)$ satisfying $f(1) = 0$),
- The $p$-powered Wasserstein distances \cite{46} $W_p^p$,
- The Rényi divergences \cite{57} for $\alpha \in [0,1]$,
- Bregman divergences \cite{3} (Exercises 2.3.29 and 2.3.30) provided that the generator $F$ satisfies $\nabla^2 F(y) + \nabla^3 F(y)(y - x) \succeq (\nabla^2 F(x)\nabla^2 F)^{-1}(y)$ where $\succeq$ denotes the Löwner ordering,
- etc.

A joint convex function is separately convex but the converse is false. However, a separately convex bivariate function that is positively homogeneous of degree one is joint convex (but this result does not hold in higher dimensions \cite{8}).

Conversely, CROT yields a lower bound for joint concave distances (e.g., fidelity in quantum computing \cite{44}).

Figure 2 illustrates the CROT distance between statistical mixtures (not having the same number of components).
4 Experiments

4.1 Total Variation distance

Since TV is a metric $f$-divergence \cite{25} bounded in $[0,1]$, so is MCOT. The closed-form formula for the total variation between univariate Gaussian distributions is reported in \cite{34} (using the erf function), and the other formula for the total variation between Rayleigh distributions and Gamma distributions is given in \cite{43}.

Figure 4 illustrates the performances of the various lower/upper bounds on the total variation between mixtures of Gaussian, Gamma, and Rayleigh distributions with respect to the true value which is estimated using Monte Carlo samplings.

The acronyms of the various bounds are as follows:

- CELB: Combinatorial Envelope Lower Bound \cite{42} (applies only for 1D mixtures)
- CEUB: Combinatorial Envelope Upper Bound \cite{42} (applies only for 1D mixtures)
- CGQLB: Coarse-Grained Quantization Lower Bound \cite{42} for 1000 bins (applies only for $f$-divergences that satisfy the information monotonicity property)
- CROT: Chain Rule Optimal Transport $H_\delta$ (this paper)
- Sinkhorn CROT: Entropy-regularized CROT \cite{7} $S_\delta \leq H_\delta$, with $\lambda = 1$ and $\epsilon = 10^{-8}$ (for convergence of the Sinkhorn-Knopp iterative matrix scaling algorithm).

Next, we consider the renown MNIST handwritten digit database \cite{29} of 70,000 handwritten digit $28 \times 28$ grey images\footnote{http://yann.lecun.com/exdb/mnist/} and the Fashion-MNIST images with exactly the same sample size and dimensions but different image contents \cite{59}. We first use PCA to reduce the original dimensionality $d = 28 \times 28 = 784$ to $D \in \{10, 50\}$. Then we extract two subsets of samples, and estimate respectively two GMMs composed of 10 multivariate Gaussian distributions with a diagonal covariance matrix. The GMMs are learned by the Expectation-Maximization (EM) algorithm implementation of scikit-learn \cite{47}. Notice that we did not use the labels in our estimation, and therefore the mixture components do not necessarily correspond to different digits.

We approximate the TV between $D$-dimensional GMMs using Monte Carlo by performing stochastic integration of the following integrals:

$$\text{TV}(p, q) := \frac{1}{2} \int |p(x) - q(x)| dx$$

$$= \frac{1}{2} \int p(x) \left| \frac{p(x) - q(x)}{p(x) + q(x)} \right| dx + \frac{1}{2} \int q(x) \left| \frac{p(x) - q(x)}{p(x) + q(x)} \right| dx$$

$$\approx \frac{1}{2m} \sum_{x_i \sim p(x)} \left| \frac{p(x_i) - q(x_i)}{p(x_i) + q(x_i)} \right| + \frac{1}{2m} \sum_{y_i \sim q(x)} \left| \frac{p(y_i) - q(y_i)}{p(y_i) + q(y_i)} \right|$$

$$= \frac{1}{2m} \sum_{x_i \sim p(x)} \frac{1 - \exp(r(x_i))}{1 + \exp(r(x_i))} + \frac{1}{2m} \sum_{x_i \sim q(x)} \frac{1 - \exp(r(y_i))}{1 + \exp(r(y_i))},$$

where $\{x_i\}_{i=1}^m$ and $\{y_i\}_{i=1}^m$ are i.i.d. samples drawn from $p(x)$ and $q(x)$ respectively, and $r(x) = |\log p(x) - \log q(x)|$. In our experiments, we set $m = 0.5 \times 10^4$. 

Figure 3: TV distance between two 10-component GMMs estimated on the MNIST dataset: (1) shows the $10 \times 10$ matrix TV distance between the first mixture components and the second mixture components (red means large distance and blue means a small distance). (2-4) displays the $10 \times 10$ optimal transport matrix $W$ (red means larger weights, blue means smaller weights). The optimal transport matrix is estimated by EMD (2), the Sinkhorn algorithm with weak regularization (3) and the Sinkhorn with strong regularization (4).

To compute the CROT, we use the EMD and Sinkhorn implementations provided by the POT [15] library (Python Optimal Transport). For Sinkhorn, we set the entropy regularization strength as follows: Sinkhorn (1) means median($M$) and Sinkhorn (10) means median($M$)/10, where $M$ is the metric cost matrix. For example, to compute CROT-TV, $M$ is the pairwise TV distance matrix from all components in the first mixture model to all components in the second mixture. The maximum number of Sinkhorn iterations is 1000, with a stop threshold of $10^{-10}$.

To get some intuitions, see Figure 3 for the cost matrix and the corresponding optimal transport matrix, where the cost is defined by TV distance, and the dataset is PCA-processed MNIST. We see that the transportation scheme tries to assign higher weights to small cost pairs (blue region in the cost matrix).

Figure 3(1) shows the $10 \times 10$ TV distance between mm1’s components and mm2’s components red means large distance, blue means a small distance Figure 3

Our experiments yield the following observations: As the sample size $\tau$ decreases, the TV distances between GMMs turn larger because the GMMs are pulled towards the two different empirical distributions. As the dimension $D$ increases, TV increases because in a high dimensional space the GMM components are less likely to overlap. We check that CROT-TV is an upper bound of TV. We verify that Sinkhorn divergences are upper bounds of CROT. These observations are consistent across two data sets. The distances of Fashion-MNIST are in general larger than the corresponding distances in MNIST, which can be intuitively explained by that the “data manifold” of Fashion-MNIST has a more complicated structure than MNIST.

4.2 Square root of the symmetric $\alpha$-Jensen-Shannon divergence

TV is bounded in $[0, 1]$ which makes it difficult to appreciate the quality of the CROT upper bounds in general. We shall consider a different parametric distance $D_\alpha$ that is upper bounded by an arbitrary bound: $D_\alpha(p,q) \leq C_\alpha$.

It is well known that the square root of the Jensen-Shannon divergence is a metric [16] (satisfying the triangle inequality). In [32], a generalization of the Jensen-Shannon divergence was proposed,
Sinkhorn (1) Sinkhorn (10)

Table 1: TV distances between two GMMs with 10 components each estimated on PCA-processed images. \( D \) is the dimensionality of the PCA. The two GMMs are estimated based on non-overlapping samples, with the parameter \( 0 < \tau \leq 1 \) specifying the relative sample size used to estimated the GMMs. For example, \( \tau = 1 \) means each GMM is estimated on half of all available images. Sinkhorn (\( \lambda \)) denotes the CROT distance estimated by the Sinkhorn algorithm, where the regularization strength is proportional to \( 1/\lambda \). For each configuration, the two GMMs are repeatedly estimated based on 100 pairs of random subsets of the full dataset, with the mean and standard deviation reported.

| Data  | \( D \) | \( \tau \) | TV     | CROT-TV | Sinkhorn (10) | Sinkhorn (1)  |
|-------|--------|----------|--------|---------|---------------|---------------|
| MNIST | 10     | 1        | 0.16 ± 0.08 | 0.26 ± 0.14 | 0.27 ± 0.14 | 0.78 ± 0.05  |
|       | 10     | 0.1      | 0.29 ± 0.05 | 0.43 ± 0.08 | 0.44 ± 0.08 | 0.84 ± 0.02  |
|       | 50     | 1        | 0.35 ± 0.08 | 0.43 ± 0.10 | 0.44 ± 0.10 | 0.78 ± 0.03  |
|       | 50     | 0.1      | 0.54 ± 0.04 | 0.64 ± 0.05 | 0.67 ± 0.06 | 0.84 ± 0.02  |
| Fashion | 10   | 1        | 0.19 ± 0.09 | 0.23 ± 0.12 | 0.24 ± 0.12 | 0.81 ± 0.03  |
| MNIST | 10     | 0.1      | 0.33 ± 0.07 | 0.40 ± 0.09 | 0.40 ± 0.09 | 0.86 ± 0.02  |
|       | 50     | 1        | 0.44 ± 0.11 | 0.48 ± 0.12 | 0.50 ± 0.13 | 0.88 ± 0.03  |
|       | 50     | 0.1      | 0.60 ± 0.07 | 0.64 ± 0.08 | 0.67 ± 0.09 | 0.92 ± 0.02  |

Table 2: Square root of the Jensen-Shannon divergence between two 10-component GMMs estimated on PCA-processed images.

| Data  | \( D \) | \( \tau \) | \( \sqrt{\text{JS}_{0.5}} \) | CROT-\( \sqrt{\text{JS}_{0.5}} \) | Sinkhorn (10) | Sinkhorn (1)  |
|-------|--------|----------|----------------|----------------|---------------|---------------|
| MNIST | 10     | 1        | 0.25 ± 0.11 | 0.36 ± 0.17 | 0.37 ± 0.17 | 0.94 ± 0.05  |
|       | 10     | 0.1      | 0.39 ± 0.05 | 0.55 ± 0.07 | 0.56 ± 0.08 | 1.00 ± 0.02  |
|       | 50     | 1        | 0.51 ± 0.11 | 0.54 ± 0.12 | 0.56 ± 0.13 | 0.93 ± 0.04  |
|       | 50     | 0.1      | 0.69 ± 0.05 | 0.76 ± 0.07 | 0.79 ± 0.07 | 1.00 ± 0.03  |
| Fashion | 10   | 1        | 0.33 ± 0.15 | 0.31 ± 0.13 | 0.33 ± 0.14 | 0.96 ± 0.04  |
| MNIST | 10     | 0.1      | 0.46 ± 0.09 | 0.48 ± 0.09 | 0.49 ± 0.10 | 1.01 ± 0.03  |
|       | 50     | 1        | 0.60 ± 0.12 | 0.57 ± 0.14 | 0.59 ± 0.15 | 1.03 ± 0.04  |
|       | 50     | 0.1      | 0.75 ± 0.07 | 0.76 ± 0.09 | 0.80 ± 0.10 | 1.08 ± 0.02  |
Figure 4: Performance of the CROT distance and the Sinkhorn CROT distance for upper bounding the total variation distance between mixtures of (1) Gaussian, (2) Gamma, and (3) Rayleigh distributions.
Figure 5: Performance of the CROT distance and the Sinkhorn CROT distance for upper bounding the square root of the $\alpha$-Jensen-Shannon distance between mixtures of (1) Gaussian, (2) Gamma, and (3) Rayleigh distributions.
given by
\[ \text{JS}_\alpha(p : q) := \frac{1}{2} \text{KL}(p : (pq)_\alpha) + \frac{1}{2} \text{KL}(q : (pq)_\alpha), \]  
(23)
where \((pq)_\alpha := (1 - \alpha)p + \alpha q\). \text{JS}_\alpha unifies (twice) the Jensen-Shannon divergence (obtained when \(\alpha = \frac{1}{2}\)) with the Jeffreys divergence (\(\alpha = 1\)) [32]. A nice property is that the skew \(K\)-divergence is upper bounded as follows:
\[ \text{KL}(p : (pq)_\alpha) \leq \int p \log \frac{p}{(1 - \alpha)p} \leq -\log(1 - \alpha) \]
for \(\alpha \in (0, 1)\), so that \(\sqrt{\text{JS}_\alpha(p : q)} \leq -\frac{1}{2} \log(1 - \alpha) - \frac{1}{2} \log \alpha\) for \(\alpha \in (0, 1)\).

Thus, we have the square root of the symmetrized \(\alpha\)-divergence that is upper bounded by
\[ \sqrt{\text{JS}_\alpha(p : q)} \leq C_\alpha = \sqrt{-\frac{1}{2} \log(1 - \alpha) - \frac{1}{2} \log \alpha}. \]

However, \(\sqrt{\text{JS}_\alpha(p : q)}\) is not a metric in general [45]. Indeed, in the extreme case of \(\alpha = 1\), it is known that any positive power of the Jeffreys divergence does not yield a metric.

Observe that \(\text{JS}_\alpha\) is a \(f\)-divergence since \(K_\alpha(p : q) := \text{KL}(p : (pq)_\alpha)\) is a \(f\)-divergence for the generator \(f(u) = -\log((1 - \alpha) + \alpha u)\), and we have \(\text{KL}(q : (pq)_\alpha) = K_{1-\alpha}(q : p)\). Since \(I_f(q : p) = I_{f^\circ}(p : q)\) for \(g(u) = uf(1/u)\), it follows that the \(f\)-generator \(f_{\text{JS}_\alpha}\) for the \(\text{JS}_\alpha\) divergence is:
\[ f_{\text{JS}_\alpha}(u) = -\log ((1 - \alpha) + \alpha u) - \log \left(\alpha + \frac{1 - \alpha}{u}\right). \]  
(24)

Figure 5 and table 2 display the experimental results obtained for the \(\alpha\)-JS divergences. One can have similar observations with the TV results.

4.3 Wasserstein \(W_p\) CROT on GMMs

The \(p\)-th power of the \(L_p\)-Wasserstein distance, \(W_p^p\), is joint convex for \(p \geq 1\) (see Eq. 20 p. 6 of [46]). Thus we can apply the CROT distance between two GMMs \(m_1\) and \(m_2\) to get the following upper bound:
\[ W_p(m_1, m_2) \leq H_{W_p^p}(m_1, m_2), \quad \alpha \geq 1. \]

We also have \(W_p \leq W_q\) for \(1 \leq p \leq q < \infty\).

The OT distance \(W_2\) between Gaussian measures [11, 56] is available in closed-form:
\[ W_2(N(\mu_1, \Sigma_1), N(\mu_1, \Sigma_1)) = \sqrt{||\mu_1 - \mu_2||^2 + \text{tr}(\Sigma_1 + \Sigma_2 - 2(\Sigma_1^{\frac{1}{2}} \Sigma_2 \Sigma_1^{\frac{1}{2}})^\frac{1}{2})}. \]

This \(H_{W_p^p}\) CROT distance generalizes [5] that considered the \(W_2\) distance between GMMs using discrete OT. They proved that \(H_{W_2}(m_1, m_2)\) is a metric, and \(W_2(m_1, m_2) \leq \sqrt{H_{W_2}(m_1, m_2)}\). These results generalize to mixture of elliptical distributions [11]. However, we do not know a closed-form formula for \(W_p\) between Gaussian measures when \(p \neq 2\).
Given two high-dimensional mixture models \( m_1 \) and \( m_2 \), we draw respectively \( n \) i.i.d. samples from \( m_1 \) and \( m_2 \), so that \( m_1(x) \approx \frac{1}{n} \sum_{i=1}^{n} \delta(x_i) \) and \( m_2(x) \approx \frac{1}{n} \sum_{j=1}^{n} \delta(y_j) \). Then, we have

\[
W_p(m_1, m_2) \approx W_p \left( \frac{1}{n} \sum_{i=1}^{n} \delta(x_i), \frac{1}{n} \sum_{j=1}^{n} \delta(y_j) \right) \leq H_{W_p}^{1/p} \left( \frac{1}{n} \sum_{i=1}^{n} \delta(x_i), \frac{1}{n} \sum_{j=1}^{n} \delta(y_j) \right).
\]

Note that \( W_p(\delta(x_i), \delta(x_j)) = \|x_i - x_j\|_2 \) and therefore the RHS of (25) can be evaluated. We use UB(\( W_2 \)) to denote this empirical upper bound that will hold if \( n \to \infty \). In our experiments \( n = 10^3 \).

See Table 3 for the \( W_2 \) distances evaluated on the two investigated data sets. The column LB(\( W_2 \)) is a lower bound based on the first and second moments of the mixture models [18]. We can clearly see that \( \sqrt{H_{W_2}^{1/2}} \) provides a tighter upper bound than UB(\( W_2 \)). To compute UB(\( W_2 \)) one need to draw a potentially large number of random samples to make the approximation in (25) and the computation of the EMD is costly. Therefore one should use \( \sqrt{H_{W_2}^{1/2}} \) for its better and more efficient approximation.

### 4.4 Rényi CROT on GMMs

We investigate Rényi \( \alpha \)-divergence [39, 38] defined by

\[
R_\alpha(p : q) = \frac{1}{1 - \alpha} \log \int p(x)^\alpha q(x)^{1-\alpha} dx,
\]

which encompasses KL divergence at the limit \( \alpha \to 1 \). Notice that for multivariate Gaussian densities \( p \) and \( q \), \( R_\alpha(p : q) \) can be undefined for \( \alpha > 1 \) as the integral may diverge. In this case the CROT-R\( \alpha \) divergence is undefined.

Table 4 shows \( R_\alpha \) for \( \alpha \in \{0.1, 0.5, 0.9\} \) and the corresponding CROT estimated on MNIST and Fashion-MNIST datasets. The observation is consistent with the other distance metrics.

### 5 Conclusion and perspectives

In this work, we defined the generic Chain Rule Optimal Transport (CROT) distance (Definition 1) \( H_\delta \) for a ground distance \( \delta \) that encompasses the Wasserstein distance between point sets (Earth Mover Distance [51]) and the Mixture Component Optimal Transport (MCOT) distance [30], and proved that \( H_\delta \) is a metric whenever \( \delta \) is a metric (Theorem 3). We then dealt with statistical mixtures, and showed that \( H_\delta(m_1 : m_2) \geq \delta(m_1 : m_2) \) (Theorem 5) whenever \( \delta \) is joint convex. This holds in particular for statistical \( f \)-divergences \( I_f(p : q) = \int p(x)f(q(x)/p(x)) dx \):

\[
H_{I_f}(m_1 : m_2) \geq I_f(m_1 : m_2).
\]

We also considered the smoothened Sinkhorn CROT distance \( S_\delta(m_1 : m_2) \) for fast calculations of \( H_\delta(m_1 : m_2) \) via matrix scaling algorithms (Sinkhorn-Knopp algorithm), with \( H_\delta(m_1 : m_2) \leq S_\delta(m_1 : m_2) \).

There are many venues to explore for further research: For example, we may consider the chain rule factorization for \( d \)-variate densities (which gives rise to a hierarchy of CROT distances). This is
Table 3: $W_2$ distances between two 10-component GMMs estimated on PCA-processed images.

| Data   | $D$ | $\tau$ | UB($W_2$)       | LB($W_2$)       | $\sqrt{\text{CROT}-W_2^2}$ | Sinkhorn (10) | Sinkhorn (1) |
|--------|-----|--------|-----------------|-----------------|----------------------------|---------------|--------------|
| MNIST  | 10  | 1      | 1.91 ± 0.02     | 0.03 ± 0.00     | 0.84 ± 0.57                | 0.88 ± 0.58   | 7.13 ± 0.11  |
|       | 10  | 0.1    | 1.93 ± 0.02     | 0.09 ± 0.02     | 1.48 ± 0.38                | 1.54 ± 0.39   | 7.29 ± 0.11  |
|       | 50  | 1      | 7.51 ± 0.03     | 0.07 ± 0.01     | 2.17 ± 0.93                | 2.39 ± 0.97   | 12.02 ± 0.15 |
|       | 50  | 0.1    | 7.53 ± 0.04     | 0.21 ± 0.02     | 4.04 ± 0.86                | 4.33 ± 0.91   | 12.69 ± 0.22 |
|       | 10  | 1      | 1.71 ± 0.05     | 0.03 ± 0.01     | 1.19 ± 0.62                | 1.24 ± 0.63   | 10.36 ± 0.08 |
| Fashion| 10  | 0.1    | 1.74 ± 0.05     | 0.10 ± 0.02     | 1.61 ± 0.63                | 1.68 ± 0.64   | 10.43 ± 0.15 |
| MNIST  | 50  | 1      | 7.47 ± 0.04     | 0.07 ± 0.01     | 3.12 ± 1.01                | 3.21 ± 1.02   | 15.31 ± 0.20 |
|       | 50  | 0.1    | 7.50 ± 0.04     | 0.22 ± 0.02     | 4.32 ± 1.02                | 4.45 ± 1.05   | 15.99 ± 0.29 |

Table 4: Rényi divergences between two 10-component GMMs estimated on PCA-processed images.

| Data   | $D$ | $\tau$ | $R_\alpha$       | CROT-$R_\alpha$  | Sinkhorn (10) | Sinkhorn (1) |
|--------|-----|--------|------------------|-------------------|---------------|--------------|
| MNIST  | 10  | 1      | 0.01 ± 0.01      | 0.07 ± 0.05       | 0.08 ± 0.05   | 0.80 ± 0.02  |
|        | 10  | 0.1    | 0.03 ± 0.02      | 0.15 ± 0.04       | 0.16 ± 0.04   | 0.84 ± 0.04  |
|        | 50  | 1      | 0.09 ± 0.06      | 0.25 ± 0.09       | 0.29 ± 0.10   | 1.40 ± 0.07  |
|        | 50  | 0.1    | 0.18 ± 0.09      | 0.42 ± 0.09       | 0.46 ± 0.10   | 1.43 ± 0.09  |
| Fashion| 10  | 1      | 0.04 ± 0.03      | 0.11 ± 0.06       | 0.12 ± 0.06   | 1.59 ± 0.05  |
| MNIST  | 10  | 0.1    | 0.06 ± 0.05      | 0.34 ± 0.23       | 0.37 ± 0.22   | 4.09 ± 0.12  |
|        | 50  | 1      | 0.31 ± 0.13      | 1.07 ± 0.41       | 1.28 ± 0.43   | 6.73 ± 0.31  |
|        | 50  | 0.1    | 0.69 ± 0.14      | 1.92 ± 0.40       | 2.16 ± 0.42   | 7.01 ± 0.33  |
| Fashion| 10  | 1      | 0.17 ± 0.12      | 0.52 ± 0.29       | 0.55 ± 0.29   | 7.54 ± 0.14  |
| MNIST  | 10  | 0.1    | 0.28 ± 0.13      | 0.87 ± 0.28       | 0.92 ± 0.29   | 7.79 ± 0.23  |
|        | 50  | 1      | 0.54 ± 0.24      | 1.45 ± 0.48       | 1.55 ± 0.48   | 10.53 ± 0.26 |
|        | 50  | 0.1    | 0.89 ± 0.21      | 2.16 ± 0.39       | 2.27 ± 0.40   | 10.79 ± 0.38 |

| Data   | $D$ | $\tau$ | $R_{0.9}$       | LB($R_{0.9}$)  | Sinkhorn (10) | Sinkhorn (1) |
|--------|-----|--------|-----------------|---------------|---------------|--------------|
| MNIST  | 10  | 1      | 0.14 ± 0.09     | 0.76 ± 0.42   | 0.80 ± 0.42   | 7.18 ± 0.19  |
|        | 10  | 0.1    | 0.31 ± 0.09     | 1.35 ± 0.37   | 1.42 ± 0.37   | 7.53 ± 0.35  |
|        | 50  | 1      | 0.61 ± 0.32     | 1.90 ± 0.82   | 2.25 ± 0.85   | 12.46 ± 0.66 |
|        | 50  | 0.1    | 1.33 ± 0.30     | 3.51 ± 0.80   | 3.90 ± 0.82   | 12.96 ± 0.86 |
| Fashion| 10  | 1      | 0.32 ± 0.23     | 1.07 ± 0.60   | 1.12 ± 0.61   | 14.25 ± 0.38 |
| MNIST  | 10  | 0.1    | 0.50 ± 0.26     | 1.69 ± 0.66   | 1.77 ± 0.67   | 14.74 ± 0.54 |
|        | 50  | 1      | 1.07 ± 0.43     | 2.76 ± 0.96   | 2.93 ± 0.97   | 21.41 ± 0.78 |
|        | 50  | 0.1    | 1.76 ± 0.45     | 4.18 ± 1.06   | 4.40 ± 1.09   | 22.16 ± 1.02 |
all the more interesting because the Wasserstein $W_p$ distance admits a simple closed-form solution in the 1D case:

$$W_p(X,Y) = \left( \int_0^1 |F_X^{-1}(u) - F_Y^{-1}(u)|^p du \right)^{\frac{1}{p}},$$

where $F_X$ and $F_Y$ are the cumulative distribution functions (CDFs) of $X$ and $Y$, respectively.

We would also like to apply CROT to infinite Gaussian mixtures [49] and graphical models [26]. It would also be interesting to consider the Sinkhorn CROT vs. CROT in applications [30] that deal with mixtures of features. Yet another direction is to explore the use of the CROT distance in deep learning.

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Lemma 6 to get $p$ with equality when

\begin{equation}
Eq. 27
\end{equation}

Proof. Consider a strictly convex and differentiable function $F(x)$ on $(0, \infty)$. Then we have

\[ F(b) - F(a) \geq F'(a)(b-a), \]

for any $a, b \in (0, \infty)$, with equality iff. $a = b$. Indeed, this inequality is related to the non-negativeness of the scalar Bregman divergence $B_F(b, a) = F(b) - F(a) - (b - a)F'(a) \geq 0$.

Plugging $F(x) = -\log x$ (with $F'(x) = -\frac{1}{x}$ and $F''(x) = \frac{1}{x^2} > 0$), $a = q(x)$ and $b = p(x)$ in Eq. 27 we get

\[ \log q(x) - \log p(x) \geq \frac{q(x) - p(x)}{q(x)}. \]

Multiplying both sides of the inequality by $-p(x) < 0$ (and reversing the inequality), we end up with

\[ p(x) \log \frac{p(x)}{q(x)} \leq \frac{p^2(x)}{q(x)} - p(x). \]

Then taking the integral over the support $\mathcal{X}$ of the distributions yields:

\[ \text{KL}(p : q) \leq \int_{\mathcal{X}} \frac{p(x)^2}{q(x)} \, d\mu(x) - 1, \]

with equality when $p(x) = q(x)$ almost everywhere. Notice that the right-hand side integral $\int_{\mathcal{X}} \frac{p(x)^2}{q(x)} \, d\mu(x)$ may diverge (e.g., when KL is infinite).

Now, let us consider two mixtures $m(x) = \sum_{i=1}^{k} w_i p_i(x)$ and $m'(x) = \sum_{i=1}^{k'} w_i' p_i'(x)$. Apply Lemma 6 to get

\[ \text{KL}(m : m') \leq \sum_{i,j} w_i w_j \frac{p_i(x)p_j(x)}{m'(x)} \, d\mu(x) - 1. \]

Let us upper bound $A_{ij} = \int \frac{b_i(x)p_i(x)}{m'(x)} \, d\mu(x)$ to upper bound

\[ \text{KL}(m : m') \leq \sum_{i,j} w_i w_j A_{ij} - 1. \]

For bounding the terms $A_{ij}$, we interpret the mixture density as an arithmetic weighted mean that is greater or equal than a geometric mean (AGM inequality). Therefore we get:

\[ \int \frac{p_i(x)p_j(x)}{m'(x)} \, d\mu(x) \leq \int \frac{p_i(x)p_j(x)}{\prod_{l=1}^{k'} w_i' p_i'(x)} \, d\mu(x). \]
When the mixture components belong to a same exponential family \(36\), we get a closed-form upper bound since \(\theta_i + \theta_j - \sum_{l=1}^{k'} w'_l \theta'_l \in \Theta\): Let \(\bar{\theta}' = \sum_{l=1}^{k'} w'_l \theta'_l\) denote the barycenter of the natural parameters of the mixture components of \(m'\). We have:

\[
\frac{p(x; \theta_i)p(x; \theta_j)}{\prod_{l=1}^{k'} w'_l p(x; \theta'_l)} = \exp\left( (\theta_i + \theta_j - \bar{\theta}')^\top t(x) - F(\theta_i) - F(\theta_j) + \sum_{l=1}^{k'} w'_l F(\theta'_l) + k(x) \right).
\]

Taking the integral over the support we find that

\[
A_{ij} \leq \exp\left( F(\theta_i + \theta_j - \bar{\theta}') - F(\theta_i) - F(\theta_j) + \sum_{l=1}^{k'} w'_l F(\theta'_l) \right).
\]

Overall, we get the upper bound:

\[
\text{KL}(m : m') \leq \left( \sum_{i,j} w_i w_j \exp\left( F(\theta_i + \theta_j - \bar{\theta}') - F(\theta_i) - F(\theta_j) + \sum_{l=1}^{k'} w'_l F(\theta'_l) \right) \right) - 1. \tag{28}
\]

In general, we have the following upper bound for \(f\)-divergences \(12\):

**Property 7** (\(f\)-divergence upper bound). The \(f\)-divergence between two densities \(p\) and \(q\) with respect to \(\mu\) is upper bounded as follows: \(I_f(p : q) \leq \int (q(x) - p(x)) f'(\frac{q(x)}{p(x)}) \, d\mu(x)\).

**Proof.** Let us use the non-negative property of scalar Bregman divergences:

\[
B_F(a : b) = F(a) - F(b) - (a - b)F'(b) \geq 0.
\]

Let \(F(x) = f(x)\) (with \(F(1) = f(1) = 0\)), and \(a = 1\) and \(b = \frac{q}{p}\). It follows that

\[
B_F \left( 1 : \frac{q}{p} \right) = -f \left( \frac{q}{p} \right) - \left( 1 - \frac{q}{p} \right) f' \left( \frac{q}{p} \right) \geq 0.
\]

That is,

\[
pf \left( \frac{q}{p} \right) \leq p \left( \frac{q}{p} - 1 \right) f' \left( \frac{q}{p} \right).
\]

Taking the integral over the support, we get

\[
I_f(p : q) \leq \int (q - p) f' \left( \frac{q}{p} \right) \, d\mu.
\]

\(\square\)

For example, when \(f(u) = -\log u\) (with \(f'(u) = -\frac{1}{u}\)), we recover the former upper bound:

\[
\text{KL}(p : q) \leq \int (p - q) \frac{p}{q} \, d\mu = \int \frac{p^2}{q} \, d\mu - 1.
\]

Notice that \(\int \frac{p^2}{q} \, d\mu - 1\) is a \(f\)-divergence for the generator \(f(u) = \frac{1}{u} - 1\).