# ON THE GEOMETRY OF MIXTURES OF PRESCRIBED DISTRIBUTIONS

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## ABSTRACT

We consider the space of w-mixtures that are finite statistical mixtures sharing the same prescribed component distributions, like Gaussian mixture models sharing the same components. The information geometry induced by the Kullback-Leibler (KL) divergence yields a dually flat space where the KL divergence between two w-mixtures amounts to a Bregman divergence for the negative Shannon entropy generator, called the Shannon information. Furthermore, we prove that the skew Jensen-Shannon statistical divergence between w-mixtures amount to skew Jensen divergences on their parameters and state several divergence inequalities between w-mixtures and their closures.

## 1. INTRODUCTION AND BACKGROUND

Let  $M^1_+(\Omega)$  denote the space of probability measures defined on a  $\sigma$ -algebra  $\Omega$  of an observation space  $\mathcal{X}$ . Consider a *base measure*  $\mu \in M^1_+(\Omega)$  (usually the Lebesgue or counting measure), and let  $P_0, \ldots, P_{k-1}$  be k prescribed probability distributions, all dominated by  $\mu$  ( $P_i \ll \mu$ ), with  $p_i = \frac{\mathrm{d}P_i}{\mathrm{d}\mu}$  the Radon-Nikodym derivative of  $P_i$  with respect to  $\mu$ . The density  $m(x; w) \in M^1_+(\Omega)$  of a w-mixture is defined by  $m(x; w) := \sum_{i=0}^{k-1} w_i p_i(x)$ , with  $w := (w_0, \ldots, w_{k-1}) \in \Delta^\circ_{k-1}$ , where  $\Delta^\circ_{k-1}$  is the (k-1)-dimensional open probability simplex sitting in  $\mathbb{R}^k$ . Thus w-mixtures are strictly convex weighted combinations of fixed component distributions: They form special subfamilies of finite statistical mixtures [1] that are closed by convex combinations.

Given multiple datasets  $\mathcal{O}_1, \ldots, \mathcal{O}_n$ , a set of *w*-mixtures  $m_1 = m(x; w_1), \ldots, m_n = m(x, w_n)$  (called comixs [2]) can be learned *simultaneously* by generalizing the Expectation-Maximization (EM) or the Classification EM (CEM) algorithms. In particular, one can learn *w*-Gausian Mixture Models [2] (*w*-GMMs) where the prescribed mixture components are fixed Gaussian distributions.

The class of statistical f-divergences [3, 4, 5] between two distributions  $p, q \ll \mu$  defined on support  $\mathcal{X}$  is defined by

$$I_f(p:q) := \int_{\mathcal{X}} p(x) f\left(\frac{q(x)}{p(x)}\right) d\mu(x) \ge f(1), \quad (1)$$

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with f a convex function satisfying f(1) = 0. We have [6]  $I_f(p:q) \leq \lim_{\epsilon \to 0} f(\epsilon) + \epsilon f(\frac{1}{\epsilon})$ . For discrete distributions with probability mass functions  $p := (p_0, \ldots, p_{d-1})$  and q := $(q_0, \ldots, q_{d-1})$ , it comes that  $I_f(p : q) = \sum_{i=0}^{d-1} p_i f(\frac{q_i}{p_i})$ . The f-divergences include the KL divergence (f(u)) = $-\log u$ ), the  $\chi^2$ -divergence, the Hellinger divergence, the  $\alpha$ -divergences, the total variation  $TV(p,q) := \frac{1}{2} \int_{\mathcal{X}} |p(x)| - \frac{1}{2} \int_{\mathcal{X}} |p(x)| + \frac{1}{2} \int_{\mathcal{X}} |p($  $q(x)|d\mu(x)$  (with  $f(u) = \frac{1}{2}|1-u|$ , the only f-divergence metric [7] satisfying the triangle inequality), etc. The dual divergence  $I_f^*(p:q) := I_f(q:p)$  is obtained by taking the dual generator  $f^{\diamond}(u):=uf\left(\frac{1}{u}\right)$ :  $I_{f^{\diamond}}(p:q)=I_{f}(q:p)=$  $I_{f}^{*}(p:q)$ . Thus f-divergences can always be symmetrized [8] by taking the generator  $s(u) = f(u) + f^{\diamond}(u)$ . Examples of symmetric *f*-divergences are the Jeffreys divergence [9]  $J(p;q) := \mathrm{KL}(p:q) + \mathrm{KL}(q:p)$  and the Jensen-Shannon divergence [10] JS(p:q) := K(p:q) + K(q:p) with K(p:q) = K(p;q) + K(q;p)q):=KL $(p:\frac{p+q}{2}) = \int p(x) \log \frac{2p(x)}{p(x)+q(x)} d\mu(x)$ . Depending on the generator f, the f-divergence may be either (1) unbounded when the integral diverges:  $I_f(p:q) := +\infty$  (e.g., KL between a standard Cauchy distribution and a standard normal distributions), or (2) always bounded (e.g., Jensen-Shannon divergence bounded by  $\log 2$ ).

The *f*-divergences between statistical mixtures [11, 12] is not available in closed form although it can be easily upper bounded by using the joint convexity property of *f*divergences:  $I_f(m : m') \leq \sum_{i,j} w_i w'_j I_f(p_i : p'_j)$  for two mixture models  $m(x) = \sum_i w_i p_i(x)$  and m'(x) = $\sum_j w'_j p'_j(x)$ . In practice, to bypass this intractability, one *estimates* the *f*-divergence using Monte Carlo (MC) stochastic integration [13] (Chapter 17): Let *s* iid. samples  $x_1, \ldots, x_s \sim$ p(x), and define the estimator  $\hat{I}_f^s(p:q) := \frac{1}{s} \sum_{i=1}^s f\left(\frac{q(x_i)}{p(x_i)}\right)$ . It follows from the Law of Large Numbers (LLN) that  $\lim_{s\to\infty} \hat{I}_f^s(p:q) = I_f(p:q)$  provided that the variance  $\operatorname{Var}_p\left[f\left(\frac{q(x)}{p(x)}\right)\right]$  is bounded. The MC estimator is consistent (but the MC approximation does not hold when  $I_f(p:q) = \infty$ ). Furthermore, using the Central Limit Theorem (CLT), the MC estimator is shown to be *normally* distributed:  $\hat{I}_f^s(p:q) \sim \mathcal{N}\left(I_f(p:q), \frac{1}{s}\operatorname{Var}_p\left[f\left(\frac{q(x)}{p(x)}\right)\right]\right)$ .

### 1.1. Contributions

In §2, we describe the dually flat geometry of the space of w-mixtures induced by the Kullback-Leibler (KL) divergence. It proves that the KL divergence between any two w-mixtures is equivalent to a Bregman divergence induced by the negative Shannon entropy generator. As a byproduct, this allows us to prove that the KL-averaging integration of w-mixtures used in distributed estimation [14] can be performed optimally without information loss. In §2.2, we show that the skew Jensen-Shannon divergences between w-mixtures amount to an equivalent skew Jensen  $\alpha$ -divergences on their parameters. Finally, we consider several divergence inequalities between w-mixtures and their closures in §3.2.

## 2. GEOMETRY OF W-MIXTURES

We slightly depart from the constructions sketched in the textbooks [15, 9], in order to ease sanity checks.

When the k prescribed component distributions  $p_0(x), \ldots, p_{k-1}(x)$  are *linearly independent*, the space  $\mathcal{M} = \{m(x; w), w \in \Delta_{k-1}^{\circ}\}$  of w-mixtures forms a *mixture family* in information geometry [9, 16] with:

$$m(x;w) = m(x;\eta) = \sum_{i=1}^{k-1} \eta_i p_i(x) + \left(1 - \sum_{i=1}^{k-1} \eta_i\right) p_0(x),$$
(2)

with  $\eta_i = w_i$  for  $i \in [k-1] := \{1, \ldots, k-1\}$  and  $w_0 = 1 - \sum_{i=1}^{k-1} \eta_i = 1 - \sum_{i=1}^{k-1} w_i$ . Let D = k-1 denote the order of the mixture family, that is its number of degrees of freedom. We have  $m(x;w) = m(x;\eta)$ , where vector w is k-dimensional while vector  $\eta$  is (k-1)-dimensional. Let  $f_i(x) = p_i(x) - p_0(x)$  for  $i \in [D]$ , and  $c(x) = p_0(x)$ . Then  $\mathcal{M}$  can be written in the canonical form of a mixture family in information geometry [9]:  $\mathcal{M} = \left\{ m(x;\eta) = \sum_{i=1}^{k-1} \eta_i f_i(x) + c(x), \quad \eta \in \Delta_D^{\circ} \right\}$ , where the  $f_i(x)$ 's and c(x) are linearly independent. By convention, we define  $\eta_0 = 1 - \sum_{i=1}^{D} \eta_i$ , the weight of  $p_0$ . Beware that  $\eta_0$  is not a vector component of  $\eta = (\eta_1, \ldots, \eta_D) \in \Delta_D^{\circ}$ , the D = (k-1)-dimensional open probability simplex sitting in  $\mathbb{R}^d$ .

We consider  $\mathcal{M}$  as a smooth manifold of  $\eta$ -mixtures. The Shannon differential entropy [17] of a mixture m(x):

$$h(m) := -\int_{\mathcal{X}} m(x) \log m(x) \mathrm{d}\mu(x) \tag{3}$$

is usually not available in closed-form [11, 12] because of the log-sum term. Both lower and upper bounds on the entropy of mixtures are reported in [11, 18]. For  $\eta$ -mixtures, the parametric function  $E(\eta) = -h(m(x; \eta))$ , is strictly convex and differentiable. Thus we can form a *dually flat manifold* [15, 9] where the Kullback-Leibler divergence between two mixtures

 $m(x; \eta_1)$  and  $m(x; \eta_2)$  amounts to calculate a *Bregman divergence* [19]  $B_{F^*}(\eta_1 : \eta_2)$  for the *negative Shannon information generator* shifted by one [9]:

$$F^*(\eta) = \int (m(x;\eta) \log m(x;\eta) - m(x;\eta)) d\mu(x), (4)$$
$$= \int m(x;\eta) \log m(x;\eta) d\mu(x) - 1.$$
(5)

Since the Shannon entropy is strictly concave, the negative Shannon entropy called *Shannon information* [20] is strictly convex (and a dually flat manifold can be built from *any*  $C^3$ convex function [5]). Let  $m_1(x) = m(x; \eta_1)$  and  $m_2(x) =$  $m(x; \eta_2)$  for short. We have

$$\begin{aligned} \mathrm{KL}(m_1:m_2) &= \int m(x;\eta_1) \log \frac{m(x;\eta_1)}{m(x;\eta_2)} \mathrm{d}\mu(x), \\ &= F^*(\eta_1) - F^*(\eta_2) - \langle \eta_1 - \eta_2, \nabla F^*(\eta_2) \rangle \\ &= B_{F^*}(\eta_1:\eta_2), \end{aligned}$$

where  $\langle x, y \rangle = x^{\top} y$  denotes the scalar product of  $\mathbb{R}^{D}$ . Although the Shannon information of a *w*-mixture is a convex function of  $\eta$ , it is not available in closed-form [21, 22]. The  $\eta$  parameter is traditionally called the "*expectation*" parameter in information geometry (although this stems from a property of the exponential family manifolds [9]). The dual parameters  $\theta = (\theta^{1}, \ldots, \theta^{D})$ , called the *natural parameters*, are defined by

$$\theta^{i}(\eta) = (\nabla_{\eta} F^{*}(\eta))_{i} = \int \left(p_{i}(x) - p_{0}(x)\right) \log m(x;\eta) \mathrm{d}\mu(x),$$
(6)

since  $(\nabla_{\eta}m(x;\eta))_i = p_i(x) - p_0(x)$  and swapping  $\nabla \int = \int \nabla$  (under regularity condition of Leibniz integral rule). The extra constant  $-1 = -\int m(x;\eta) d\mu(x)$  term in Eq. 4 is added to get a nice expression of the  $\theta^i$ 's in Eq. 6. The dual Legendre convex conjugate [23]  $F(\theta)$  of  $F^*(\eta)$  defined by the Legendre-Fenchel transform  $F(\theta) = \sup_{\theta} \{ \langle \theta, \eta \rangle - F^*(\eta) \}$  is

$$F(\theta) = -\int (p_0(x)\log m(x;\eta) - m(x;\eta))d\mu(x), (7)$$
  
=  $-\int p_0(x)\log m(x;\eta)d\mu(x) + 1$  (8)

Function  $F(\theta)$  is convex with respect to  $\theta$ , and the gradients of the convex conjugates are reciprocal, allowing one to convert *theoretically* from one coordinate system into the dual one:  $\eta = \nabla F(\theta)$  and  $\theta = \nabla F^*(\eta)$ . However, since neither F or  $F^*$  are available in closed forms (except for the multinomial family that are w-mixtures with prescribed Dirac component distributions), those conversions are computationally intractable. It follows that the KL divergence between two  $\eta$ -mixture distributions of  $\mathcal{M}$  can be equivalently written as

$$\begin{aligned} \mathrm{KL}(m_1:m_2) &= \int m(x;\eta_1) \log \frac{m(x;\eta_1)}{m(x;\eta_2)} \mathrm{d}\mu(x), \\ &= B_{F^*}(\eta_1:\eta_2) = B_F(\theta_2:\theta_1), \\ &= D_{F^*,F}(\eta_1:\theta_2) = D_{F,F^*}(\theta_2:\eta_1), \end{aligned}$$

where  $D_{F^*,F}(\eta_1 : \theta_2) = F^*(\eta_1) + F(\theta_2) - \langle \eta_1, \theta_2 \rangle$  denotes the *canonical divergence* [9] in dually flat spaces written using the mixed  $\theta/\eta$ -coordinate systems.

**Theorem 1** (KL of *w*-mixtures as a Bregman divergence). The Kullback-Leibler divergence between two  $\eta$ -mixtures (or *w*-mixtures) is equivalent to a Bregman divergence defined for the convex Shannon information generator on the  $\eta$ parameters.

The information geometry of  $(\mathcal{M}, \text{KL})$  is said *dually flat* [9] because the dual Christoffel symbol coefficients  $\Gamma_{ijk}$  and  $\Gamma^*_{ijk}$  have all their coefficients equal to zero [24]. Thus geodesics (autoparallel curves) are visualized as straight Euclidean lines in either the  $\eta$ - or the  $\theta$ -affine coordinate systems.

**Corollary 1** (KL of *w*-GMMS as a Bregman divergence). The KL between Gaussian Mixture Models sharing the same components (*w*-GMM [2]) is equivalent (theoretically) to a Bregman divergence.

## 2.1. Application: Optimal KL-averaging integration

Let us consider a *computer cluster* [26] of m machines  $M_1, \ldots, M_m$  with the independently and identically sampled data-set  $\mathcal{O}$  partitioned into m pieces:  $\mathcal{O}_1, \ldots, \mathcal{O}_m$  with  $|\mathcal{O}_i| = n_i$ . Dataset  $\mathcal{O}_i$  is stored *locally* in the memory of machine  $M_i$ . Liu and Ihler [14] proposed (1) to estimate the m models locally (say, via Maximum Likelihood Estimators, MLEs,  $\hat{\eta}_i$ 's on the local samples  $\mathcal{O}_i$ ), and then (2) to merge/aggregate those local model estimates on a *central node* by performing *KL-averaging integration*. When the models all belong to the same exponential family (e.g., Gaussian models), they showed that the KL-averaging model integration yields no information loss: For exponential families with log-density  $t(x)^{\top}\theta - F(\theta)$  (with  $\theta$  the natural parameters, sufficient statistics t(x) and  $F(\theta)$  the lognormalizer), the KL-averaging integration [14] yields  $\hat{\theta}^{\text{KL}} =$  $\nabla F^{-1}\left(\frac{1}{m}\sum_{i=1}^{m}\nabla F(\hat{\theta}_i)\right)$  without information loss (with MLE  $\hat{\eta}_i = \nabla F(\hat{\theta}_i) = \frac{1}{n_i} \sum_{x \in \mathcal{O}_i} t(x)$ . Notice that it requires to manipulate explicitly both the log-normalizer  $F(\theta)$ and its inverse gradient function  $\nabla F^{-1}$ , see [14]. Interestingly, they also report experiments on GMMs [14] that are not exponential families with information loss.

However, for  $\eta$ -mixtures (mixture families), the KLaveraging integration [14, 27] is defined by the following optimization problem:

$$\hat{\eta}^{\text{KL}} = \arg\min_{\eta} \sum_{i=1}^{m} \text{KL}(m(x; \hat{\eta}_i) : m(x; \eta)), \quad (10)$$

$$= \arg \min_{\eta} \sum_{i=1}^{m} B_{F^*}(\hat{\eta}_i : \eta).$$
 (11)

Since the *right-sided Bregman centroid* [28] is always the center of mass *whatever* the chosen Bregman generator<sup>1</sup>, we end up with the *optimal integration* (best parameter) for  $\eta$ -mixtures:  $\hat{\eta}^{\text{KL}} = \frac{1}{m} \sum_{i=1}^{m} \hat{\eta}_i$  (or equivalently,  $\hat{w}^{\text{KL}} = \frac{1}{m} \sum_{i=1}^{m} \hat{w}_i$ ).

**Theorem 2** (Optimal KL-averaging integration). *The KL-averaging integration of w-mixtures can be performed optimally without information loss.* 

Note that the local model estimators of mixtures may not be consistent nor efficient. In fact, the global Maximum Likelihood (ML) optimization requires to tackle an untractable log-sum maximization for mixtures, and the exact MLE solution for these mixtures maybe transcendental [29]. (In a separate report, we study how *w*-mixtures can be inferred efficiently.)

#### 2.2. Skew Jensen-Shannon divergences of w-mixtures

Let the skew  $\alpha$ -Jensen-Shannon divergence be defined by

$$JS_{\alpha}(p:q):=(1-\alpha)KL(p:m_{\alpha})+\alpha KL(q:m_{\alpha}),$$

for  $\alpha \in [0, 1]$ , and  $m_{\alpha} = (1 - \alpha)p + \alpha q$ . Define the  $\alpha$ -Jensen divergences [30, 31] by  $J_{F^*,\alpha}(\eta_1 : \eta_2) := (1 - \alpha)F^*(\eta_1) + \alpha F^*(\eta_2) - F^*((1 - \alpha)\eta_1 + \alpha\eta_2)$ , for the Shannon information  $F^*(\eta) = -h(m(x;\eta))$ . We have in the limit cases [30, 31] for  $m_1(x) = m(x;\eta_1)$  and  $m_2(x) = m(x;\eta_2)$ :

$$\lim_{\alpha \to 1^{-}} \frac{J_{F^*,\alpha}(\eta_1 : \eta_2)}{\alpha(1-\alpha)} = B_{F^*}(\eta_1 : \eta_2) = \mathrm{KL}(m_1 : m_2)$$
$$\lim_{\alpha \to 0^{+}} \frac{J_{F^*,\alpha}(\eta_1 : \eta_2)}{\alpha(1-\alpha)} = B_{F^*}(\eta_2 : \eta_1) = \mathrm{KL}(m_2 : m_1)$$

Since the combination of w-mixtures is a w-mixture,  $m_{\alpha}(x):=(1-\alpha)m(x;\eta_1)+\alpha m(x;\eta_2)=m(x;\eta_{\alpha}=(1-\alpha)\eta_1+\alpha\eta_2)$ , plugging Shannon entropy h, we get  $J_{F^*,\alpha}(\eta_1:\eta_2)=h(m_{\alpha})-(1-\alpha)h(m_1)-\alpha h(m_2)$ . Therefore we rewrite

$$J_{F^*,\alpha}(\eta_1:\eta_2) = \int \left( (1-\alpha)m_1(x)\log\frac{m_1(x)}{m_\alpha(x)} + \alpha m_2(x)\log\frac{m_2(x)}{m_\alpha(x)} \right) \mathrm{d}\mu(x)$$

and get  $J_{F^*,\alpha}(\eta_1:\eta_2) = (1-\alpha) \operatorname{KL}(m_1:m_\alpha) + \alpha \operatorname{KL}(m_2:m_\alpha) = \operatorname{JS}_{\alpha}(m_1:m_2)$ . In particular, when  $\alpha = \frac{1}{2}$ ,

<sup>&</sup>lt;sup>1</sup>Here, it is specially interesting since  $F^*$  (the negative entropy) is not available in closed form, and we bypass its use.

 $J_{F^*,\frac{1}{2}}(\eta_1:\eta_2) = \frac{1}{2} JS(m_1:m_2)$  is the Jensen-Shannon divergence [10], and when  $\alpha \to 1$ ,  $\frac{1}{1-\alpha} J_{F^*,\alpha}(\eta_1:\eta_2) = KL(m_1:m_2)$ .

**Theorem 3.** The  $\alpha$ -Jensen-Shannon statistical divergences between  $\eta$ -mixtures amount to  $\alpha$ -Jensen divergences between their corresponding  $\eta$ -mixture parameters:  $JS_{\alpha}(m(x; \eta_1) : m(x; \eta_2)) = J_{F^*,\alpha}(\eta_1 : \eta_2).$ 

# 3. ON CLOSURES AND DIVERGENCES

## **3.1.** Divergence inequalities for *w*-mixtures

**Theorem 4** (Upper bound on *f*-divergences of *w*-mixtures). The *f*-divergence  $I_f(m(x;w) : m(x;w'))$  between any two *w*-mixtures is upper bounded by  $I_f(w : w') = \sum_{i=0}^{k-1} w_i f(\frac{w'_i}{w_i}).$ 

*Proof.* We use a generalization of the log-sum inequality for any convex function f (see [32], p. 448): For two finite positive number sequences  $A = \{a_i\}_{i=0}^{k-1}$  and B = $\{b_i\}_{i=0}^{k-1}$ , we have  $\sum_i a_i f\left(\frac{b_i}{a_i}\right) \ge af\left(\frac{b}{a}\right)$ . It follows that  $m(x;w)f\left(\frac{m(x;w')}{m(x;w)}\right) \le \sum_{i=0}^{k-1} w_i p_i(x) f\left(\frac{w'_i p_i(x)}{w_i p_i(x)}\right) =$  $\sum_{i=0}^{k-1} w_i f\left(\frac{w'_i}{w_i}\right) p_i(x)$  Carrying out integration on the support  $\mathcal{X}$ , we get  $I_f(m(x;w):m(x;w')) \le I_f(w:w')$  since  $\int_{\mathcal{X}} p_i(x) d\mu(x) = 1$ . Recall that the KL divergence is a fdivergence obtained for the generator  $f(u) = -\log u$ .

# 3.2. Closures of *w*-mixtures

The manifold  $\mathcal{M}$  of w-mixtures is parameterized by the *open* probability simplex  $\Delta_{k-1}^{\circ}$ . When topologically closing the manifold  $\mathcal{M}$ , we consider  $\overline{\Delta}_{k-1}$ . Take a *l*-face of the (d-1)-dimensional simplex  $\Delta_{k-1}^{\circ}$ . When l > 0, the sub-simplex  $\sigma \in \overline{\Delta}_{k-1}$  is a *l*-dimensional simplex, and  $\sigma^{\circ}$  parameterizes a *w*-mixture family of order l > 0. In the extreme case, we consider order-1 *w*-mixture induced by a simplex edge  $\sigma_1 \in \Delta_{k-1}^{\circ}$  with extremity component distributions p and q. Define  $m^{\epsilon}(p,q) = (1-\epsilon)p + \epsilon q = p + \epsilon(q-p) = m^{1-\epsilon}(q:p)$  for  $\epsilon \in [0,1]$ . In the limit cases, the *w*-mixtures  $m^{\epsilon}$  yields (with  $w \in \Delta_1^{\circ}$ ):  $\lim_{\epsilon \to 0} m^{\epsilon}(p,q) = \lim_{\epsilon \to 1} m^{\epsilon}(q,p) = p$  and  $\lim_{\epsilon \to 1} m^{\epsilon}(p,q) = \lim_{\epsilon \to 0} m^{\epsilon}(q,p) = q$ . Let  $I_f^{\epsilon}(p:q)$ : q:= $I_f(m^{\epsilon}(p,q):m^{\epsilon}(q,p))$ . How "far" is  $I_f^{\epsilon}(p:q)$  from its closure  $I_f(p:q)$ ?

On one hand, we have the following theorem:

**Theorem 5** (Total variation continuity). We have the following identity  $\mathrm{TV}^{\epsilon}(p,q) = |1 - 2\epsilon| \mathrm{TV}(p,q)$  (since  $m^{\epsilon}(p,q) - m^{\epsilon}(q,p) = (1 - 2\epsilon)(p-q)$ ) that yields  $\lim_{\epsilon \to 0} \mathrm{TV}^{\epsilon}(p,q) = \lim_{\epsilon \to 1} \mathrm{TV}^{\epsilon}(p,q) = \mathrm{TV}(p,q)$ .

On the other hand,  $\mathrm{KL}^{\epsilon}(p:q) := \mathrm{KL}(m^{\epsilon}(p,q):m^{\epsilon}(q,p))$ has been shown to amount to a (univariate) Bregman divergence. That is,  $\mathrm{KL}^{\epsilon}(p:q) = B_{F^*}(\epsilon:1-\epsilon)$  for 1D generator  $F^*(\eta) = \int_{\mathcal{X}} (p(x) + \eta(q(x) - p(x))) \log(p(x) + \eta(q(x) - p(x))) d\mu(x)$ . By using the fact that the Bregman divergence is the tail of a first-order Taylor expansion [9], we get using Lagrange exact remainder:  $\mathrm{KL}^{\epsilon}(p : q) = \frac{1}{2}(1 - 2\epsilon)^2(F^*)''(\eta)$ , for  $\eta \in [\epsilon, 1 - \epsilon]$  (assuming  $\epsilon \leq \frac{1}{2}$ ). However, the KL between p and q may potentially be infinite so that in general  $\forall \epsilon \neq 0$ ,  $\mathrm{KL}^{\epsilon}(p:q) \neq \mathrm{KL}(p:q)$  (Bregman divergences are always finite). Using the *joint convexity* of the KL divergence, we can show that

$$\mathrm{KL}^{\epsilon}(p:q) \le \mathrm{KL}(p:q) + \epsilon^2 J(p;q), \tag{12}$$

where J denotes the Jeffreys divergence.

Let us relate the *f*-divergence between the 1D  $\eta$ -mixture and its extremities (closure) as follows:

**Theorem 6** (*f*-divergence inequalities). We have

$$I_f^{\epsilon}(p:q) \leq (1-\epsilon)I_f(p:q) + \epsilon I_f(q:p),$$
(13)

$$I_f^{\epsilon}(p:q) \leq (1-\epsilon)f\left(\frac{\epsilon}{1-\epsilon}\right) + \epsilon f\left(\frac{1-\epsilon}{\epsilon}\right).$$
 (14)

When  $I_f$  is symmetric  $(f = f^\diamond)$ ,  $I_f^\epsilon(p:q) \le I_f(p:q)$ . That is, mixing distributions decrease symmetrized f-divergences.

*Proof.* Apply the convex-sum inequality on  $A:=\{(1 - \epsilon)p(x), \epsilon q(x)\}$  and  $B:=\{(1 - \epsilon)q(x), \epsilon p(x)\}$ , so that  $a = m^{\epsilon}(p,q)$  and  $b = m^{\epsilon}(q,p)$ . First, let  $a_0:=(1 - \epsilon)p(x)$ ,  $b_0:=(1 - \epsilon)q(x)$ , and  $a_1:=\epsilon q(x)$  and  $b_1:=\epsilon p(x)$ . We get Ineq. 13. Second, let  $a_0:=(1 - \epsilon)p(x)$ ,  $b_0:=\epsilon p(x)$ , and  $a_1:=\epsilon q(x)$  and  $b_1:=(1 - \epsilon)q(x)$ . We get Ineq. 14. Note that when  $\epsilon \to 0$ , the second right-hand-side inequality yields  $f(0) + 0f(\infty)$ , similar to  $I_f \leq f(0) + \frac{f(\infty)}{\infty}$  of [6].

Supplementary material at

https://FrankNielsen.github.io/wmixture/

### 4. REFERENCES

- G. McLachlan and D. Peel, *Finite Mixture Models*, Wiley series in probability and statistics: Applied probability and statistics. Wiley, 2004.
- [2] Olivier Schwander, Stéphane Marchand-Maillet, and Frank Nielsen, "Comix: Joint estimation and lightspeed comparison of mixture models," in *IEEE International Conference on Acoustics, Speech and Signal Processing* (ICASSP), 2016, pp. 2449–2453.
- [3] Imre Csiszár, "Eine informationstheoretische ungleichung und ihre anwendung auf den beweis der ergodizitat von markoffschen ketten," *Magyar. Tud. Akad. Mat. Kutató Int. Közl*, vol. 8, pp. 85–108, 1963.
- [4] Syed Mumtaz Ali and Samuel D Silvey, "A general class of coefficients of divergence of one distribution from another," *Journal of the Royal Statistical Society. Series B* (*Methodological*), pp. 131–142, 1966.

- [5] Frank Nielsen, "What is... an information projection," *Notices of the AMS*, vol. 65, no. 3, pp. 321–324, 2018.
- [6] F. Liese and I. Vajda, Convex Statistical Distances, Teubner, Leipzig, 1987.
- [7] Mohammadali Khosravifard, Dariush Fooladivanda, and T Aaron Gulliver, "Confliction of the convexity and metric properties in *f*-divergences," *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences*, vol. 90, no. 9, pp. 1848–1853, 2007.
- [8] Frank Nielsen, "A family of statistical symmetric divergences based on Jensen's inequality," *arxiv*:1009.4004, 2010.
- [9] Shun-ichi Amari, *Information Geometry and Its Applications*, vol. 194, Springer, 2016.
- [10] Jianhua Lin, "Divergence measures based on the Shannon entropy," *IEEE Transactions on Information theory*, vol. 37, no. 1, pp. 145–151, 1991.
- [11] Frank Nielsen and Ke Sun, "Guaranteed bounds on the Kullback-Leibler divergence of univariate mixtures," *IEEE Signal Processing Letters*, vol. 23, no. 11, pp. 1543–154, 2016.
- [12] Frank Nielsen and Ke Sun, "Combinatorial bounds on the  $\alpha$ -divergence of univariate mixture models," *IEEE ICASSP*, pp. 4476-4480, 2017.
- [13] Ian Goodfellow, Yoshua Bengio, and Aaron Courville, Deep Learning, MIT Press, 2016, http://www. deeplearningbook.org.
- [14] Qiang Liu and Alexander T Ihler, "Distributed estimation, information loss and exponential families," in Advances in Neural Information Processing Systems, 2014, pp. 1098–1106.
- [15] Ovidiu Calin and Constantin Udriste, *Geometric modeling in probability and statistics*, Springer, 2014.
- [16] Frank Nielsen and Richard Nock, "On *w*-mixtures: Finite convex combinations of prescribed component distributions," *CoRR*, vol. abs/1708.00568, 2017.
- [17] Thomas M Cover and Joy A Thomas, *Elements of information theory*, John Wiley & Sons, 2012.
- [18] Artemy Kolchinsky and Brendan D. Tracey, "Estimating mixture entropy with pairwise distances," *Entropy*, vol. 19, no. 7, 2017.
- [19] Arindam Banerjee, Srujana Merugu, Inderjit S Dhillon, and Joydeep Ghosh, "Clustering with Bregman divergences," *Journal of machine learning research*, vol. 6, no. Oct, pp. 1705–1749, 2005.

- [20] Frank Nielsen, "The dual geometry of Shannon information and its applications," https://www. youtube.com/watch?v=aGxZoKSk6CQ, 2016.
- [21] Sumio Watanabe, Keisuke Yamazaki, and Miki Aoyagi, "Kullback information of normal mixture is not an analytic function," *Technical report of IEICE (in Japanese)*, pp. 41–46, 2004.
- [22] Kamyar Moshksar and Amir K. Khandani, "Arbitrarily tight bounds on differential entropy of gaussian mixtures," *IEEE Transactions on Information Theory*, vol. 62, no. 6, pp. 3340–3354, June 2016.
- [23] Frank Nielsen, "Cramér-Rao lower bound and information geometry," In *Connected at Infinity II*, pp. 18-37, Hindustan Book Agency, 2013.
- [24] Shun-ichi Amari and Andrzej Cichocki, "Information geometry of divergence functions," *Bulletin of the Polish Academy of Sciences: Technical Sciences*, vol. 58, no. 1, pp. 183–195, 2010.
- [25] Richard Nock and Frank Nielsen, "Fitting the smallest enclosing Bregman ball," in *ECML*. Springer, 2005, pp. 649–656.
- [26] Frank Nielsen, "Introduction to HPC with MPI for Data Science," Springer, 2016.
- [27] Shun-ichi Amari, "Integration of stochastic models by minimizing α-divergence," *Neural computation*, vol. 19, no. 10, pp. 2780–2796, 2007.
- [28] Frank Nielsen and Richard Nock, "Sided and symmetrized Bregman centroids," *IEEE transactions on Information Theory*, vol. 55, no. 6, pp. 2882–2904, 2009.
- [29] Carlos Améndola, Mathias Drton, and Bernd Sturmfels, "Maximum likelihood estimates for gaussian mixtures are transcendental," in *International Conference* on Mathematical Aspects of Computer and Information Sciences. Springer, 2015, pp. 579–590.
- [30] Jun Zhang, "Divergence function, duality, and convex analysis," *Neural Computation*, vol. 16, no. 1, pp. 159– 195, 2004.
- [31] Frank Nielsen and Sylvain Boltz, "The Burbea-Rao and Bhattacharyya centroids," *IEEE Transactions on Information Theory*, vol. 57, no. 8, pp. 5455–5466, 2011.
- [32] Imre Csiszár and Paul C Shields, "Information theory and statistics: A tutorial," *Foundations and Trends* (R) *in Communications and Information Theory*, vol. 1, no. 4, pp. 417–528, 2004.