Discrepancies, dissimilarities, divergences, and distances

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This is a working document which will be frequently updated with materials concerning the discrepancy between two distributions.

This document is also available in the PDF `Distance.pdf`

There are many other acronyms used in the literature for referencing a dissimilarity; For example, the following 5 D's: Discrepancies, deviations, dissimilarities, divergences, and distances.

Contents

1 Statistical distances between densities with computationally intractable normalizers

Consider a density $p(x) = \frac{\tilde{p}(x)}{Z_p}$ where $\tilde{p}(x)$ is an unnormalized *computable* density and $Z_p = \int p(x)\mathrm{d}\mu(x)$ the *computationally intractable* normalizer (also called in statistical physics the partition function or free energy). A statistical distance $D[p_1 : p_2]$ between two densities $p_1(x) = \frac{\tilde{p}_1(x)}{Z_{p_1}}$

and $p_2(x) = \frac{\tilde{p}_2(x)}{Z_{p_2}}$ with computationally intractable normalizers Z_{p_1} and Z_{p_2} is said *projective* (or two-sided *homogeneous*) if and only if

$$\forall \lambda_1 > 0, \lambda_2 > 0, \quad D[p_1 : p_2] = D[\lambda_1 p_1 : \lambda_2 p_2].$$

In particular, letting $\lambda_1 = Z_{p_1}$ and $\lambda_2 = Z_{p_2}$, we have

$$D[p_1 : p_2] = D[\tilde{p}_1 : \tilde{p}_2].$$

Notice that the rhs. does not rely on the computationally intractable normalizers. These projective distances are useful in statistical inference based on minimum distance estimators [2] (see next Section).

Here are a few statistical projective distances:

- **γ-divergences** ($\gamma > 0$) [10, 6]:

$$D_\gamma[p : q] := \log \left(\int_{\mathbb{R}} q^{\alpha+1} \right) - \left(1 + \frac{1}{\alpha} \right) \log \left(\int_{\mathbb{R}} q^\alpha p \right) + \frac{1}{\alpha} \log \left(\int_{\mathbb{R}} p^{\alpha+1} \right), \quad \gamma \geq 0$$

When $\gamma \to 0$, we have [6] $D_\gamma[p : q] = D_{\mathrm{KL}}[p : q]$, the Kullback-Leibler divergence (KLD). For example, we can estimate the KLD between two densities of an exponential-polynomial family by Monte Carlo stochastic integration of the γ-divergence for a small value of γ [27].

The γ-divergences (projective, Bregman-type=Cross-entropy-entropy) and the density power divergence [1] (non-projective, Bregman-type divergence):

$$D_\alpha^{\mathrm{dpd}}[p : q] := \int_{\mathbb{R}} q^{\alpha+1} - \left(1 + \frac{1}{\alpha} \right) \int_{\mathbb{R}} q^\alpha p + \frac{1}{\alpha} \int_{\mathbb{R}} p^{\alpha+1}, \quad \alpha \geq 0,$$

can be encapsulated into the family of Φ-power divergences [37] (functional density power divergence class):

$$D_{\phi,\alpha}[p : q] := \phi \left(\int_{\mathbb{R}} q^{\alpha+1} \right) - \left(1 + \frac{1}{\alpha} \right) \phi \left(\int_{\mathbb{R}} q^\alpha p \right) + \frac{1}{\alpha} \phi \left(\int_{\mathbb{R}} p^{\alpha+1} \right), \quad \alpha \geq 0,$$

where $\phi(e^x)$ convex and strictly increasing, ϕ continuous and twice continuously differentiable with finite second order derivatives. We have $D_{\phi,0}[p : q] = \phi'(1) \int_{\mathbb{R}} p(x) \log \frac{p(x)}{q(x)} d\mu(x) = \phi'(1) D_{\mathrm{KL}}[p : q]$.

- **Cauchy-Schwarz divergence** [9] (CSD, projective)

$$D_{\mathrm{CS}}[p : q] = -\log \left(\frac{\int p(x) q(x) d\mu(x)}{\sqrt{\int p(x)^2 d\mu(x) \int q(x)^2 d\mu(x)}} \right) = D_{\mathrm{CS}}[\lambda_1 p : \lambda_2 q], \forall \lambda_1 > 0, \lambda_2 > 0,$$

and **Hölder divergences** [35] (HD, projective, which generalizes the CSD):

$$D_{\alpha,\gamma}^{\mathrm{Hölder}}[p : q] = -\log \left(\frac{\int_{\mathcal{X}} p(x)^{\gamma/\alpha} q(x)^{\gamma/\beta} dx}{\left(\int_{\mathcal{X}} p(x)^\gamma dx \right)^{1/\alpha} \left(\int_{\mathcal{X}} q(x)^\gamma dx \right)^{1/\beta}} \right), \quad \frac{1}{\alpha} + \frac{1}{\beta} = 1.$$

We have

$$\forall \lambda_1 > 0, \lambda_2 > 0, D_{\alpha,\gamma}^{\text{Hölder}}[\lambda_1 p : \lambda_2 q] = D_{\alpha,\gamma}^{\text{Hölder}}[p : q],$$

and

$$D_{2,2}^{\text{Hölder}}[p : q] = D_{\text{CS}}[p : q].$$

Hölder divergences between two densities p_{θ_p} and p_{θ_q} of an exponential family with cumulant function $F(\theta)$ is available in closed-form [35]:

$$D_{\alpha,\gamma}^{\text{Hölder}}[p : q] = \frac{1}{\alpha} F(\gamma \theta_p) + \frac{1}{\beta} F(\gamma \theta_q) - F\left(\frac{\gamma}{\alpha} \theta_p + \frac{\gamma}{\beta} \theta_q\right)$$

The CSD is available in closed-form between mixtures of an exponential family with a conic natural parameter [18]: This includes the case of Gaussian mixture models [11].

- **Hilbert distance** [34] (projective): Consider two probability mass functions $p = (p_1, \dots, p_d)$ and $q = (q_1, \dots, q_d)$ of the d-dimensional probability simplex. Then the Hilbert distance is

$$D^{\text{Hilbert}}[p : q] = \log \left(\frac{\max_{i \in \{1,\dots,d\}} \frac{p_i}{q_i}}{\min_{j \in \{1,\dots,d\}} \frac{p_j}{q_j}} \right).$$

We have

$$\forall \lambda_1 > 0, \lambda_2 > 0, D^{\text{Hilbert}}[\lambda_1 p : \lambda_2 q] = D^{\text{Hilbert}}[p : q].$$

The Hilbert projective simplex distance can be extended to the cone of positive-definite matrices [34] (and its subspace of correlation matrices called the elliptope) as follows:

$$D^{\text{Hilbert}}[P : Q] = \log \left(\frac{\lambda_{\max}(PQ^{-1})}{\lambda_{\min}(PQ^{-1})} \right),$$

where $\lambda_{\max}(X)$ and $\lambda_{\min}(X)$ denote the largest and smallest eigenvalue of matrix X, respectively.

2 Statistical distances between empirical distributions and densities with computationally intractable normalizers

When estimating the parameter $\hat{\theta}$ for a parametric family of distributions $\{p_\theta\}$ from i.i.d. observations $\mathcal{S} = \{x_1, \dots, x_n\}$, we can define a minimum distance estimator (MDE):

$$\hat{\theta} = \arg \min_\theta D[p_{\mathcal{S}} : p_\theta],$$

where $p_{\mathcal{S}} = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$ is the empirical distribution (normalized). Thus we need only a right-sided projective divergence to estimate models with computationally intractable normalizers. For example, the Maximum Likelihood Estimator (MLE) is a MDE wrt. the KLD:

$$\hat{\theta}_{\text{MLE}} = \arg \min_\theta D_{\text{KL}}[p_{\mathcal{S}} : p_\theta].$$

It is thus interesting to study the impact of the choice of the distance D to the properties of the corresponding estimator (e.g., γ-divergences yields provably robust estimators [6]).

- **Hyvärinen divergence** [7] (also called **Fisher divergence**):

$$D^{\text{Hyvärinen}}[p : p_\theta] := \frac{1}{2} \int \|\nabla_x \log p(x) - \nabla_x \log p_\theta(x)\|^2 \, p(x) \mathrm{d}x.$$

The Hyvarinen divergence has been extended for order-α Hyvarinen divergences [22] (for $\alpha > 0$):

$$D_\alpha^{\text{Hyvärinen}}[p : q] := \frac{1}{2} \int p(x)^\alpha \left(\nabla_x \log p(x) - \nabla_x \log q(x)\right)^2 \mathrm{d}x, \quad \alpha > 0.$$

3 The Jensen-Shannon divergence and some generalizations

3.1 Origins of the Jensen-Shannon divergence

Let $(\mathcal{X}, \mathcal{F}, \mu)$ be a measure space, and $(w_1, P_1), \ldots, (w_n, P_n)$ be n weighted probability measures dominated by a measure μ (with $w_i > 0$ and $\sum w_i = 1$). Denote by $\mathcal{P} := \{(w_1, p_1), \ldots, (w_n, p_n)\}$ the set of their weighted Radon-Nikodym densities $p_i = \frac{\mathrm{d}P_i}{\mathrm{d}\mu}$ with respect to μ.

A *statistical divergence* $D[p : q]$ is a measure of dissimilarity between two densities p and q (i.e., a 2-point distance) such that $D[p : q] \geq 0$ with equality if and only if $p(x) = q(x)$ μ-almost everywhere. A *statistical diversity index* $D(\mathcal{P})$ is a measure of variation of the weighted densities in $\mathcal{P}$ related to a measure of centrality, i.e., a n-point distance which generalizes the notion of 2-point distance when $\mathcal{P}_2(p, q) := \{(\frac{1}{2}, p_1), (\frac{1}{2}, p_2)\}$:

$$D[p : q] := D(\mathcal{P}_2(p, q)).$$

The fundamental measure of dissimilarity in information theory is the *I-divergence* (also called the *Kullback-Leibler divergence*, KLD, see Equation (2.5) page 5 of [12]):

$$D_{\text{KL}}[p : q] := \int_\mathcal{X} p(x) \log \left(\frac{p(x)}{q(x)}\right) \mathrm{d}\mu(x).$$

The KLD is asymmetric (hence the delimiter notation ":" instead of ',') but can be symmetrized by defining the Jeffreys *J-divergence* (Jeffreys divergence, denoted by I_2 in Equation (1) in 1946's paper [8]):

$$D_J[p, q] := D_{\text{KL}}[p : q] + D_{\text{KL}}[q : p] = \int_\mathcal{X} (p(x) - q(x)) \log \left(\frac{p(x)}{q(x)}\right) \mathrm{d}\mu(x).$$

Although symmetric, any positive power of Jeffreys divergence fails to satisfy the triangle inequality: That is, D_J^α is never a metric distance for any $\alpha > 0$, and furthermore D_J^α cannot be upper bounded.

In 1991, Lin proposed the asymmetric *K-divergence* (Equation (3.2) in [14]):

$$D_K[p : q] := D_{\text{KL}} \left[p : \frac{p+q}{2}\right],$$

and defined the *L-divergence* by analogy to Jeffreys's symmetrization of the KLD (Equation (3.4) in [14]):

$$D_L[p, q] = D_K[p : q] + D_K[q : p].$$

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By noticing that

$$D_L[p, q] = 2h\left[\frac{p+q}{2}\right] - (h[p] + h[q]),$$

where h denotes Shannon entropy (Equation (3.14) in [14]), Lin coined the (skewed) *Jensen-Shannon divergence* between two weighted densities $(1 - \alpha, p)$ and (α, q) for $\alpha \in (0, 1)$ as follows (Equation (4.1) in [14]):

$$D_{\text{JS},\alpha}[p, q] = h[(1 - \alpha)p + \alpha q] - (1 - \alpha)h[p] - \alpha h[q]. \tag{1}$$

Finally, Lin defined the *generalized Jensen-Shannon divergence* (Equation (5.1) in [14]) for a finite weighted set of densities:

$$D_{\text{JS}}[\mathcal{P}] = h\left[\sum_i w_i p_i\right] - \sum_i w_i h[p_i].$$

This generalized Jensen-Shannon divergence is nowadays called the *Jensen-Shannon diversity index.*

To contrast with the Jeffreys' divergence, the Jensen-Shannon divergence (JSD) $D_{\text{JS}} := D_{\text{JS},\frac{1}{2}}$ is upper bounded by $\log 2$ (does not require the densities to have the same support), and $\sqrt{D_{\text{JS}}}$ is a metric distance [4, 5]. Lin cited precursor work [42, 15] yielding definition of the Jensen-Shannon divergence: The Jensen-Shannon divergence of Eq. 1 is the so-called "increments of entropy" defined in (19) and (20) of [42].

The Jensen-Shannon diversity index was also obtained very differently by Sibson in 1969 when he defined the *information radius* [40] of order α using Rényi α-means and Rényi α-entropies [38]. In particular, the information radius IR_1 of order 1 of a weighted set $\mathcal{P}$ of densities is a diversity index obtained by solving the following variational optimization problem:

$$\text{IR}_1[\mathcal{P}] := \min_c \sum_{i=1}^n w_i D_{\text{KL}}[p_i : c]. \tag{2}$$

Sibson solved a more general optimization problem, and obtained the following expression (term K_1 in Corollary 2.3 [40]):

$$\text{IR}_1[\mathcal{P}] = h\left[\sum_i w_i p_i\right] - \sum_i w_i h[p_i] := D_{\text{JS}}[\mathcal{P}].$$

Thus Eq. 2 is a variational definition of the Jensen-Shannon divergence.

3.2   Some extensions of the Jensen-Shannon divergence

- **Skewing the JSD.**

  The K-divergence of Lin can be skewed with a scalar parameter $\alpha \in (0, 1)$ to give

  $$D_{K,\alpha}[p : q] := D_{\text{KL}}[p : (1 - \alpha)p + \alpha q]. \tag{3}$$

  Skewing parameter α was first studied in [13] (2001, see Table 2 of [13]). We proposed to unify the Jeffreys divergence with the Jensen-Shannon divergence as follows (Equation 19 in [17]):

  $$D_{K,\alpha}^J[p : q] := \frac{D_{K,\alpha}[p : q] + D_{K,\alpha}[q : p]}{2}. \tag{4}$$

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When $\alpha = \frac{1}{2}$, we have $D_{K,\frac{1}{2}}^J = D_{\mathrm{JS}}$, and when $\alpha = 1$, we get $D_{K,1}^J = \frac{1}{2}D_J$.

Notice that

$$D_{\mathrm{JS}}^{\alpha,\beta}[p;q] := (1-\beta)D_{\mathrm{KL}}[p : (1-\alpha)p + \alpha q] + \beta D_{\mathrm{KL}}[q : (1-\alpha)p + \alpha q]$$

amounts to calculate

$$h^\times[(1-\beta)p + \beta q : (1-\alpha)p + \alpha q] - ((1-\beta)h[p] + \beta h[q])$$

where

$$h^\times[p,q] := \int -p(x)\log q(x)\mathrm{d}\mu(x)$$

denotes the *cross-entropy*. By choosing $\alpha = \beta$, we have $h^\times[(1-\beta)p + \beta q : (1-\alpha)p + \alpha q] = h[(1-\alpha)p + \alpha q]$, and thus recover the skewed Jensen-Shannon divergence of Eq. 1.

In [21] (2020), we considered a positive *skewing vector* $\alpha \in [0,1]^k$ and a unit positive weight w belonging to the standard simplex Δ_k, and defined the following *vector-skewed Jensen-Shannon divergence*:

$$D_{\mathrm{JS}}^{\alpha,w}[p:q] := \sum_{i=1}^k D_{\mathrm{KL}}[(1-\alpha_i)p_+\alpha_i q : (1-\bar\alpha)p + \bar\alpha q], \tag{5}$$

$$= h[(1-\bar\alpha)p + \bar\alpha q] - \sum_{i=1}^k h[(1-\alpha_i)p_+\alpha_i q], \tag{6}$$

where $\bar\alpha = \sum_{i=1}^k w_i\alpha_i$. The divergence $D_{\mathrm{JS}}^{\alpha,w}$ generalizes the (scalar) skew Jensen-Shannon divergence when $k = 1$, and is a Ali-Silvey-Csiszár f-divergence upper bounded by $\log\frac{1}{\bar\alpha(1-\bar\alpha)}$ [21].

- **A priori mid-density**. The JSD can be interpreted as the total divergence of the densities to the *mid-density* $\bar p = \sum_{i=1}^n w_i p_i$, a statistical mixture:

$$D_{\mathrm{JS}}[\mathcal{P}] = \sum_{i=1}^n w_i D_{\mathrm{KL}}[p_i : \bar p] = h[\bar p] - \sum_{i=1}^n w_i h[p_i].$$

Unfortunately, the JSD between two Gaussian densities is not known in closed form because of the definite integral of a log-sum term (i.e., K-divergence between a density and a mixture density $\bar p$). For the special case of the Cauchy family, a closed-form formula [29] for the JSD between two Cauchy densities was obtained. Thus we may choose a *geometric mixture distribution* [19] instead of the ordinary arithmetic mixture $\bar p$. More generally, we can choose any weighted mean M_α (say, the geometric mean, or the harmonic mean, or any other power mean) and define a generalization of the K-divergence of Equation 3:

$$D_K^{M_\alpha}[p:q] := D_K[p : (pq)_{M_\alpha}], \tag{7}$$

where

$$(pq)_{M_\alpha}(x) := \frac{M_\alpha(p(x),q(x))}{Z_{M_\alpha}(p:q)}$$

is a statistical M-mixture with $Z_{M_\alpha}(p, q)$ denoting the normalizing coefficient:

$$Z_{M_\alpha}(p : q) = \int M_\alpha(p(x), q(x)) \mathrm{d}\mu(x)$$

so that $\int (pq)_{M_\alpha}(x) \mathrm{d}\mu(x) = 1$. These M-mixtures are well-defined provided the convergence of the definite integrals.

Then we define a generalization of the JSD [19] termed (M_α, N_β)-*Jensen-Shannon divergence* as follows:

$$D_{\mathrm{JS}}^{M_\alpha, N_\beta}[p : q] := N_\beta \left(D_K[p : (pq)_{M_\alpha}], D_K[q : (pq)_{M_\alpha}] \right), \tag{8}$$

where N_β is yet another weighted mean to average the two M_α-K-divergences. We have $D_{\mathrm{JS}} = D_{\mathrm{JS}}^{A,A}$ where $A(a, b) = \frac{a+b}{2}$ is the arithmetic mean. The geometric JSD yields a closed-form formula between two multivariate Gaussians, and has been used in deep learning [3]. More generally, we may consider the Jensen-Shannon symmetrization of an arbitrary distance D as

$$D_{M_\alpha, N_\beta}^{\mathrm{JS}}[p : q] := N_\beta \left(D[p : (pq)_{M_\alpha}], D[q : (pq)_{M_\alpha}] \right). \tag{9}$$

- **A posteriori mid-density**. We consider a generalization of Sibson's information radius [40]. Let $S_w(a_1, \ldots, a_n)$ denote a generic weighted mean of n positive scalars $a_1, \ldots, a_n$, with weight vector $w \in \Delta_n$. Then we define the *S-variational Jensen-Shannon diversity index* [24] as

$$D_{\mathrm{vJS}}^{S_w}(\mathcal{P}) := \min_c S_w \left(D_{\mathrm{KL}}[p_1 : c], D_{\mathrm{KL}}[p_n : c] \right). \tag{10}$$

When $S_w = A_w$ (with $A_w(a_1, \ldots, a_n) = \sum_{i=1}^n w_i a_i$ the arithmetic weighted mean), we recover the ordinary Jensen-Shannon diversity index. More generally, we define the *S-Jensen-Shannon index of an arbitrary distance D* as

$$D_{S_w}^{\mathrm{vJS}}(\mathcal{P}) := \min_c S_w \left(D[p_1 : c], \ldots, D[p_n : c] \right). \tag{11}$$

When $n = 2$, this yields a Jensen-Shannon-symmetrization of distance D.

The variational optimization defining the JSD can also be constrained to a (parametric) family of densities $\mathcal{D}$, thus defining the $(S, \mathcal{D})$-*relative Jensen-Shannon diversity index*:

$$D_{\mathrm{vJS}}^{S_w, \mathcal{D}}(\mathcal{P}) := \min_{c \in \mathcal{D}} S_w \left(D_{\mathrm{KL}}[p_1 : c], \ldots, D_{\mathrm{KL}}[p_n : c] \right). \tag{12}$$

The relative Jensen-Shannon divergences are useful for clustering applications: Let p_{θ_1} and p_{θ_2} be two densities of an exponential family $\mathcal{E}$ with cumulant function $F(\theta)$. Then the $\mathcal{E}$-relative Jensen-Shannon divergence is the Bregman information of $\mathcal{P}_2(p, q)$ for the conjugate function $F^*(\eta) = -h[p_\theta]$ (with $\eta = \nabla F(\theta)$). The $\mathcal{E}$-relative JSD amounts to a *Jensen divergence* for F^*:

$$D_{\text{vJS}}[p_{\theta_1}, p_{\theta_2}] \quad = \quad \min_{\theta} \frac{1}{2} \left\{ D_{\text{KL}}[p_{\theta_1} : p_\theta] + D_{\text{KL}}[p_{\theta_2} : p_\theta] \right\}, \tag{13}$$

$$= \quad \min_{\theta} \frac{1}{2} \left\{ B_F[\theta : \theta_1] + B_F[\theta : \theta_2] \right\}, \tag{14}$$

$$= \quad \min_{\eta} \frac{1}{2} \left\{ B_{F^*}[\eta_1 : \eta] + B_{F^*}[\eta_2 : \eta] \right\}, \tag{15}$$

$$= \quad \frac{F^*(\eta_1) + F^*(\eta_2)}{2} - F^*(\eta^*), \tag{16}$$

$$=: \quad J_{F^*}(\eta_1, \eta_2), \tag{17}$$

since $\eta^* := \frac{\eta_1 + \eta_2}{2}$ (a right-sided *Bregman centroid* [26]).

4   Statistical distances between mixtures

Pearson [36] first considered a unimodal Gaussian mixture of two components for modeling distributions crabs in 1894. Statistical mixtures [16] like the Gaussian mixture models (GMMs) are often met in information sciences, and therefore it is important to assess their dissimilarities. Let $m(x) = \sum_{i=1}^{k} w_i p_i(x)$ and $m'(x) = \sum_{i=1}^{k'} w_i' p_i'(x)$ be two finite statistical mixtures. The KLD between two GMMs m and m' is not analytic [41] because of the log-sum terms:

$$D_{\text{KL}}[m : m'] = \int m(x) \log \frac{m(x)}{m'(x)} \mathrm{d}x.$$

However, the KLD between two GMMs with the same prescribed components $p_i(x) = p_i'(x) = p_{\mu_i, \Sigma_i}(x)$ (i.e., $k = k'$, and only the normalized positive weights may differ) is provably a Bregman divergence [28] for the differential negentropy $F(\theta)$:

$$D_{\text{KL}}[m(\theta) : m(\theta')] = B_F(\theta, \theta'),$$

where $m(\theta) = \sum_{i=1}^{k-1} w_i p_i(x) + (1 - \sum_{i=1}^{k-1} w_i) p_k(x)$ and $F(\theta) = \int m(\theta) \log m(\theta) \mathrm{d}x$. The family $\{m_\theta \quad \theta \in \Delta_{k-1}^\circ\}$ is called a mixture family in information geometry, where Δ_{k-1}° denotes the $(k-1)$-dimensional open standard simplex. However, $F(\theta)$ is usually not available in closed-form because of the log-sum integral. In some special cases like the mixture of two prescribed Cauchy distributions, we get a closed-form formula for the KLD, JSD, etc. [30, 25]. Thus when dealing with mixtures (like GMMs), we either need efficient approximating (§4.1), bounding (§4.2) KLD techniques, or new distances (§4.3) that yields closed-form formula between mixture densities.

4.1   Approximating and/or fast statistical distances between mixtures

- The Jeffreys divergence (JD) $D_J[m, m'] = D_{\text{KL}}[m : m'] + D_{\text{KL}}[m' : m]$ between two (Gaussian) MMs is not available in closed-form, and can be estimated using Monte Carlo integration as

$$\hat{D}_J^{\mathcal{S}_s}[m, m'] := \frac{1}{s} \sum_{i=1}^{s} 2 \frac{(m(x_i) - m'(x_i))}{m(x_i) + m'(x_i)} \log \left(\frac{m(x_i)}{m'(x_i)} \right),$$

where $\mathcal{S}_s = \{x_1, \ldots, x_s\}$ are s IID samples from the mid mixture $m_{12}(x) := \frac{1}{2}(m(x) + m'(x))$ (with $\lim_{s \to \infty} \hat{D}_J^{\mathcal{S}_s}[m, m'] = D_J[m, m']$). In [23], the mixtures m and m' are converted into

densities of an exponential-polynomial family. The JD between densities p_θ and $p_{\theta'}$ of an exponential family with cumulant function F is available in closed-form:

$$D_J[p_\theta, p_{\theta'}] = (\theta' - \theta) \cdot (\eta' - \eta),$$

with $\eta = \nabla F(\theta)$ and $\theta = \nabla F^*(\eta)$, where F^* denotes the convex conjugate. Any smooth density r (includes a mixture $r = m$) is converted into close densities $p_{\theta_r^{\mathrm{MLE}}}$ and $p^{\eta_r^{\mathrm{SME}}}$ of a exponential-polynomial family using extensions of the Maximum Likelihood Estimator (MLE) and Score Matching Estimator (SME). Then JD between mixtures is approximated as follows

$$D_J[m, m'] \simeq (\theta'^{\mathrm{SME}} - \theta^{\mathrm{SME}}) \cdot (\eta'^{\mathrm{MLE}} - \eta^{\mathrm{MLE}}).$$

- Given a finite set of mixtures $\{m_i(x)\}$ sharing the same components (e.g., points on a mixture family manifold), we precompute the KLD between pairwise components to obtain fast approximation of the KLD $D_{\mathrm{KL}}[m_i : m_j]$ between any two mixtures m_i and m_j, see [39].

4.2 Bounding statistical distances between mixtures

- **Log-Sum-Exp bounds**: In [31, 32], we lower and upper bound the cross-entropy between mixtures using the fact that the log-sum term $\log m(x)$ and be interpreted as a LSE function. We then compute lower envelopes and upper envelopes of density functions using technique of computational geometry to report deterministic lower and upper bounds on the KLD and α-divergences. These bounds are said combinatorial because we decompose the support into elementary intervals. Bounds between the Total Variation Distance (TVD) between univariate mixtures are reported in [33].

4.3 Newly designed statistical distances yielding closed-form formula for mixtures

- **Statistical Minkowski distances** [20]: Consider the Lebesgue space

$$L_\alpha(\mu) := \left\{ f \in \mathbb{F} \ : \ \int_{\mathcal{X}} |f(x)|^\alpha \mathrm{d}\mu(x) < \infty \right\}$$

for $\alpha \geq 1$, where $\mathbb{F}$ denotes the set of all real-valued measurable functions defined on the support $\mathcal{X}$. Minkowski's inequality writes as $\|p + q\|_\alpha \leq \|p\|_\alpha + \|q\|_\alpha$ for $\alpha \in [1, \infty)$. The statistical Minkowski difference distance between $p, q \in L_\alpha(\mu)$ is defined as

$$D_\alpha^{\mathrm{Minkowski}}[p, q] := \|p\|_\alpha + \|q\|_\alpha - \|p + q\|_\alpha \geq 0. \tag{18}$$

The statistical Minkowski log-ratio distance is defined by:

$$L_\alpha^{\mathrm{Minkowski}}[p, q] := -\log \frac{\|p + q\|_\alpha}{\|p\|_\alpha + \|q\|_\alpha} \geq 0. \tag{19}$$

These statistical Minkowski distances are symmetric, and $L_\alpha[p, q]$ is scale-invariant. For even integers $\alpha \geq 2$, $D_\alpha^{\mathrm{Minkowski}}[m : m']$ is available in closed-form.

- We show that the Cauchy-Schwarz divergence (CSD), the quadratic Jensen-Rényi divergence (JRD), and the total square Distance (TSD) between two GMMs, and more generally two mixtures of exponential families, can be obtained in closed-form in [18].

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