Corrigendum and addendum to:

"Sided and symmetrized Bregman centroids"

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Abstract

We correct and extend the results presented in [12].

1 Dissimilarities, dual centroids, and dual information radii

Let D(P:Q) denote the dissimilarity between two points P and Q of a space \mathbb{G} such that $D(P:Q) \geq 0$ with equality if and only if P=Q. By analogy with the notion of Fréchet barycenters in metric spaces [7], we define the D-barycenters or D-centroid $C_D(\mathcal{P})$ of a weighted point set $\mathcal{P} = \{P_1, \ldots, P_n\}$ with respect to D as

$$C_D(\mathcal{P}) := \arg\min_{X \in \mathbb{G}} \sum_{i=1}^n w_i D(P_i : X), \tag{1}$$

where $w_i > 0$ and $\sum_{i=1}^n w_i = 1$ (i.e., w belongs to the (n-1)-dimensional standard simplex Δ_{n-1}). The centroids are special cases of barycenters obtained for the uniform weighting $w_i = \frac{1}{n}$. Notice that $C_D(\mathcal{P})$ is generally a subset of points of \mathbb{G} , and may not necessarily exist nor be unique. For example, the centroid of two antipodal points on the unit Euclidean sphere is a great circle. In Riemannian geometry, other notions of barycenters have been defined [1]: Karcher local barycenters, exponential barycenters, etc.

Since D may be asymmetric $D(P:Q) \neq D(Q:P)$ (oriented dissimilarity, hence the delimiter notation ":"), we define the dual dissimilarity $D^*(P:Q) := D(Q:P)$, and the dual D-barycenter or left-sided D-barycenter:

$$C_D^*(\mathcal{P}) := \arg\min_{X \in \mathbb{G}} \sum_{i=1}^n w_i D(X : P_i), \tag{2}$$

$$= \arg\min_{X \in \mathbb{G}} \sum_{i=1}^{n} w_i D^*(P_i : X), \tag{3}$$

$$= C_{D^*}(\mathcal{P}). \tag{4}$$

Notice that the dual of the dual dissimilarity is the original (primal) dissimilarity: $D^{**} = D$ (involutive property of duality).

Let $C_D(\mathcal{P})$ be the primal *D*-barycenter (right-sided *D*-barycenter) and $C_D^*(\mathcal{P})$ be the dual *D*-barycenter (left-sided *D*-barycenter). The dual *D*-barycenter with respect to *D* amounts to the (primal) D^* -barycenter for the dual dissimilarity D^* . When *D* is the squared Euclidean distance, both primal and dual centroids coincide to the center of mass.

The (primal) information radius [13] is defined by

$$I_D(\mathcal{P}) := \sum_{i=1}^n w_i D(P_i : C), \quad C \in C_D(\mathcal{P}), \tag{5}$$

while the dual information radius is defined by

$$I_D^*(\mathcal{P}) := \sum_{i=1}^n w_i D(C:P_i), \quad C \in C_D^*(\mathcal{P}).$$
 (6)

In general, we have $I_D^*(\mathcal{P}) \neq I_{D^*}(\mathcal{P})$ because the left-sided and right-sided centroids may not coincide. (They coincide by default when the dissimilarity is symmetric.) The information radius for the squared Euclidean distance represents the variance of the point set.

2 Bregman centroids and Bregman information

Let $F(\theta)$ be a strictly convex and differentiable real-valued function for $\theta \in \Theta$, where $\Theta \subset \mathbb{R}^D$ denotes the open parameter space. We define the *Bregman divergence* [6] with respect to generator F as:

$$B_F(\theta:\theta') := F(\theta) - F(\theta') - (\theta - \theta')^\top \nabla F(\theta'), \tag{7}$$

for $\theta, \theta' \in \Theta$.

Bregman divergences are canonical smooth dissimilarities of dually flat space in information geometry [2, 8]: That is, we can build a canonical Bregman divergence from any dually flat space, and a Bregman divergence yields a dually flat space [3]. In a dually flat space (or Bregman manifold [9]), the dissimilarity between two points P and Q is expressed by

$$D_F(P:Q) := B_F(\theta(P):\theta(Q)), \tag{8}$$

where $\theta(\cdot)$ is a global (affine) coordinate system used to define the potential function $F(\theta)$, see [2, 8]. The dual divergence amounts to a dual Bregman divergence B_{F^*} as follows:

$$D_F^*(P:Q) = D(Q:P) = B_F(\theta(Q):\theta(P)) = B_{F^*}(\eta(P):\eta(Q)) = D_{F^*}(P:Q), \tag{9}$$

where F^* is the Legendre-Fenchel convex conjugate [9], and $\eta(\theta) = \nabla F(\theta)$ the dual affine global coordinate system [2, 8]. We can introduce the *Legendre-Fenchel divergence* from the dual potential functions F and F^* as follows:

$$A_F(\theta : \eta') := F(\theta) + F^*(\eta') - \theta^\top \eta' \ge 0$$
 (10)

with equality if and only if $\eta' = \nabla F(\theta)$, or equivalently $\theta = \nabla F^*(\eta')$.

Thus, in a Bregman manifold, we have the dual divergences that can be expressed using the dual coordinate systems either by Bregman divergences or by Legendre-Fenchel divergences as follows:

$$D_F(P:Q) = B_F(\theta(P):\theta(Q)) = A_F(\theta(P):\eta(Q)) =: D_F^*(Q:P), \tag{11}$$

$$D_F^*(P:Q) = B_{F^*}(\eta(P):\eta(Q)) = A_{F^*}(\eta(P):\theta(Q)) =: D_F(Q:P).$$
(12)

Theorem 1 Theorem 3.1 and Theorem 3.2 of [12] Let $\theta_i = \theta(P_i)$ and $\eta_i = \eta(P_i)$ be the primal and dual coordinates of point P_i for $P_i \in \mathcal{P} = \{P_1, \dots, P_n\}$. Let $\bar{\theta} = \sum_{i=1}^n w_i \theta_i$ and $\bar{\eta} = \sum_{i=1}^n w_i \eta_i$ denote the center of mass in the primal θ -coordinate system and dual η -coordinate system, respectively. The right-sided Bregman centroid $C_{D_F}(\mathcal{P})$ and the left-sided Bregman centroid $C_{D_F}^*(\mathcal{P})$ exist and are both unique, and we have $\theta(C_{D_F}(\mathcal{P})) = \bar{\theta}$ and $\eta(C_{D_F}^*(\mathcal{P})) = \bar{\eta}$.

Proof: We have

$$C_{D_F}(\mathcal{P}) = \arg\min_{X \in \mathbb{G}} \sum_{i=1}^{n} w_i D_F(P_i : X), \tag{13}$$

$$= \arg\min_{X \in \mathbb{G}} \sum_{i=1}^{n} w_i A_F(\theta_i : \eta(X)), \tag{14}$$

$$= \arg\min_{X \in \mathbb{G}} E(X) = (\sum_{i=1}^{n} w_i F(\theta_i)) + F^*(\eta(X)) - \bar{\theta}^{\top} \eta(X).$$
 (15)

A point $X \in C_{D_F}(\mathcal{P})$ if and only if $\nabla_{\eta(X)} = 0$: $\nabla_{\eta} F^*(\eta(X)) = \bar{\theta}$. That is:

$$\eta(X) = (\nabla F^*)^{-1}(\bar{\theta}) = (\nabla F^*)^{-1}(\sum_{i=1}^n w_i \nabla F^*(\eta_i)).$$
(16)

The right-sided centroid is unique since the Hessian $\nabla^2_{\eta(X)}E(X)$ is $\nabla^2 F^*(\eta(X))$, and $\nabla^2 F^*$ is positive-definite $(F^*$ is a strictly convex conjugate). The right-sided centroid is expressed in the θ -coordinate system as $\theta(C_{D_F}(\mathcal{P})) = (\nabla F^*)(\eta(C_{D_F}(\mathcal{P}))) = (\nabla F^*)((\nabla F^*)^{-1}(\bar{\theta})) = \bar{\theta}$.

The proof for the left-sided centroid is similar, and we have $\theta(C_{D_F}^*(\mathcal{P})) = (\nabla F)^{-1}(\bar{\eta}) = (\nabla F)^{-1}(\sum_{i=1}^n w_i \nabla F(\theta_i))$ so that $C_{D_F}^*(\mathcal{P})$ expressed in the η -coordinate system is $\bar{\eta}$. \square To summarize, we have:

In term of Bregman divergences, the right-sided Bregman centroid is the center of mass [4]. The Bregman information radius is called *Bregman information* in [4]. It was shown in [11, 5] that the only *symmetrized Bregman divergences* are squared Mahalanobis divergences. Thus the left-sided centroid and right-sided Bregman centroids coincide only for squared Mahalanobis divergences, and the dual Bregman information radii differ in the general case.

Corollary 1 Correct Corollary 3.3 of [12] The information radius $I_{D_F}(\mathcal{P}) = J_F(\theta_1, \dots, \theta_n; w_1, \dots, w_n)$ where J_F denotes the Jensen diversity index [10]:

$$J_F(\theta_1, \dots, \theta_n; w_1, \dots, w_n) := \sum_{i=1}^n w_i F(\theta_i) - F\left(\sum_{i=1}^n w_i \theta_i\right) \ge 0.$$
 (17)

The dual information radius $I_{D_F}^*(\mathcal{P}) = I_{D_F}^*(\mathcal{P}) = J_{F^*}(\eta_1, \dots, \eta_n; w_1, \dots, w_n)$ differs from the primal information radius except when D_F is a squared Mahalanobis divergence.

Thus we have:

$$I_{D_F}(\mathcal{P}) = \sum_{i=1}^n w_i F(\theta_i) - F\left(\sum_{i=1}^n w_i \theta_i\right), \tag{18}$$

$$I_{D_F^*}(\mathcal{P}) = \sum_{i=1}^n w_i F^*(\eta_i) - F^* \left(\sum_{i=1}^n w_i \eta_i\right).$$
 (19)

Example 1 When $F(\theta) = \frac{1}{2}\theta^{\top}Q\theta$ for a positive-definite matrix $Q \succ 0$, we have the convex conjugate $F^*(\eta) = \frac{1}{2}\eta^{\top}Q^{-1}\eta$. We have $\theta_i = Q^{-1}\eta_i$ and $\theta_i = Q\theta_i$. It follows that $\bar{\theta} = \sum_{i=1}^n w_i\theta_i = Q^{-1}\bar{\eta}$ and $\bar{\eta} = \sum_{i=1}^n w_i\eta_i = Q\bar{\theta}$. Thus we check that the information radii coincide when dealing with squared Mahalanobis Bregman divergences:

$$I_{D_F}(\mathcal{P}) = \sum_{i=1}^n w_i \frac{1}{2} \theta_i^\top Q \theta_i - \frac{1}{2} \bar{\theta}^\top Q \bar{\theta}, \tag{20}$$

$$= \sum_{i=1}^{n} w_i \frac{1}{2} (Q^{-1} \eta_i)^{\top} Q(Q^{-1} \eta_i) - \frac{1}{2} (Q^{-1} \bar{\eta})^{\top} Q(Q^{-1} \bar{\eta}), \tag{21}$$

$$= \sum_{i=1}^{n} w_i \eta_i^{\top} Q^{-1} \eta_i - \frac{1}{2} \bar{\eta} Q^{-1} \bar{\eta}, \tag{22}$$

$$= I_{D_{F^*}}(\mathcal{P}) = I_{D_F^*}(\mathcal{P}). \tag{23}$$

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