Generalizing Fidelity and Bures-Wasserstein distance based on the Riemannian Geometry of the Bures-Wasserstein Manifold

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1. Introduciton

We propose a generalization of fidelity and Bures distance motivated by the Riemannian geometry of the Bures-Wasserstein manifold. This *generalized fidelity* recovers various quantum fidelities and exhibits interesting geometric properties. We will denote the open set of all $d \times d$ positive definite matrices by $\mathbb{P}_d$. Generalized fidelity and generalized Bures distance have well-motivated Riemannian geometric interpretation, which sheds new light on the geometry of various known quantum fidelities.

The Bures-Wasserstein distance is well studied in classical machine due to its relation to Wasserstein distance between probability measures. Our results are thus placed at the intersection of quantum information and classical machine learning, thus making it well-suited for QTML. Because how the generalized Bures distance varies as the base (defined below) changes, we believe these results can have applications such as metric learning.

2. Definitions: Generalized Fidelity

Let $P, Q, R \in \mathbb{P}_d$. The *generalized fidelity* and the squared generalized Bures distance *between P and Q at R* are respectively defined as

$$\mathrm{F}_R(P,Q) := \mathrm{Tr}\left[\sqrt{R^{\frac{1}{2}}PR^{\frac{1}{2}}}R^{-1}\sqrt{R^{\frac{1}{2}}QR^{\frac{1}{2}}}\right] \quad \text{and} \quad \mathrm{B}_R(P,Q) := \mathrm{Tr}[P+Q] - 2\Re\,\mathrm{F}_R(P,Q). \tag{1}$$

Here and hereafter, R is called the *base* of the generalized fidelity (and generalized Bures distance). The generalized Bures distance has the geometric interpretation of being the distance between P and Q if we *linearized the manifold at R*. In particular, linearzing R at specific points lead to recovery of various known fidelities.

3. Recovering named fidelities from Generalized fidelity

For particular choices of the base R, we can recover Uhlmann, Holevo, and Matsumoto fidelity as shown below.

$$R \in \{P,Q\} \implies \mathrm{F}_R(P,Q) = \mathrm{F}_\mathrm{U}(P,Q) := \mathrm{Tr}[\sqrt{P^{1/2}QP^{1/2}}], \tag{2}$$

$$R = \mathbb{I} \implies \mathrm{F}_R(P,Q) = \mathrm{F}_\mathrm{H}(P,Q) := \mathrm{Tr}[P^{1/2}Q^{1/2}], \quad \text{and} \tag{3}$$

$$R \in \{P^{-1},Q^{-1}\} \implies \mathrm{F}_R(P,Q) = \mathrm{F}_\mathrm{M}(P,Q) := \mathrm{Tr}[P\#Q]. \tag{4}$$

We note that these are not the only bases at which these fidelities are recovered by generalized fidelity. Other scenarios are discussed in next section.

4. Geodesic properties of the generalized fidelity

Fix P and Q and allow the base R to vary. Then, as R traverses the manifold of positive definite matrices along certain paths, interesting invariance and covariance properties are exhibited. We look at paths related to 3 Riemannian metrics: The Euclidean (or *flat*) metric, the Bures-Wasserstein metric, and the Affine-invariant metric. These metrics define geodesics on the manifold of positive definite matrices. The geodesic (between points A and B in $\mathbb{P}_d$) is denoted as $\gamma_{AB}^{\mathrm{Metric}} : [0,1] \to \mathbb{P}_d$ where 'Metric' can be 'Euc', 'BW', or 'AI' to denote the three metrics mentioned above. The convex combination of the endpoints gives the Euclidean geodesic: $\gamma_{PQ}^{\mathrm{Euc}}(t) := (1-t)P + tQ$. The other two geodesics are

$$\gamma_{PQ}^{\mathrm{BW}}(t) := [(1-t)\mathbb{I} + tP^{-1}\#Q]P[(1-t)\mathbb{I} + tP^{-1}\#Q] \quad \text{and} \quad \gamma_{PQ}^{\mathrm{AI}}(t) := P^{1/2}(P^{-1/2}QP^{-1/2})^t P^{1/2}. \tag{5}$$

We show that, for any $t \in [0,1]$,

$$R = \gamma_{PQ}^{\mathrm{BW}}(t) \quad \text{or} \quad R = (\gamma_{P^{-1}Q^{-1}}^{\mathrm{BW}}(t))^{-1} \implies \mathrm{F}_R(P,Q) = \mathrm{F}_\mathrm{U}(P,Q), \tag{6}$$

$$R = \gamma_{P^{-1}Q^{-1}}^{\mathrm{AI}}(t) \quad \text{or} \quad R = \gamma_{P^{-1}Q^{-1}}^{\mathrm{Euc}}(t) \quad \text{or} \quad R = (\gamma_{PQ}^{\mathrm{Euc}}(t))^{-1} \implies \mathrm{F}_R(P,Q) = \mathrm{F}_\mathrm{M}(P,Q). \tag{7}$$

Consider the geodesic $\gamma^{\mathrm{AI}}_{PP^{-1}}(t) = P^{1-2t}$. As the base $R \equiv R_t = P^{1-2t}$ moves along this path, it takes the form

$$\mathrm{F}_{R_t}(P,Q) = \mathrm{Tr}\left[P^{\frac{t}{2}}\sqrt{P^{\frac{1}{2}-t}QP^{\frac{1}{2}-t}}P^{\frac{t}{2}}\right]. \tag{8}$$

For $t = 0, \frac{1}{2}$, and 1, we recover Uhlmann, Holevo, and Matsumoto fidelity. Moroever, we numerically observe a monotonic dependence on t: for $t, t' \in [0,1]$ such that $t \geq t'$ we observe $\mathrm{F}_{R_t}(P,Q) \leq \mathrm{F}_{R_{t'}}(P,Q)$. We also prove existence of pairs of paths where the generalized fidelity changes in a *covariant fashion*. In particular, if for any $t \in [0,1]$, $R = \gamma^{\mathrm{BW}}_{PQ^{-1}}(t)$ and $R' = \gamma^{\mathrm{BW}}_{QP^{-1}}(t)$,

$$\mathrm{F}_R(P,Q) = \mathrm{F}_{R'}(P,Q). \tag{9}$$

5. Other results

Other results we study include joint convexity of Bures distance and squared Bures distance along generalized geodesic, a block-matrix characterization of generalized fidelity and squared generalized Bures distance, and Uhlmann-like theorem for generalized fidelity, and relation between multivariate generalized fidelity and Bures-Wasserstein barycenters. Finally we define an analogous generaliztion to Renyi divergence which recovers various divergences like Petz-, Sandwich-, Reverse sandwich-, and geometric Rényi relative entropies.