On the Riemannian metric of α-entropies of density matrices[1]

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Recently several authors have studied Riemannian metrics on density matrices which represent the (mixed) states of a quantum mechanical system. Uhlmann ([18, 19]) was led by the idea of the extension of the Berry phase to mixed states, Balian et al. ([1]) advocated an information-geometric approach to non-equilibrium statistical mechanics, Braunstein and Caves ([2]) used statistical distinguishability to define a metric, parameter estimation, and in particular, generalization of the Cramér-Rao inequality in the quantum setting were considered by Yuen and Lax ([21]), Nagaoka ([11]), Petz and Toth ([16]), extension of the metrics to the boundary was investigated by Sudár ([17]) and Dittmann ([4]).

To avoid boundary problems, the manifold $\mathcal{M}_n$ of invertible finite density matrices is considered here and the tangent space is identified with the space of all selfadjoint traceless matrices. A Riemannian metric is an inner product $K_D(\,\cdot\,,\,\cdot\,)$ on the tangent space $T_D(\mathcal{M}_n)$ which depends smoothly on the footpoint $D \in \mathcal{M}_n$. In the literature two metrics have appeared often. The Kubo-Mori inner product

$$K_D^{\mathrm{KM}}(A,B) = \int_0^\infty \mathrm{Tr}\, A(D+s)^{-1}B(D+s)^{-1}\, ds \tag{1}$$

and the metric of the symmetric logarithmic derivative

$$K_D^{\mathrm{SL}}(A,B) = \mathrm{Tr}\,(GB), \tag{2}$$

where G is determined by the equation $DG + GD = 2A$.

If a distance between density matrices expresses statistical distinguishability then this distance must decrease under coarse-graining which is a completely positive mapping preserving the trace and hence sends density matrix into density matrix. We call a Riemannian metric monotone if the differential of any coarse-graining is a contraction, that is

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$$K_{\mathbf{T}(D)}\big(\mathbf{T}(A), \mathbf{T}(A)\big) \le K_D(A, A)\,, \tag{3}$$

for every coarse-graining $\mathbf{T}$ and tangent vector A. It was proved in [13] that the Kubo-Mori metric is monotone. A characterization of all monotone metrics was obtained afterwards in [14] (see also [15]). A monotone metric is covariant under unitary conjugation, hence it suffices to know $K_D(A, A)$ in the case when the density D is diagonal.

Theorem 1. [14] Let $D = \mathbf{Diag}(p_1, p_2, \ldots, p_n) \in \mathcal{M}_n$ and $A = (A_{ij}) \in T_D(\mathcal{M}_n)$ then

$$K_D(A, A) = C \sum_{k=1}^{n} p_k^{-1} A_{kk}^2 + 2 \sum_{j<k} c(p_j, p_k) |A_{jk}|^2 \tag{4}$$

determines a monotone metric if and only if C is an arbitrary constant and the function $c(\lambda, \mu)$ is expressed as

$$c(\lambda, \mu) = \frac{1}{y f(x/y)} \tag{5}$$

by means of an operator monotone function $f : \mathbb{R}^+ \to \mathbb{R}$ satisfying the condition

$$f(t) = t f(t^{-1})\,. \tag{6}$$

Some examples of functions f satisfying the hypothesis of Theorem 1 are the following.

$$\frac{x-1}{\log x}, \quad \frac{2x^{\alpha+1/2}}{1+x^{2\alpha}}, \quad \frac{x-1}{\log x}\,\frac{2\sqrt{x}}{1+x}, \quad \left(\frac{x-1}{\log x}\right)^2 \frac{2}{1+x}, \quad \frac{1+x}{2} \tag{7}$$

where $0 \le \alpha \le 1/2$. This list was expected implicitly in [10] and the first function yields the metric K^{KM}, the last gives K^{SL}. Another remark concerns the case when D and A commute. Then (4) becomes

$$K_D(A, A) = C \operatorname{Tr} D^{-1} A^2 \tag{8}$$

and there is no ambiguity up to the normalization constant. This feature reminds Chentsov's uniqueness result from probability theory ([3]) which corresponds to commutativity in the density matrix setting. Theorem 1 and the theory of operator monotone functions give that the metric K^{SL} of symmetric logarithmic derivative is the smallest possible and this is the metric studied in [2, 4, 11, 18, 19].

The Kubo-Mori inner product has been used in quantum statistical mechanics since the late 1950's, however, it appeared as a possible Riemmanian metric in the work [8] in connection with the quantum relative entropy. For the densities D_1 and D_2, the relative entropy is

$$S(D_1, D_2) = \operatorname{Tr} D_1 (\log D_1 - \log D_2) \tag{9}$$

(see [12] for the background). Ingarden et al. ([8]) observed that

$$\frac{\partial^2}{\partial t \partial u} S(D+tA, D+uB)\Big|_{t=u=0} = K_D^{\mathrm{KM}}(A,B). \tag{10}$$

This approach was extended by Hasegawa ([5]). He started with the α-divergence

$$S_\alpha(D_1, D_2) = \frac{4}{1-\alpha^2} \mathrm{Tr}\, (I - D_2^{\frac{1+\alpha}{2}} D_1^{-\frac{1+\alpha}{2}}) D_1 \quad (\alpha \neq \pm 1) \tag{11}$$

and took its Hessian

$$\frac{\partial^2}{\partial t \partial u} S_\alpha(D+tA, D+uB)\Big|_{t=u=0} = K_D^\alpha(A,B) \tag{12}$$

to get a family of metrics. (Note that the limit $\alpha \to -1$ in (11) yields relative entropy (9) and (12) reduces to K_D^{KM} in that limit.) If D, A and B commute then $K_D^\alpha(A,B) = \mathrm{Tr}\, D^{-1}AB$ in accordance with (8). To perform the partial differentiations in (12) we may benefit from the formula

$$\frac{\partial}{\partial t}\Big|_{t=0} f(X + tY + \mathrm{i}t[X,Z]) = Yf'(X) + \mathrm{i}[f(X), Z], \tag{13}$$

where f is assumed to be a smooth function, X, Y and Z are selfadjoint matrices and $[X,Y]=0$. In particular, we get

$$K_D^\alpha(\mathrm{i}[D,X], \mathrm{i}[D,X]) = \frac{2}{1-\alpha^2} \mathrm{Tr}\, \left([D^{\frac{1-\alpha}{2}}, X][D^{\frac{1+\alpha}{2}}, X]\right). \tag{14}$$

It is worthwile to point out the similarity to the skew information proposed by Wigner, Yanase and Dyson (apart from a constant factor), see [20] or p. 49 in [12].

Theorem 2. The Riemannian metric K^α is monotone for $-1 \le \alpha \le 1$.

Proof. $\alpha = \pm 1$ is the case of the Kubo-Mori metric which is known to be monotone, so let $|\alpha| < 1$.

First we calculate the function c of two variables and the function f of one variable from Theorem 1 and corresponding to the metric K^α. We find

$$c(\lambda, \mu) = \frac{4}{1-\alpha^2} \frac{\left(\lambda^{\frac{1+\alpha}{2}} - \mu^{\frac{1+\alpha}{2}}\right)\left(\lambda^{\frac{1-\alpha}{2}} - \mu^{\frac{1-\alpha}{2}}\right)}{(\lambda-\mu)^2}$$

and using the notation $\beta = (1-\alpha)/2$ we have

$$f_\alpha(x) = \beta(1-\beta) \frac{(x-1)^2}{(x^\beta - 1)(x^{1-\beta} - 1)}. \tag{15}$$

It suffices to prove that this function is operator monotone. In fact, we are going to show that $1/f_\alpha(x)$ is operator monotone decreasing for $0 < \beta < 1$.

We benefit from the following two integral formulas

$$\frac{x^\beta - 1}{x-1} = \beta \int_0^1 \left(x + s(1-x)\right)^{\beta-1} ds, \qquad z^\beta = \frac{\sin \pi\beta}{\pi} \int_0^\infty \frac{\lambda^{\beta-1} z}{\lambda + z}\, d\lambda.$$

(The first one is elementary and the second one is often used to express the fractional powers of a positive operator.) By combination of the two formulas we obtain

$$\frac{1}{\beta(1-\beta)}\,\frac{(x^{\beta}-1)(x^{(1-\beta)}-1)}{(x-1)^2} =$$
$$\frac{\sin\pi\beta}{\pi}\int_0^\infty d\lambda\,\lambda^{\beta-1}\int_0^1 ds\int_0^1 dt\,\frac{1}{x\big(\lambda(1-t)+(1-s)\big)+(\lambda t+s)}\,.$$

Here the integrand is operator monotone decreasing for all possible values of $0 \le t, s \le 1$ and $\lambda > 0$, because the inverse is so. Consequently, $1/f_\alpha(z)$ is operator monotone decreasing and $f_\alpha(z)$ is operator monotone. □

In terms of the skew information the theorem above means the following. Let T be a stochastic mapping, D be a density, and K be selfadjoint. If $T([D,K]) = [T(D),H]$ for some selfadjoint H, then

$$\mathrm{Tr}\,\left([T(D)^{\frac{1-\alpha}{2}},H][T(D)^{\frac{1+\alpha}{2}},H]\right) \le \mathrm{Tr}\,\left([D^{\frac{1-\alpha}{2}},K][D^{\frac{1+\alpha}{2}},K]\right)$$

for every $-1 < \alpha < 1$. Since monotonicity of an entropy quantity is usually stronger than convexity, our result extends the Lieb convexity theorem (equivalent to the concavity of the skew information, see [9]).

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