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NEW QUANTUM DIVERGENCES GENERATED BY MONOTONICITY INEQUALITY

TRUNG HOA DINH, ANH VU LE, HIROYUKI OSAKA AND NGOC YEN PHAN*

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Abstract. In this paper, we introduce a new class of quantum divergences generated by monotonicity inequality. We also consider some related inverse problems for matrix means. As a consequence, we obtain some new characterizations of the trace property via monotonicity inequality.

1. Introduction

A continuous function f is said to be *operator monotone* on $\mathscr{I} \subset \mathbb{R}$ if for any Hermitian matrices A and B with spectra in $\mathscr{I}$,

$$A \leqslant B \quad \Longrightarrow \quad f(A) \leqslant f(B).$$

Operator monotone functions were introduced by Loewner in 1930 [14]. In 1980, Kubo and Ando [13] introduced the theory of operator means on the set of $B(H)^+ \times B(H)^+$, where $B(H)^+$ is the set of positive invertible operators in a Hilbert space H. The main result in their paper is the one-to-one correspondence between operator means σ and operator monotone functions f_σ on $(0,\infty)$ defined by

$$A\sigma B = A^{1/2} f_\sigma (A^{-1/2}BA^{-1/2})A^{1/2}. \tag{1}$$

For $f(x) = (1+x)/2, g(x) = \sqrt{x}, h(x) = 2x/(1+x)$, we have well-known arithmetic, geometric and harmonic means, respectively. Notice that the geometric mean $A\#B = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$ was firstly defined by Puzs and Woronowicz [17] in 1975 as a unique solution of the algebraic Riccati equation $XA^{-1}X = B$.

Let f and g be operator monotone functions on $(0,\infty)$ such that $f(x) \leqslant g(x)$ for $x > 0$. According to (1) there are corresponding operator means σ_f and σ_g such that for any positive definite matrices A and B, $A\sigma_f B \leqslant A\sigma_g B$. Then we have

$$\Phi(A,B) = \operatorname{Tr}(A\sigma_g B - A\sigma_f B) \geqslant 0. \tag{2}$$

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* Corresponding author.

The quantity $\Phi(A,B)$ in (2) could be considered as a distance-like function that expresses the gap between two data points A and B which are positive definite matrices. In general, $\Phi(A,B)$ does not necessarily satisfy the symmetry condition nor triangle inequality.

In the past few years, quantum divergences have been actively studied [16]. Mostly, people studied different types of matrix generalizations of the difference between the arithmetic and the geometric means of positive numbers

$$\frac{a+b}{2} - \sqrt{ab}, \quad a,b \geqslant 0.$$

For example, the quantum Hellinger distance [2] defined as

$$\Phi(A,B) = \operatorname{Tr}(A\nabla B - A\#B).$$

Recently, Pitrik and Virosztek [16] considered a more general version of quantum Hellinger divergence by replacing the geometric mean with a Kubo-Ando mean σ:

$$\Phi_\sigma(A,B) = \operatorname{Tr}(A\nabla B - A\sigma B).$$

They showed that $\Phi_\sigma(A,B)$ belongs to the family of *f-maximal quantum divergence* [16], and hence it is jointly convex, and satisfies the Data Processing Inequality. Recall that the class of f-maximal divergence consists of elements of the form $\operatorname{Tr}(Af(A^{-1/2}BA^{-1/2}))$, where $A,B > 0$, and f is operator convex function from $(0,\infty)$ to $(0,\infty)$ (see, for example, in [10]).

Recently, the first author and co-authors [6] introduced some new quantum divergences one of which was of the form

$$\Phi(A,B) = \operatorname{Tr}\left(P_\alpha(p,A,B) - A\#_\alpha B\right),$$

where $P_\alpha(p,A,B) = A^{\frac{1}{2}}((1-\alpha)I + \alpha(A^{-\frac{1}{2}}BA^{-\frac{1}{2}})^p)^{\frac{1}{p}}A^{\frac{1}{2}}(\alpha \in [0,1])$ is the Kubo-Ando matrix power mean, and $A\#_\alpha B = A^{1/2}(A^{-1/2}BA^{-1/2})^\alpha A^{1/2}$ is the weighted geometric mean of A and B. In our knowledge, this is the first non-trivial quantum divergence of the form (2), where σ_g is not the arithmetic mean.

Now let $f : [0,\infty) \to [0,\infty)$ be monotone increasing. Then, for any positive $A,B \in \mathscr{P}_n$ with $A \leqslant B$,

$$\operatorname{Tr}(f(A)) \leqslant \operatorname{Tr}(f(B)). \tag{3}$$

This fact is well-known in the literature, but we give a short proof here for the readers' convenience. According to the Weyl's monotonicity principle, from the assumption we have $\lambda_k(A) \leqslant \lambda_k(B)$ for $1 \leqslant k \leqslant n$, where $(\lambda_1(A), \ldots \lambda_n(A))$ is the list of eigenvalues of A in the decreasing order. Since $f : [0,\infty) \to [0,\infty)$ is monotone increasing, we have $f(\lambda_k(A)) \leqslant f(\lambda_k(B))$ for $1 \leqslant k \leqslant n$. Hence,

$$\operatorname{Tr}(f(A)) = \sum_{i=1}^{n} f(\lambda_k(A)) \leqslant \sum_{k=1}^{n} f(\lambda_k(B)) = \operatorname{Tr}(f(B)).$$

It is natural to ask when the quantity

$$\Psi_f(A,B) = \mathrm{Tr}\,(f(A)) - \mathrm{Tr}\,(f(B)) \tag{4}$$

is a quantum divergence.

Notice that for $A \geqslant B > 0$, according to a result in [9] the following inverse problem

$$\begin{cases} A = \frac{X+Y}{2} \\ B = X\#Y \end{cases} \tag{5}$$

has a positive solution (X,Y). For $0 \leqslant B \leqslant A$, the system (5) was solved by Uchiyama [18]. He also showed that, actually, (5) has a unique positive solution. Therefore, for $0 \leqslant B \leqslant A$, the trace distance between A and B is nothing but the quantum Hellinger distance between the corresponding X and Y. Namely,

$$||A-B||_1 = \mathrm{Tr}\,(A-B) = \mathrm{Tr}\,(X\nabla Y - X\#Y) = \Phi(X,Y).$$

And the quantity (4) has the following form in term of matrix means:

$$\Psi_f(A,B) = \mathrm{Tr}\,(f(A)) - \mathrm{Tr}\,(f(B)) = \mathrm{Tr}\,(f(X\nabla Y) - f(X\#Y)) := \Phi_f(X,Y). \tag{6}$$

Since for each pair (A,B) such that $A \geqslant B > 0$ there exists a pair of positive definite matrices (X,Y) satisfying (5). Reversely, each pair of positive definite matrices (A,B) defines a pair of (A,B) by the relation in (5). Therefore, instead of considering the quantity $\Psi_f(A,B)$ we investigate when $\Phi_f(X,Y)$ is a quantum divergence.

In this paper, for a continuously differentiable and monotone increasing function f, we show that $\Phi_f(X,Y)$ is a quantum divergence. We also generalize the result to any operator mean σ instead of the geometric mean $\#$. Namely, for a Kubo-Ando mean σ the quantity

$$\Phi_{f,\sigma}(X,Y) = \mathrm{Tr}\,[f(X\nabla Y) - f(X\sigma Y)] \tag{7}$$

is a quantum divergence, where $X,Y \in \mathscr{P}_n$, and $f : [0,\infty) \to [0,\infty)$ is continuously differentiable and monotone increasing.

In the relation with (5), notice that some inverse problems and the characterization problems was considered in [5]. In [7] the first authors and co-authors obtained new characterizations of operator monotone functions by inequalities of the form

$$f(A\#B) \leqslant f(A\sigma B)$$

for some symmetric Kubo-Ando operator mean σ. In fact, they solved a similar inverse problem for $\#$ and σ. In this paper, we also consider some related inverse problems for matrix means, and obtain some new characterizations of the trace property in the relation with quantum divergence (7).

2. Generalized Hellinger divergences generated by monotone functions

DEFINITION 1. (Fréchet derivative) Let V, W be Banach spaces and let $f : V \to W$ be a function. The Fréchet derivative of f at a point x_0 (if it exists) is a bounded linear operator $Df(x_0) : V \to W$ such that

$$\lim_{\|h\|\to 0} \frac{\|f(x_0+h) - f(x_0) - Df(x_0)(h)\|_W}{\|h\|_V} = 0.$$

DEFINITION 2. [2] A smooth function Φ from $\mathscr{P}_n \times \mathscr{P}_n$ to the set of nonnegative real numbers is call a *quantum divergence* if

(i) $\Phi(A,B) = 0$ if and only if $A = B$;

(ii) The derivative with respect to the second variable vanishes on the diagonal,

$$D\Phi(A,X)|_{X=A} = 0;$$

(iii) The second derivative is positive on the diagonal,

$$D^2\Phi(A,X)|_{X=A}(Y,Y) \geqslant 0 \quad \text{for all Hermitian matrix} \quad Y.$$

Before moving to the main result, we need some preparations.

LEMMA 1. [15, Proposition 4.5] *Let σ be an operator mean such that $! \leqslant \sigma \leqslant \nabla$. Then, the correspondent representing function $f'_\sigma(1) = \frac{1}{2}$.*

LEMMA 2. *Let A be positive definite matrix, and σ be an operator mean in the sense of Kubo-Ando such that $! \leqslant \sigma \leqslant \nabla$. Then, the first derivative of the function $g(X) = A\sigma X$ is given by the following formula*

$$Dg(X)(Y) = bY + \int_0^\infty (\lambda + XA^{-1})^{-1} Y (\lambda + A^{-1}X)^{-1} d\mu(\lambda), \tag{8}$$

where $f_\sigma(x) = a + bx + \int_0^\infty \left(\frac{\lambda}{\lambda^2+1} - \frac{1}{\lambda+x}\right) d\mu(\lambda)$ is the integral representation of the representing function of the mean σ. Furthermore,

$$Dg(X)(Y)|_{X=A} = \frac{Y}{2}. \tag{9}$$

Proof. For any Hermitian matrix Y, the derivative of the function $X \mapsto f_\sigma(X)$ is given by

$$Df_\sigma(X)(Y) = bY + \int_0^\infty (\lambda + X)^{-1} Y (\lambda + X)^{-1} d\mu(\lambda).$$

Since $g(X)=A^{1/2}f_\sigma(A^{-1/2}XA^{-1/2})A^{1/2}$, we have

$$\begin{aligned}
&Dg(X)(Y)\\
&=A^{1/2}\Big(bA^{-1/2}YA^{-1/2}+\int_0^\infty(\lambda+A^{-1/2}XA^{-1/2})^{-1}(A^{-1/2}YA^{-1/2})\\
&\quad\times(\lambda+A^{-1/2}XA^{-1/2})^{-1}d\mu(\lambda)\Big)A^{1/2}\\
&=bY+\int_0^\infty(\lambda+XA^{-1})^{-1}Y(\lambda+A^{-1}X)^{-1}d\mu(\lambda).
\end{aligned}$$

As a consequence, we get

$$Dg(X)(Y)|_{X=A}=\left(b+\int_0^\infty(\lambda+1)^{-2}d\mu(\lambda)\right)Y=f'_\sigma(1)Y=\frac{Y}{2}.\quad\square$$

LEMMA 3. *For a natural number n, the derivative of the map $X\mapsto(A\sigma X)^n$ is calculated by the following formula*

$$D(g(X)^n)(B)|_{X=A}=\frac{1}{2}\sum_{i=0}^{n-1}A^iBA^{n-1-i}. \tag{10}$$

Therefore,

$$D(\mathrm{Tr}\,((A\sigma X)^n)|_{X=A}(B)=n\mathrm{Tr}\left(A^{n-1}\frac{B}{2}\right).$$

Proof. The derivative of the map $U\mapsto U^n$ is as follows

$$D(U^n)(B)=\sum_{i=0}^{n-1}U^iBU^{n-1-i}.$$

By Lemma 2 and the chain rule, we have

$$D(g(X)^n)(B)=\sum_{i=0}^{n-1}(A\sigma X)^iD(A\sigma X)(B)(A\sigma X)^{n-1-i}.$$

Consequently,

$$\begin{aligned}
D(g(X)^n)(B)|_{X=A}&=\sum_{i=0}^{n-1}A^iD(A\sigma X)(B)|_{X=A}A^{n-1-i}\\
&=\frac{1}{2}\sum_{i=0}^{n-1}A^iBA^{n-1-i}.
\end{aligned}$$

Therefore,

$$\begin{aligned} D(\operatorname{Tr}((A\sigma X)^n)|_{X=A}(B) &= \operatorname{Tr}\left(\frac{1}{2}\sum_{i=0}^{n-1} A^iBA^{n-1-i}\right) \\ &= \sum_{i=0}^{n-1} \operatorname{Tr}\left(\frac{1}{2}A^{n-1}B\right) \\ &= n\operatorname{Tr}\left(A^{n-1}\frac{B}{2}\right). \quad \square \end{aligned}$$

We also need to calculate the second derivative of the matrix function $\operatorname{Tr}(g(X)^n)$. By the definition,

$$D^2\operatorname{Tr}(F(A\sigma X))(Y,Z) = \frac{d}{dt}|_{t=0} D(\operatorname{Tr}(F(A\sigma(X+tZ))))(Y). \tag{11}$$

LEMMA 4. *The second derivative of the function* $\operatorname{Tr}((A\sigma X)^n)$ *on the diagonal is given by*

$$D^2(\operatorname{Tr}((X\sigma Y)^n)(A,A)(Z,Z) = n\operatorname{Tr}\left(\frac{1}{4}\sum_{i=0}^{n-2} A^iZA^{n-2-i}Z + 2f''_\sigma(1)ZA^{-1}ZA^{n-1}\right). \tag{12}$$

Proof. On account of Lemmas 2 and 3, we have

$$\begin{aligned} &D\operatorname{Tr}((A\sigma X)^n)(Y) \\ &= \operatorname{Tr}\Big(\sum_{i=0}^{n-1}(A\sigma X)^i D(A\sigma X)(Y)(A\sigma X)^{n-1-i}\Big) \\ &= \sum_{i=0}^{n-1}\operatorname{Tr}\left((A\sigma X)^i\left(bY + \int_0^\infty (\lambda + XA^{-1})^{-1}Y(\lambda + A^{-1}X)^{-1}d\mu(\lambda)\right)(A\sigma X)^{n-1-i}\right) \\ &= \sum_{i=0}^{n-1}\operatorname{Tr}\left((A\sigma X)^{n-1}\left(bY + \int_0^\infty (\lambda + XA^{-1})^{-1}Y(\lambda + A^{-1}X)^{-1}d\mu(\lambda)\right)\right) \\ &= n\operatorname{Tr}\left((A\sigma X)^{n-1}\left(bY + \int_0^\infty (\lambda + XA^{-1})^{-1}Y(\lambda + A^{-1}X)^{-1}d\mu(\lambda)\right)\right). \end{aligned}$$

By the definition of the second derivative, we have

$$D^2\operatorname{Tr}((A\sigma X)^n)(Y,Z) = \frac{d}{dt}|_{t=0} D\operatorname{Tr}((A\sigma(X+tZ))^n)(Y).$$

For this, we again use the integral representation of the function f_σ,

$$\begin{aligned} &f_\sigma(A^{-1/2}(X+tZ)A^{-1/2}) \\ &= a + A^{-1/2}(X+tZ)A^{-1/2} + \int_0^\infty \frac{\lambda}{\lambda^2+1} - (\lambda + A^{-1/2}(X+tZ)A^{-1/2})^{-1}d\mu(\lambda). \end{aligned}$$

Consequently,

$$\frac{df_\sigma}{dt}(A^{-1/2}(X+tZ)A^{-1/2})|_{t=0}$$
$$=A^{-1/2}ZA^{-1/2}+\int_0^\infty(\lambda+A^{-1/2}XA^{-1/2})^{-1}A^{-1/2}ZA^{-1/2}(\lambda+A^{-1/2}XA^{-1/2})^{-1}d\mu(\lambda).$$

Therefore,

$$\begin{aligned}\frac{d(A\sigma(X+tZ))}{dt}|_{t=0}&=A^{1/2}\frac{df_\sigma(A^{-1/2}(X+tZ)A^{-1/2})}{dt}|_{t=0}A^{1/2}\\&=Z+\int_0^\infty(\lambda+XA^{-1})Z(\lambda+A^{-1}X)d\mu(\lambda).\end{aligned}$$

We are almost ready to compute the following derivative

$$\begin{aligned}&\frac{d}{dt}|_{t=0}(A\sigma(X+tZ))^{n-1}\\&=D((A\sigma X)^{n-1})(Z)\\&=\sum_{i=0}^{n-2}(A\sigma X))^iD(A\sigma X)(Z)(A\sigma X)^{n-2-i}\\&=\sum_{i=0}^{n-2}(A\sigma X)^i\left(bZ+\int_0^\infty(\lambda+XA^{-1})^{-1}Z(\lambda+A^{-1}X)^{-1}d\mu(\lambda)\right)(A\sigma X)^{n-2-i}.\end{aligned}$$

Therefore,

$$\frac{d}{dt}|_{t=0}(A\sigma(X+tZ)^{n-1})|_{A=X}=\frac{1}{2}\sum_{i=0}^{n-2}A^iZA^{n-2-i}. \tag{13}$$

Similarly, we can compute the following derivative which was obtained in [2, Theorem 2]

$$\frac{d}{dt}|_{t=0}\left(bY+\int_0^\infty(\lambda+XA^{-1})^{-1}Y(\lambda+A^{-1}X)^{-1}d\mu(\lambda)\right)(A,A)(Z,Z)=2f''_\sigma(1)ZA^{-1}Z. \tag{14}$$

From (13) and (14), we get

$$D^2(\mathrm{Tr}\,(g(X)^n))(A,A)(Z,Z)=n\mathrm{Tr}\left(\frac{1}{4}\sum_{i=0}^{n-2}A^iZA^{n-2-i}Z+2f''_\sigma(1)ZA^{-1}ZA^{n-1}\right). \quad \square$$

REMARK 1. Let $p(t)=a_0+a_1t+\cdots+a_nt^n$. Then we have by Lemmas 3 and 4, we have

$$\begin{aligned}D(\mathrm{Tr}\,(p(A\sigma X)))|_{X=A}(Z)&=(a_1+2a_2+\cdots+na_n)\mathrm{Tr}\left(A^{n-1}\frac{Z}{2}\right)\\&=p'(1)\mathrm{Tr}\left(A^{n-1}\frac{Z}{2}\right)\end{aligned}$$

and

$$\begin{aligned}
&D^2(\mathrm{Tr}\,(p(X\sigma Y))(A,A)(Z,Z)\\
&=(a_1+2a_2+\cdots+na_n)\mathrm{Tr}\left(\frac{1}{4}\sum_{i=0}^{n-2}A^iZA^{n-2-i}Z+2f_\sigma''(1)ZA^{-1}ZA^{n-1}\right)\\
&=p'(1)\mathrm{Tr}\left(\frac{1}{4}\sum_{i=0}^{n-2}A^iZA^{n-2-i}Z+2f_\sigma''(1)ZA^{-1}ZA^{n-1}\right).
\end{aligned}$$

We recall some basic properties on operator monotonicity.

LEMMA 5. *Let σ be an operator mean such that $! \leqslant \sigma \leqslant \nabla$, and A be a positive definite matrix. If $I\sigma A = I\nabla A$, then $A = I$.*

Proof. Since $! \leqslant \sigma \leqslant \nabla$ we have that $f_\sigma'(1) = 1/2$, that means, the representing function $(1+t)/2$ of the arithmetic mean is the tangent line to the graph of f_σ at $t = 1$. And since the function f_σ is concave, the graph of f_σ is below its tangent line $(1+t)/2$. Indeed, we always can find a small neighborhood $(a,b) \subset (0,\infty)$ of 1 such that $f_\sigma(t) < (1+t)/2$ for any $t \in (a,b) \setminus \{1\}$. Now, if there exists $t_1 \neq 1$ such that $f_\sigma(t_1) = 1$, then from the concavity of the function f_σ, for any $\lambda \in (0,1)$ we have

$$f_\sigma(\lambda 1 + (1-\lambda)t_1) \geqslant \lambda f_\sigma(1) + (1-\lambda)f_\sigma(t_1) = 1.$$

From here, there exists $\lambda \in (0,1)$ such that the point $\lambda 1 + (1-\lambda)t_1 \in (a,b)$, i.e., $f_\sigma(\lambda 1 + (1-\lambda)t_1) < f_\sigma(1) = 1$ which is a contradiction. Therefore, $f_\sigma(t) = 1$ if and only if $t = 1$. As a consequence, if $I\sigma A = I\nabla A$, then $f_\sigma(\lambda_A) = (1+\lambda_A)/2$ for all eigenvalues λ_A of A. From here, $\lambda_A = 1$. That means, A is the identity matrix. □

LEMMA 6. *Let $g : [0,\infty) \to [0,\infty)$ with $g(0) = 0$ be a continuous strictly increasing map. Suppose that g^{-1} is operator monotone. Then, for any positive operators X, Y and operator monotone $\sigma \leqslant \nabla$ if $g(X\nabla Y) = g(X\sigma Y)$, then $X = Y$.*

Proof. From [1, Theorem X.1.6] we know that if $g(X\nabla Y) = g(X\sigma Y)$ then $X\nabla Y = X\sigma Y$. Since $X^{-1/2}(X\nabla Y)X^{-1/2} = I\sigma X^{-1/2}YX^{-1/2}$, we have $I\nabla X^{-1/2}YX^{-1/2} = I\sigma X^{-1/2}YX^{-1/2}$. Set $A = X^{-1/2}YX^{-1/2}$. Then from Lemma 5 we have $A = I$. That is, $X = Y$. □

LEMMA 7. *Let $g : [0,\infty) \to [0,\infty)$ with $g(0) = 0$ be a strictly increasing function in C^∞-class. Then, for any finite interval $[a,b] \subset [0,\infty)$ containing 1, and for any ε, there exists a polynomial p such that $\max_{t\in[a,b]} |g(t) - p(t)| < \varepsilon$ such that $p'(1) \geqslant 0$.*

Proof. Recall that for the points $(t_i, f(t_i))$ $(i = 1,2,\cdots,n)$, the Lagrange interpolation polynomial $P_n(t)$ is

$$P_n(t) = \sum_{i=1}^{n} g(t_i)L_i(t),$$

where each Lagrange basis polynomial $L_i(t)$ is $L_i(t)=\prod_{j=1,j\neq i}^{n}\frac{t-t_j}{t_i-t_j}$. It is well-known that for such function g, for any $\varepsilon>0$ there exists a Lagrange polynomial $P_n(t)$ such that $\max_{t\in[a,b]}|g(t)-P_n(t)|<\varepsilon$. Also, in this case we have

$$g(t)=P_n(t)+\frac{g^{(n+1)}(\varepsilon(t))}{(n+1)!}(t-t_1)(t-t_2)\cdots(t-t_n).$$

Differentiating both sides, we get

$$g'(t)=P_n'(t)+\left(\frac{g^{(n+1)}(\varepsilon(t))}{(n+1)!}(t-t_1)(t-t_2)\cdots(t-t_n)\right)'.$$

Since the function $g(t)$ is strictly increasing on $[a,b]$, $g'(1)>0$. Therefore, we can choose n as big as $\left(\frac{g^{(n+1)}(\varepsilon(t))}{(n+1)!}(t-t_1)(t-t_2)\cdots(t-t_n)\right)'|_{t=1}<g'(1)$. From here, we obtain that $P_n'(1)>0$. $\square$

Using the calculations from Remark 1, Lemma 7 ensures that the condition $P_n'(1)>0$ holds, which is essential for the validity of the following theorem.

THEOREM 1. *Let σ be a operator mean such that $!\leqslant\sigma\leqslant\nabla$ and f_σ be a C^2-class representing function of σ. Let $g:[0,\infty)\to[0,\infty)$ be strictly increasing function with $g'(1)\in(0,1)$ such that g^{-1} is operator monotone function on $(0,\infty)$. Then the quantity $\Phi_{g,\sigma}(X,Y)=\mathrm{Tr}\,(g(X\nabla Y)-g(X\sigma Y))$ is a quantum divergence, where $X,Y\in\mathscr{P}_n$.*

Proof. Firstly, notice that from operator monotonicity of the function g^{-1}, we have that g^{-1} is in the class $C^\infty(0,\infty)$. Therefore, its inverse, which is the function g is also in the class $C^\infty(0,\infty)$.

It is sufficient to prove the theorem for the case where $g(t)=t^n$ for any natural number n. The general case then follows by applying Lemma 7, which ensures that any function g satisfying the conditions of the theorem can be approximated by a sequence of Lagrange polynomial with positive derivatives at 1.

Since $X\nabla Y\geqslant X\sigma Y$ for all $X,Y\in\mathscr{P}_n$ and g is increasing monotonic, we have $\mathrm{Tr}\,(g(X\nabla Y))\geqslant\mathrm{Tr}(g(X\sigma Y))$. Again, by Lemma 6, $\Phi_{g,\sigma}(X,Y)=0$ if and only if $X=Y$. Therefore, $\Phi_{g,\sigma}(X,Y)$ satisfies the first condition in Definition 2.

From Lemma 2, one can see that the function $\Phi_{g,\sigma}(X,Y)$ also satisfies the second condition in Definition 2. Indeed,

$$\begin{aligned}D\Phi_{g,\sigma}(A,X)|_{X=A}&=\mathrm{Tr}\,(Dg\,(A\nabla X)\,|_{X=A}-Dg(A\sigma X)|_{X=A})\\&=g'(1)\mathrm{Tr}\,(Y/2-Y/2)=0.\end{aligned}$$

Finally, we will check the third condition for any Hermitian Z. Indeed, from Lemma 4 one can see that

$$D^2\Phi_{g,\sigma}(A,A)(Z,Z)=g'(1)\mathrm{Tr}\left(-2f_\sigma''(1)ZA^{-1}ZA^{n-1}\right)\geqslant 0.\quad\square$$

Now, let $A_1, A_2, \dots, A_m$ be positive definite matrices and $w = (w_1, w_2, \dots, w_m)$ be a probability vector such that $\sum_{i=1}^{m} w_i = 1$, we consider the least squares problem with respect to the new quantum divergence

$$\min_{X>0} \sum_{i=1}^{m} \omega_i \mathrm{Tr}\left[g(A_i \nabla X) - g(A_i \sigma X)\right].$$

Given that we could not find the explicit barycenter of $A_1, A_2, \cdots, A_n$, but if it exists, it should satisfy some special equation.

THEOREM 2. *Suppose that operator mean σ and the function g satisfy the conditions in Theorem 1. If the function $F(X) = \sum_{i=1}^{m} \omega_i \mathrm{Tr}\left[g(A_i \nabla X) - g(A_i \sigma X)\right]$ attains its minimum at X_0 then X_0 should be a positive solution of the following matrix equation*

$$\sum_{i=1}^{m} \frac{\omega_i}{2} g'(A_i \nabla X)$$
$$= \sum_{i=1}^{m} \omega_i \left(g'(A_i \sigma X) b + \int_0^\infty (\lambda + A_i^{-1} X)^{-1} g'(A_i \sigma X)(\lambda + X A_i^{-1})^{-1} d\mu(\lambda) \right),$$

where $f_\sigma(x) = a + bx + \int_0^\infty \left(\frac{\lambda}{\lambda^2+1} - \frac{1}{\lambda+x} \right) d\mu(\lambda)$ is the integral representation of the representing function f_σ of the mean σ.

Proof. Again, we firstly consider the case when the function $g(t) = t^n$ for some natural number n. In this case, for any Hermitian matrix B, according to Lemma 3 we have

$$\mathrm{Tr}\left(Dg(A_i \nabla X)(B)\right) = \frac{n}{2} \mathrm{Tr}\left((A_i \nabla X)^{n-1} B\right), \tag{15}$$

and

$$\mathrm{Tr}\left(D(g(X)^n)(B)\right)$$
$$= n \mathrm{Tr}\left((A_i \sigma X)^{n-1} D(A_i \sigma X)(B)\right)$$
$$= n \left(\mathrm{Tr}\left((A_i \sigma X)^{n-1} bB\right) + \int_0^\infty \mathrm{Tr}\left((A_i \sigma X)^{n-1} (\lambda + X A_i^{-1})^{-1} B (\lambda + A_i^{-1} X)^{-1} d\mu(\lambda)\right) \right)$$
$$= n \mathrm{Tr}\left(\left((A_i \sigma X)^{n-1} b + \int_0^\infty (\lambda + A_i^{-1} X)^{-1} (A_i \sigma X)^{n-1} (\lambda + X A_i^{-1})^{-1} d\mu(\lambda) \right) B \right).$$

Consequently,

$$DF(X)(B)$$
$$= n \sum_{i=1}^{m} w_i \mathrm{Tr}\left((A_i \nabla X)^{n-1} B/2\right)$$
$$- n \sum_{i=1}^{m} w_i \mathrm{Tr}\left(\left((A_i \sigma X)^{n-1} b + \int_0^\infty (\lambda + A_i^{-1} X)^{-1} (A_i \sigma X)^{n-1} (\lambda + X A_i^{-1})^{-1} d\mu(\lambda) \right) B \right).$$

From the condition that $DF(X)(B) = 0$ for any Hermitian B it implies that

$$\begin{aligned}
&\sum_{i=1}^{m} \frac{w_i}{2}(A_i \nabla X)^{n-1} \\
&= \sum_{i=1}^{m} w_i \left((A_i \sigma X)^{n-1} b + \int_0^\infty (\lambda + A_i^{-1}X)^{-1}(A_i \sigma X)^{n-1}(\lambda + XA_i^{-1})^{-1} d\mu(\lambda) \right).
\end{aligned}$$

In general case, let P_n be the sequence of Lagrange polynomials that uniformly converses to the function g such that $P_n'(1) > 0$ starting from a big enough n. For each n, let us consider the following function

$$F_n(X) = \sum_{i=1}^{m} \omega_i \mathrm{Tr}\left(P_n(A_i \nabla X) - P_n(A_i \sigma X)\right).$$

From the previous argument, one can see that if $F_n(X)$ attains minimum at X_{0n}, then X_{0n} should be the solution of the following equation

$$\begin{aligned}
&\sum_{i=1}^{m} \frac{w_i}{2} P_n'(A_i \nabla X) \\
&= \sum_{i=1}^{m} w_i \left(P_n'(A_i \sigma X) b + \int_0^\infty (\lambda + A_i^{-1}X)^{-1} P_n'(A_i \sigma X)(\lambda + XA_i^{-1})^{-1} d\mu(\lambda) \right).
\end{aligned}$$

Now we have

$$\begin{aligned}
F(X) &= \sum_{i=1}^{m} \omega_i \mathrm{Tr}\left(g(A_i \nabla X) - g(A_i \sigma X)\right) \\
&= \sum_{i=1}^{m} \omega_i \lim_n \mathrm{Tr}\left(P_n(A_i \nabla X) - P_n(A_i \sigma X)\right).
\end{aligned}$$

The derivative $DF(X)(B)$ is given by the following

$$\begin{aligned}
&DF(X)(B) \\
&= \mathrm{Tr}\left(\sum_{i=1}^{m} \omega_i \lim_n \left(DP_n(A_i \nabla X)(B) - DP_n(A_i \sigma X)(B)\right) \right) \\
&= \mathrm{Tr}\Bigg(B \sum_{i=1}^{m} \omega_i \lim_n \Bigg(\frac{1}{2} P_n'(A_i \nabla X) \\
&\quad - \left(P_n'(A_i \sigma X) b + \int_0^\infty (\lambda + A_i^{-1}X)^{-1} P_n'(A_i \sigma X)(\lambda + XA_i^{-1})^{-1} d\mu(\lambda) \right) \Bigg) \Bigg) \\
&= \mathrm{Tr}\Bigg(B \sum_{i=1}^{m} \omega_i \Bigg(\frac{1}{2} g'(A_i \nabla X) \\
&\quad - \left(g'(A_i \sigma X) b + \int_0^\infty (\lambda + A_i^{-1}X)^{-1} g'(A_i \sigma X)(\lambda + XA_i^{-1})^{-1} d\mu(\lambda) \right) \Bigg) \Bigg).
\end{aligned}$$

Therefore, $DF(X)(B)=0$ for any Hermitian B if and only if

$$\begin{aligned}&\sum_{i=1}^{m}\frac{\omega_i}{2}g'(A_i\nabla X)\\&=\sum_{i=1}^{m}\omega_i\left(g'(A_i\sigma X)b+\int_0^{\infty}(\lambda+A_i^{-1}X)^{-1}g'(A_i\sigma X)(\lambda+XA_i^{-1})^{-1}d\mu(\lambda)\right).\quad\square\end{aligned}$$

3. Inverse problems for matrix means

In this section we focus on inverse problem for matrix means that involves operator monotone functions.

PROPOSITION 1. *Let A and B in $\mathscr{P}_n$ such that $0<3B\leqslant A$ and σ be an operator mean in the sense of Kubo-Ando such that the correspondent representative function f_σ satisfies $f'_\sigma(1)=1/2$. Then the following equation has a positive definite solution T such that $B\leqslant T\leqslant A$,*

$$T=A-T\sigma B \tag{16}$$

Proof. Let $K=\{T\in\mathscr{P}_n|B\leqslant T\leqslant A\}$. Then, K is a convex compact set in $M_n(\mathbb{C})$. Let define $G(T)=A-T\sigma B$ for $T\in\mathscr{K}$. We will show that $G(T)\in\mathscr{K}$. Note that

$$T^{1/2}f_\sigma(T^{-1/2}BT^{-1/2})T^{1/2}=T\sigma B\geqslant B\sigma B=B.$$

Since $!\leqslant\sigma\leqslant\nabla$ and $B\leqslant T\leqslant A$, we get

$$A-T\sigma B\geqslant A-A\sigma B\geqslant A-\frac{A+B}{2}=\frac{1}{2}A-\frac{B}{2}\geqslant\frac{3}{2}B-\frac{B}{2}=B$$

which implies

$$G(T)\geqslant B. \tag{17}$$

On the other hand, it is trivial that $G(T)\leqslant A$. Thus, G is a self-map on the compact and convex set $\mathscr{K}$. According to Brouwer's fixed point theorem [4, Corollary 9.2], G has a fixed point. $\square$

THEOREM 3. *Suppose f is a continuous function on $(0,\infty)$ such that $f^{-1}:(0,\infty)\to(0,\infty)$ is operator monotone and $(f^{-1})'(1)=1/2$. Suppose that $0<3f^{-1}(B)\leqslant 2f^{-1}(A)$, then the inverse problem*

$$\begin{cases}A=f\left(\frac{X+Y}{2}\right)\\ B=f(P_f(Y,X))\end{cases} \tag{18}$$

have a positive definite solution (X,Y), where $P_f(Y,X)=X^{1/2}f(X^{-1/2}YX^{-1/2})X^{1/2}$ is the operator perspective of f [12, 15].

Proof. The system (18) is equivalent to the following system

$$\begin{cases} f^{-1}(A) = \dfrac{X+Y}{2} \\ f^{-1}(B) = X^{1/2} f\left(X^{-1/2} Y X^{-1/2}\right) X^{1/2}. \end{cases} \tag{19}$$

Let $A_1 = f^{-1}(A)$, $B_1 = f^{-1}(B)$. Since $3f^{-1}(B) \leqslant 2f^{-1}(A)$, we have $B_1 = f^{-1}(B) \leqslant \frac{3}{2} f^{-1}(B) \leqslant f^{-1}(A) = A_1$, and the system (19) is written by

$$\begin{cases} A_1 = \dfrac{X+Y}{2} \\ B_1 = X^{1/2} f\left(X^{-1/2} Y X^{-1/2}\right) X^{1/2}. \end{cases} \tag{20}$$

Furthermore, the system (20) is equivalent the system

$$\begin{cases} X = 2A_1 - X^{1/2} f^{-1}\left(X^{-1/2} B_1 X^{-1/2}\right) X^{1/2} = 2A_1 - X \sigma B_1 \\ Y = X^{1/2} f^{-1}\left(X^{-1/2} B_1 X^{-1/2}\right) X^{1/2}, \end{cases} \tag{21}$$

where σ is the corresponding operator mean to f^{-1}. According to Proposition 1, the first equation in (21) has a positive solution that implies that the system (21) also has a positive solution (X,Y). $\square$

4. Concluding remark on characterization of the trace

To finish the paper, we show a new characterization of the trace property in the relation with the new quantum divergence defined in the second section. For the trace property characterization we refer to the papers [3, 8] and references therein.

THEOREM 4. *Let $p > 1$ and φ be a positive linear map on $\mathbb{M}_n$. Then for any positive matrices A, B of order n, the following equality*

$$\Phi_\varphi(A,B) = \varphi\left((A \nabla B)^p\right) - \varphi\left((A \# B)^p\right)$$

is a quantum divergence if and only if φ is a scalar multiple of the canonical trace.

Proof. Suppose that $\Phi_\varphi(A,B)$ is a quantum divergence. Then $\Phi_\varphi(A,B) \geqslant 0$ for any positive definite matrices A and B. Therefore

$$\varphi\left((A \nabla B)^p\right) \geqslant \varphi\left((A \# B)^p\right). \tag{22}$$

For arbitrary $0 < X \leqslant Y$, there exists a pair of A, B such that

$$X = A \# B \quad \text{and} \quad Y = A \nabla B.$$

On account of (22) we have

$$\varphi(X^p) \leqslant \varphi(Y^p).$$

By [3, Theorem], φ is a scalar multiple of the canonical trace.

The converse implication is a direct consequence of Theorem 1. □

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Trung Hoa Dinh
Department of Mathematics and Statistics
Troy University
Troy, AL 36082, United States
e-mail: thdinh@troy.edu

Anh Vu Le
University of Economics and Law
Vietnam National University
Ho Chi Minh City, Vietnam
e-mail: vula@uel.edu.vn

Osaka Hiroyuki
Department of Mathematical Sciences
Ritsumeikan University
Kusatsu, Shiga 525-8577, Japan
e-mail: osaka@se.ritsumei.ac.jp

Ngoc Yen Phan
Faculty of Mathematics and Computer Science
University of Science, Ho Chi Minh City
Vietnam National University
Ho Chi Minh City, Vietnam
and
Department of Mathematics and Informatics
Ho Chi Minh City University of Education
Vietnam
e-mail: 22N21106@student.hcmus.edu.vn
yenpn@hcmue.edu.vn