THE MATRIX GEOMETRIC MEANS UNDER PARTIAL TRACE

Sejong Kim*

ABSTRACT. We review a partial trace alternatively defined by the composition of positive linear maps, and see how the partial trace acts on the matrix geometric means. We also study the quantum Tsallis relative entropy under partial trace related with the fidelity.

1. Introduction

A density operator, or density matrix interchangeably, is introduced as a means of describing ensembles of quantum states. The deepest application of the density operator is as a descriptive tool for subsystems of a composite quantum system. Such description is provided by the reduced density operator, called the partial trace. It is the unique operation which gives rise to the correct description of observable quantities for subsystems of a composite system (see Section 2.4.3 and Box 2.6 in [6] for more details including quantum teleportation).

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces of physical systems, whose state is described by a density operator $\rho^{\mathcal{H}\mathcal{K}}$. The reduced density operator for system $\mathcal{H}$ is defined by

$$(1.1) \qquad \rho^{\mathcal{H}} := \mathrm{tr}_{\mathcal{K}} \, \rho^{\mathcal{H}\mathcal{K}},$$

where $\mathrm{tr}_{\mathcal{K}}$ is a map of operators known as the partial trace over system $\mathcal{K}$. The partial trace is defined by

$$(1.2) \qquad \mathrm{tr}_{\mathcal{K}}(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) := |a_1\rangle\langle a_2| \, \mathrm{tr}(|b_1\rangle\langle b_2|),$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space of $\mathcal{H}$, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of $\mathcal{K}$. Note that

$\operatorname{tr}(|b_1\rangle\langle b_2|) = \langle b_1|b_2\rangle$, which is an inner product of two vectors $|b_1\rangle$ and $|b_2\rangle$. Furthermore, the partial trace $\operatorname{tr}_{\mathcal{H}}$ can be defined in an analogous way, and both maps of partial traces are linear in its input.

In the quantum information theory, quantum relative entropy is a measure of distinguishability between two quantum states, while fidelity is a measure of the closeness between two quantum states. Note that they are both not a metric for quantum states, or density operators. In [4] the author has studied the operator versions of quantum Tsallis relative entropy that involve the weighted matrix geometric means, and established the relationships with the fidelity. In this article we review the partial trace as a composition of three special positive linear maps and see the effect of partial trace on the weighted matrix geometric means in Section 3. We further investigate the quantum Tsallis relative entropy of reduced density matrices under partial trace and connect to the fidelity in Section 4.

Let M_n be the space of all $n \times n$ matrices with complex entries, $H \subset M_n$ the space of Hermitian matrices, and $P \subset H$ the open convex cone of positive definite Hermitian matrices. For any $X, Y \in H$, we write $X \leq Y$ if $Y - X$ is positive semidefinite, and $X < Y$ if $Y - X$ is positive definite. We simply write as $X \geq O$ ($X > O$) a positive semidefinite (positive definite, respectively) Hermitian matrix X. We denote $X^{\dagger}$ as the complex conjugate transpose of X.

2. Geometric means

The *Riemannian trace metric* on P is determined locally at the point A by the differential

$$ds = \|A^{-1/2}dAA^{-1/2}\|_F,$$

where $\|\cdot\|_F$ means the Frobenius or Hilbert-Schmidt norm on H. This relation is a mnemonic for computing the length of a differentiable path $\gamma : [a, b] \to P$

$$L(\gamma) = \int_a^b \|\gamma^{-1/2}(t)\gamma'(t)\gamma^{-1/2}(t)\|_F dt.$$

Based on the above notion of length, we define the Riemannian trace metric δ between two points A and B in P as the infimum of lengths of curves connecting them. Furthermore, it has been shown in [2] that

$$\delta(A, B) = \|\log(A^{-1/2}BA^{-1/2})\|_F = \|\log(A^{-1}B)\|_F.$$

The unique Riemannian geodesic connecting from A to B is given by

$$(2.1) \qquad t \in [0,1] \mapsto A \#_t B := A^{1/2}(A^{-1/2}BA^{-1/2})^t A^{1/2},$$

called the *weighted geometric mean*, and its geodesic midpoint $A \# B := A \#_{1/2} B$ is known as the unique positive definite solution of the Riccati equation $XA^{-1}X = B$.

We list the well-known properties for the weighted geometric means [2, 5].

LEMMA 2.1. *Let $A, B, C, D \in P$ and let $t \in [0,1]$. Then the following are satisfied.*

  (1) $A \#_t B = A^{1-t}B^t$ *if A and B commute.*
  (2) $(aA)\#_t(bB) = a^{1-t}b^t(A\#_t B)$ *for any $a, b > 0$.*
  (3) $A \#_t B \leq C \#_t D$ *whenever $A \leq C$ and $B \leq D$.*
  (4) $P(A\#_t B)P^\dagger = (PAP^\dagger)\#_t(PBP^\dagger)$ *for any nonsingular matrix P.*
  (5) $A \#_t B = B \#_{1-t} A$.
  (6) $(A\#_t B)^{-1} = A^{-1}\#_t B^{-1}$.
  (7) $(A\#_s B)\#_t(A\#_u B) = A\#_{(1-t)s+tu}B$ *for any $s, u \in [0,1]$.*
  (8) $[(1-\lambda)A + \lambda B]\#_t[(1-\lambda)C + \lambda D] \geq (1-\lambda)(A\#_t C) + \lambda(B\#_t D)$ *for any $\lambda \in [0,1]$.*
  (9) $\det(A\#_t B) = \det(A)^{1-t}\det(B)^t$.
  (10) $[(1-t)A^{-1} + tB^{-1}]^{-1} \leq A\#_t B \leq (1-t)A + tB$.

We have an extended version of joint concavity (Lemma 2.1 (7)) by induction as following.

LEMMA 2.2. *Let $\omega = (w_1, \ldots, w_n)$ be a probability vector: $w_j \geq 0$ for all j and $\sum_{j=1}^{n} w_j = 1$. For any $t \in [0,1]$*

$$(2.2) \qquad \sum_{j=1}^{n} w_j A_j \#_t B_j \leq \left(\sum_{j=1}^{n} w_j A_j\right) \#_t \left(\sum_{j=1}^{n} w_j B_j\right),$$

where $A_j, B_j > O$ for all j.

REMARK 2.3. *For positive semidefinite Hermitian matrices A and B, one can define the weighted geometric mean such as*

$$A\#_t B := \lim_{\epsilon \to 0}(A + \epsilon I)\#_t(B + \epsilon I).$$

3. Partial trace

The *partial trace*, which has applications in quantum information theory, is a generalization of the trace. Whereas the trace is a scalar-valued function on operators, the partial trace is an operator-valued function. It is defined as follows (see [2, Section 4.3]).

Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces with $\dim(\mathcal{H}) = n$ and $\dim(\mathcal{K}) = m$. Let A be a linear operator on the tensor product $\mathcal{H} \otimes \mathcal{K}$. For an orthonormal basis $\{e_1, \ldots, e_m\}$ in $\mathcal{K}$ the partial trace $\operatorname{tr}_{\mathcal{K}} A$, or denoted by $A^{\mathcal{H}}$, is an operator on $\mathcal{H}$ defined by the relation

$$(3.1) \qquad \langle x, (\operatorname{tr}_{\mathcal{K}} A)y \rangle = \sum_{j=1}^{m} \langle x \otimes e_j, A(y \otimes e_j) \rangle$$

for all $x, y \in \mathcal{H}$. The partial trace $\operatorname{tr}_{\mathcal{H}} A$, denoted by $A^{\mathcal{K}}$, can be defined in an analogous way. The following are obviously satisfied.

(i) If $A \geq O(A > O)$, then so are the partial traces.
(ii) The partial trace maps are trace-preserving.

The following appeared in [2, Proposition 4.3.10] gives us another way of looking at the partial trace that is more transparent and makes several calculations easier.

PROPOSITION 3.1. *Let* $\{f_1, \ldots, f_n\}$ *and* $\{e_1, \ldots, e_m\}$ *be orthonormal bases for* $\mathcal{H}$ *and* $\mathcal{K}$, *respectively. Let* A *be a linear operator on* $\mathcal{H} \otimes \mathcal{K}$ *such that its matrix in the basis* $\{f_i \otimes e_j\}$ *is the* $n \times n$ *partitioned form of*

$$A = [A_{ij}],$$

where $A_{ij}, 1 \leq i, j \leq n$ *are* $m \times m$ *matrices. Then* $\operatorname{tr}_{\mathcal{K}} A$ *is the* $n \times n$ *matrix defined as*

$$\operatorname{tr}_{\mathcal{K}} A = [\operatorname{tr} A_{ij}].$$

The map $\operatorname{tr}_{\mathcal{K}}$ is the composition of three special maps described below (see Exercise 4.3.11, [2]). Let $A = [A_{ij}]$ be as in Proposition 3.1.

(1) Let $w = e^{2\pi i/m}$ and let $U = \operatorname{diag}(1, w, \ldots, w^{m-1})$. Let $S = U \oplus U \oplus \cdots \oplus U$ be the $n \times n$ block diagonal matrix. Let

$$(3.2) \qquad \Phi_1(A) = \frac{1}{m} \sum_{j=0}^{m-1} (S^{\dagger})^j A S^j.$$

Then

$$\Phi_1(A) = [\operatorname{diag}(A_{ij})],$$

where $\operatorname{diag}(X)$ is the diagonal part of a square matrix X.

(2) Let V be the $m \times m$ permutation matrix defined as

$$V = \begin{pmatrix} 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Let $P = V \oplus V \oplus \cdots \oplus V$ be the $n \times n$ block diagonal matrix. Let

$$(3.3) \qquad \Phi_2(A) = \frac{1}{m} \sum_{j=0}^{m-1} (P^\dagger)^j A P^j.$$

Then

$$\Phi_2\Phi_1(A) = \left[\left(\frac{1}{m} \operatorname{tr} A_{ij} \right) I_m \right],$$

where I_m is the $m \times m$ identity matrix. Thus, the effect of Φ_2 on the block matrix $\Phi_1(A)$ is to replace each of the diagonal matrices of A_{ij} by the scalar matrix with the same trace as A_{ij}.

(3) Let

$$(3.4) \qquad \Phi_3(A) = m \left[A_{ij}^{(1,1)} \right],$$

where $A_{ij}^{(1,1)}$ be the (1,1) entry of A_{ij}. Note that the matrix $\left[A_{ij}^{(1,1)} \right]$ is a principal $n \times n$ submatrix of A. We have then

$$(3.5) \qquad \Phi_3\Phi_2\Phi_1(A) = \operatorname{tr}_{\mathcal{K}} A.$$

A linear map $\Phi : M_n \to M_m$ is called *positive* if $\Phi(A) \geq O$ whenever $A \geq O$. It is easy to see that every positive linear map is monotone. Indeed, if $A \leq B$ for any $A, B \in H$ then $B - A \geq O$ and

$$O \leq \Phi(B - A) = \Phi(B) - \Phi(A).$$

The linear map Φ is called *strictly positive* if $\Phi(A) > O$ whenever $A > O$, and called *unital* if $\Phi(I_n) = I_m$. It is easy to see that the positive linear map Φ is strictly positive if $\Phi(I_n) > O$.

REMARK 3.2. The special maps Φ_1, Φ_2, and Φ_3 introduced as above are all positive linear and unital maps, and so are monotone. By Theorem 4.1.5 (ii), [2], furthermore, we have

$$(3.6) \qquad \Phi_j(A \#_t B) \leq \Phi_j(A) \#_t \Phi_j(B)$$

for all $j = 1, 2, 3$, where $A, B > O$ and $t \in [0, 1]$.

We now see how the operation of partial trace acts on the matrix geometric means.

THEOREM 3.3. *Let A and B be linear operators on the tensor product $\mathcal{H} \otimes \mathcal{K}$ whose matrix representations are positive semidefinite. For any $t \in [0, 1]$*

$$(3.7) \qquad \operatorname{tr}_{\mathcal{K}}(A \#_t B) \le (\operatorname{tr}_{\mathcal{K}} A) \#_t (\operatorname{tr}_{\mathcal{K}} B).$$

Proof. Using the fact that the map $\operatorname{tr}_{\mathcal{K}}$ is the composition of positive linear maps Φ_1, Φ_2, and Φ_3, and the inequality (3.6) we obtain the inequality (3.7) for any $A, B > O$.

If $A, B \ge O$ we have

$$\operatorname{tr}_{\mathcal{K}}[(A + \epsilon I_{nm}) \#_t (B + \epsilon I_{nm})] \le [\operatorname{tr}_{\mathcal{K}}(A + \epsilon I_{nm})] \#_t [\operatorname{tr}_{\mathcal{K}}(B + \epsilon I_{nm})]$$
$$= [\operatorname{tr}_{\mathcal{K}} A + m\epsilon I_n] \#_t [\operatorname{tr}_{\mathcal{K}} B + m\epsilon I_n]$$

for any $\epsilon > 0$. Since $\operatorname{tr}_{\mathcal{K}}$ is a continuous map, we conclude by taking the limit as $\epsilon \to 0$. $\qquad \square$

COROLLARY 3.4. *Let A and B be linear operators on the tensor product $\mathcal{H} \otimes \mathcal{K}$ whose matrix representations are positive semidefinite. For any $t \in [0, 1]$*

$$\operatorname{tr}(A \#_t B) \le \operatorname{tr}[A^{\mathcal{H}} \#_t B^{\mathcal{H}}].$$

Proof. By taking the trace in the inequality (3.7), it is proved since the partial trace map is trace-preserving. $\qquad \square$

4. Entropy and fidelity under partial trace

The state of a quantum system can be represented by a *density matrix*, a positive semidefinite Hermitian matrix with trace 1. Let D be a set of all quantum states, or density matrices, of some finite dimension. In this section we review some types of Tsallis relative entropy and see the relation with fidelity under partial trace.

For any $A, B \in P$ the *Tsallis relative operator entropy* is defined in [3, 7] by

$$(4.1) \qquad T_t(A|B) = \frac{A \#_t B - A}{t},$$

where $t \in (0, 1]$. It is the difference quotient along the geodesic from A to B, and the limit

$$(4.2) \qquad \lim_{t \to 0} T_t(A|B) = A^{1/2} \log(A^{-1/2} B A^{-1/2}) A^{1/2}$$

is the tangent vector to this geodesic at A.

For any $\rho, \sigma \in D$ the *quantum Tsallis relative entropy* is defined in [1] by

$$(4.3) \qquad D_t(\rho|\sigma) := \frac{1 - \mathrm{tr}(\rho^{1-t}\sigma^t)}{t},$$

where $t \in (0, 1]$. One can see that it is one-parameter extension of the quantum relative entropy

$$(4.4) \qquad U(\rho|\sigma) := \mathrm{tr}[\rho(\log \rho - \log \sigma)],$$

in the sense that

$$\lim_{t \to 0} D_t(\rho|\sigma) = U(\rho|\sigma).$$

LEMMA 4.1. [4, Lemma 3.3] *For any density matrices ρ and σ, and $t \in (0, 1]$*

$$(4.5) \qquad D_t(\rho|\sigma) \leq -\mathrm{tr}\, T_t(\rho|\sigma).$$

The equality holds if ρ and σ commute.

The *fidelity* between quantum states ρ and σ is defined by

$$(4.6) \qquad F(\rho, \sigma) := \mathrm{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}} = \mathrm{tr}\,|\rho^{1/2}\sigma^{1/2}|,$$

where $|A| := (AA^\dagger)^{1/2}$ is a positive part in the polar decomposition of A. Although it is not a metric on D, the fidelity represents a closeness of quantum states. Furthermore, it does give rise to a useful metric like the *Bures metric* $B(\rho, \sigma) := \sqrt{2(1 - F(\rho, \sigma))}$ or *Bures angle* $A(\rho, \sigma) := \cos^{-1} F(\rho, \sigma)$.

We discuss the relation between relative entropy and fidelity modifying Theorem 5.6 and Remark 5.7 in [4].

REMARK 4.2. Let ρ and σ be invertible density matrices. From the proof of Theorem 5.6 in [4] we have

$$F(\rho, \sigma) \leq \mathrm{tr}\, H_t(\rho, \sigma),$$

where $H_t(\rho, \sigma) := \frac{1}{2}[\rho\#_t\sigma + \sigma\#_t\rho]$ is known as the *Heinz mean*. So

$$(4.7) \qquad \begin{aligned} 2(1 - F(\rho, \sigma)) &\geq [1 - \mathrm{tr}(\rho\#_t\sigma)] + [1 - \mathrm{tr}(\sigma\#_t\rho)] \\ &\geq 1 - \mathrm{tr}(\rho\#_t\sigma) \geq 1 - \mathrm{tr}(\rho^{1-t}\sigma^t). \end{aligned}$$

The last inequality follows from Lemma 4.1. This implies that

$$(4.8) \qquad tD_t(\rho|\sigma) \leq -t\,\mathrm{tr}\, T_t(\rho|\sigma) \leq 2(1 - F(\rho, \sigma)) = B(\rho, \sigma)^2.$$

By Proposition 4.6, [4], we obtain

(4.9) $B(\rho,\sigma)^2 \leq D_{1/2}(\rho|\sigma) \leq -\operatorname{tr} T_{1/2}(\rho|\sigma) \leq 2B(\rho,\sigma)^2.$

The above inequalities work for any density matrices ρ and σ due to Remark 2.3.

THEOREM 4.3. *Let ρ and σ be any density matrices on the tensor product $\mathcal{H} \otimes \mathcal{K}$ of Hilbert spaces. For any $t \in (0,1]$*

(4.10) $\operatorname{tr}_{\mathcal{K}} T_t(\rho|\sigma) \leq T_t(\rho^{\mathcal{H}}|\sigma^{\mathcal{H}}),$

and

(4.11) $t D_t(\rho^{\mathcal{H}}|\sigma^{\mathcal{H}}) \leq B(\rho,\sigma)^2.$

   Proof. By Theorem 3.3 we have

$$\operatorname{tr}_{\mathcal{K}}(\rho \#_t \sigma - \rho) = \operatorname{tr}_{\mathcal{K}}(\rho \#_t \sigma) - \rho^{\mathcal{H}} \leq \rho^{\mathcal{H}} \#_t \sigma^{\mathcal{H}} - \rho^{\mathcal{H}}.$$

The equation (4.10) is proved because $t > 0$. Since the partial trace is a trace-preserving map, taking the trace in the above inequality implies that

$$\operatorname{tr}(\rho \#_t \sigma) - 1 \leq \operatorname{tr}(\rho^{\mathcal{H}} \#_t \sigma^{\mathcal{H}}) - 1.$$

By the inequalities (4.7) we obtain

$$t D_t(\rho^{\mathcal{H}}|\sigma^{\mathcal{H}}) = 1 - \operatorname{tr}(\rho^{\mathcal{H}} \#_t \sigma^{\mathcal{H}}) \leq 1 - \operatorname{tr}(\rho \#_t \sigma) \leq 2(1 - F(\rho,\sigma)).$$

$\square$

   REMARK 4.4. The property (4.11) can be proved alternatively as following. From Theorem 9.6 in [6] we have

$$F(\rho,\sigma) \leq F(\mathcal{E}(\rho), \mathcal{E}(\sigma))$$

for any trace-preserving quantum operation $\mathcal{E}$. Taking $\mathcal{E} = \operatorname{tr}_{\mathcal{K}}$ we obtain

$$F(\rho,\sigma) \leq F(\rho^{\mathcal{H}}, \sigma^{\mathcal{H}}).$$

Then by the inequality (4.8)

$$t D_t(\rho^{\mathcal{H}}|\sigma^{\mathcal{H}}) \leq B(\rho^{\mathcal{H}}, \sigma^{\mathcal{H}})^2 \leq B(\rho,\sigma)^2.$$

   REMARK 4.5. The *quantum trace distance* between quantum states ρ and σ is defined by

(4.12) $D(\rho,\sigma) := \dfrac{1}{2} \operatorname{tr} |\rho - \sigma|.$

A good way to understand the quantum trace distance is to compute for the special case of qubit density matrices in the Bloch vector representation

$$\rho = \frac{1}{2}(I_2 + \mathbf{x} \cdot \overrightarrow{\sigma}), \ \sigma = \frac{1}{2}(I_2 + \mathbf{y} \cdot \overrightarrow{\sigma}),$$

where $\mathbf{x} = [x_1, x_2, x_3]$ and $\mathbf{y} = [y_1, y_2, y_3]$ are vectors in R^3 with magnitude less than or equal to 1, and $\overrightarrow{\sigma} = [\sigma_x, \sigma_y, \sigma_z]$ is a vector of Pauli matrices. The quantum trace distance between ρ and σ is

$$(4.13) \qquad D(\rho, \sigma) = \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|,$$

that is, one half of the Euclidean distance between Bloch vectors $\mathbf{x}$ and $\mathbf{y}$.

By the equation (9.110) in [6] it has been proved the relation between the quantum trace distance and fidelity: for any quantum states ρ and σ

$$(4.14) \qquad 1 - F(\rho, \sigma) \leq D(\rho, \sigma) \leq \sqrt{1 - F(\rho, \sigma)^2}.$$

Theorem 4.3 implies that

$$(4.15) \qquad tD_t(\rho^{\mathcal{H}} | \sigma^{\mathcal{H}}) \leq 2D(\rho, \sigma) = \operatorname{tr} |\rho - \sigma|.$$

References

[1] S. Abe, *Nonadditive generalization of the quantum Kullback-Leibler divergence for measuring the degree of purification*, Phys. Rev. A. **68** (2003), 032302.

[2] R. Bhatia, *Positive Definite Matrices*, Princeton Series in Applied Mathematics, Princeton, NJ, 2007.

[3] S. Furuichi, K. Yanagi, and K. Kuriyama, *Fundamental properties of Tsallis relative entropy*, J. Math. Phys. **45** (2004), 4868-4877.

[4] S. Kim, *Operator entropy and fidelity associated with the geometric mean*, Linear Algebra Appl. **438** (2013), 2475-2483.

[5] J. Lawson and Y. Lim, *Metric convexity of symmetric cones*, Osaka J. Math., **44** (2007), 795-816.

[6] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, 2010.

[7] K. Yanagi, K. Kuriyama, and S. Furuichi, *Generalized Shannon inequalities based on Tsallis relative operator entropy*, Linear Algebra Appl. **394** (2005), 109-118.

*

Department of Mathematics
Chungbuk National University
Cheongju 28644, Republic of Korea
E-mail: skim@chungbuk.ac.kr