

# METRICS INDUCED BY CERTAIN HILBERT-SCHMIDT FIDELITIES ON POSITIVE SEMI-DEFINITE MATRICES

VU THE KHOI AND HO MINH TOAN

ABSTRACT. Motivated by measuring the *degree of similarity* of a pair of quantum states (density matrices), we consider the metric property of the modified Bures angles and modified Bures distances of symmetric functions which are extensions of some fidelity measures on the spaces  $\mathcal{P}$  of nonzero positive semi-definite matrices. We use the positive semi-definiteness of the Gram-type matrices to characterize the metric property of the modified Bures angles. As a consequence, we can show that the modified Bures angles induced by the geometric mean, harmonic mean, minimum and maximum of two positive numbers are metrics on  $\mathcal{P}$ . In addition, we can also show that the metric property of the modified Bures angles is stronger than that of the modified Bures distances.

## 1. INTRODUCTION

Fidelity is a useful concept in quantum information science. A fidelity measure is widely used as a measure of the *degree of similarity* of a pair of quantum states (density matrices). Recently, fidelity measure has been applied to study entanglement quantification, etc. A nice survey of this topic can be found in [1, 2] and the references therein.

If  $\mathcal{F}$  is a fidelity measure, we may expect that a metric can be constructed via some functionals of  $\mathcal{F}$ . Moreover, we may also expect to study the metric property not only on the quantum state space (the set of density matrices), but also on the space of positive semi-definite matrices Bhatia et al. [6]. The metric property of the modified Bures angle (denoted by  $\arccos \sqrt{\mathcal{F}}$ ), of the modified Bures distance ( $\sqrt{1 - \sqrt{\mathcal{F}}}$ ) and of the modified Bures sine distance ( $\sqrt{1 - \mathcal{F}}$ ) are studied and summarized in [1, Table 6]. Motivated by studying metric properties for some functionals which are considered but still undetermined in [1], we consider that

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problem for a class of real-valued symmetric functions defined on  $\mathcal{P} \times \mathcal{P}$ , where  $\mathcal{P}$  is the space of nonzero positive semi-definite matrices. Such the functions may be extensions of some fidelity measures on the quantum state spaces. This class includes the well-known fidelity measures such as  $\mathcal{F}_{\text{II}}, \mathcal{F}_{\text{AM}}, \mathcal{F}_{\text{GM}}$ , etc. (see [1]). Precisely, given a real-valued, symmetric and nonnegative function  $f$  on  $(\mathbb{R}^+)^2$ , we consider the function  $\mathcal{F}_f$  defined on  $\mathcal{P} \times \mathcal{P}$  as below:

$$\mathcal{F}_f(A, B) = \frac{\text{Tr}(AB)}{\sqrt{\text{Tr}(A^2)\text{Tr}(B^2)}} f(\text{Tr}(A^2), \text{Tr}(B^2)),$$

for every pair of nonzero positive semi-definite matrices of the same size  $A, B$ . These fidelities measures are called *Hilbert-Schmidt fidelities*, see [1, 2.6]

The first Jozsa's axioms **J1a)** and **J1b)** state that the values of a fidelity functional at a pair of positive semi-definite of the same size  $(A, B)$  must be real numbers in  $[0, 1]$  and equal to 1 if and only if  $A = B$ . The second Jozsa's axiom **J2)** is the symmetric property. Hence, these axioms ensure that the modified Bures angel  $\arccos \mathcal{F}(A, B)$  is well-defined, symmetric, nonnegative and equal to zero if and only if  $A = B$ . A real valued function  $d$  defined on  $X \times X$  is said to satisfy *the triangle inequality on  $X$*  if  $d(x, y) \leq d(x, z) + d(z, y)$  for every  $x, y, z$  in  $X$ . The difficult step which proves such a function  $d$  to be a metric on  $X$  is to check the triangle inequality. Therefore, we pay attention to the triangle inequality of the modified Bures angles  $\arccos \mathcal{F}$  and of the modified Bures distance  $\sqrt{1 - \mathcal{F}}$ , where  $\mathcal{F}$  is defined on  $\mathcal{P}$ .

In this work, we consider the metric property of the modified Bures angle  $\arccos \mathcal{F}_f$ . We will show that the modified Bures angle  $\arccos \mathcal{F}(A, B)$  satisfies the triangle inequality on  $\mathcal{P}$  if and only if the Gram-type matrix of  $\mathcal{F}$  is positive semi-definite on  $\mathcal{P}$ . As a consequence, if  $f$  is the ratio of the geometric mean and maximum mean of two positive numbers then the modified Bures angle  $\arccos \mathcal{F}_f$  is a metric on  $\mathcal{P}$ . Another application of the above equivalent conditions is to prove the triangle inequality of  $\arccos \mathcal{F}_{\text{GM}}$  on  $\mathcal{P}$ . Precisely, if  $f$  is the constant 1 then  $\mathcal{F}_1 = \mathcal{F}_{\text{GM}}$  and the modified Bures angle  $\arccos \mathcal{F}_{\text{GM}}$  is a metric on the quantum state space, *not* a metric on  $\mathcal{P}$ , even it satisfies the triangle inequality on  $\mathcal{P}$ , since  $\mathcal{F}_{\text{GM}}(A, B) = 1$  if and only if  $\{A, B\}$  is linearly dependent. In other cases, if  $f = \frac{m}{\nabla}$ , where  $\nabla$  is the arithmetic mean of two positive numbers and  $m(x, y)$  is a mean which is a member of  $\{\min\{x, y\}, \sqrt{xy}, x!y\}$  then we can show that  $\arccos \mathcal{F}_f$  is a metric on  $\mathcal{P}$ . In

addition, we also show that if the modified Bures angle  $\arccos \mathcal{F}$  is a metric, so is  $\sqrt{1 - \mathcal{F}}$ .

The paper is organized as follow: In section 2, we recall some notations and results obtained in Liang at el. [1]. Section 3 includes the characterization of metric property of the modified Bures angle  $\arccos \mathcal{F}_f$  and its applications to some nice cases where  $f$  are ratios of means of two positive numbers.

## 2. PRELIMINARIES AND NOTATIONS

**Notations.** Let  $\mathbb{R}^+$  denote the set of positive real number,  $M$  the algebra of  $n \times n$  matrices with complex coefficients,  $\mathcal{P}$  the space of nonzero positive semi-definite matrices.

The function  $\arccos(\mathcal{F})$  ( $\sqrt{1 - \mathcal{F}}$ ) is called the *modified Bures angle* of  $\sqrt{\mathcal{F}}$  (the *modified Bures distance* of  $\sqrt{\mathcal{F}}$ , respectively), see Liang at el. [1].

We recall the notations of some well-known fidelities as follows Liang at el. [1].

$$(2.1) \quad \mathcal{F}_{\text{II}}(A, B) = \frac{\text{Tr}(AB)}{\max\{\text{Tr}A^2, \text{Tr}B^2\}}$$

$$(2.2) \quad \mathcal{F}_{\text{AM}}(A, B) = \frac{2\text{Tr}(AB)}{\text{Tr}(A^2) + \text{Tr}(B^2)}$$

$$(2.3) \quad \mathcal{F}_{\text{GM}}(A, B) = \frac{\text{Tr}(AB)}{\sqrt{\text{Tr}(A^2)}\sqrt{\text{Tr}(B^2)}}$$

where  $A, B$  are nonzero positive semi-definite matrices of the same size. In [1], the fidelity defined by (2.1) is denoted by  $\mathcal{F}_2$ . To avoid confusion, in this paper, we use the notation  $\mathcal{F}_{\text{II}}$  instead.

A large class of functions which are generalizations of the fidelity measures above can be defined as follows. Let  $f$  be an arbitrary symmetric, non-vanishing function on  $\mathbb{R}^+ \times \mathbb{R}^+$ . One can define a function on  $\mathcal{P} \times \mathcal{P}$  :

$$(2.4) \quad \begin{aligned} \mathcal{F}_f(A, B) &= \text{Tr}\left(\frac{A}{\sqrt{\text{Tr}(A^2)}} \frac{B}{\sqrt{\text{Tr}(B^2)}}\right) f(\text{Tr}(A^2), \text{Tr}(B^2)) \\ &= \mathcal{F}_{\text{GM}}(A, B) f(\text{Tr}(A^2), \text{Tr}(B^2)). \end{aligned}$$

Note that the notation  $\mathcal{F}_f$  in [1] means the function  $\mathcal{F}_{\frac{\#}{f}}$  in the sense (2.4), where  $x\#y = \sqrt{xy}$ .

*Remark.* Let  $\mathcal{F}_f$  be a function defined by (2.4).

- If  $f(x, y) = 2\frac{\sqrt{xy}}{x+y}$ , then

$$\mathcal{F}_f(A, B) = \frac{2\text{Tr}(AB)}{\text{Tr}(A^2) + \text{Tr}(B^2)} = \mathcal{F}_{\text{AM}}(A, B).$$

- If  $f(x, y) = 1$ , a constant function then

$$\mathcal{F}_f(A, B) = \frac{\text{Tr}(AB)}{\sqrt{\text{Tr}(A^2)}\sqrt{\text{Tr}(B^2)}} = \mathcal{F}_{\text{GM}}(A, B).$$

- If  $f(x, y) = \frac{\sqrt{xy}}{\max\{x, y\}}$ , then

$$\mathcal{F}_f(A, B) = \frac{\text{Tr}(AB)}{\max\{\text{Tr}(A^2), \text{Tr}(B^2)\}} = \mathcal{F}_{\text{II}}(A, B).$$

We can recall here the results about metric property on the quantum state space for the functionals of the fidelity as in [1, Table 6]:

- Neither  $\arccos \sqrt{\mathcal{F}}$  nor  $\sqrt{1 - \sqrt{\mathcal{F}}}$  are metrics on the quantum state space if  $\mathcal{F}$  is a member in  $\{\mathcal{F}_{\text{II}}, \mathcal{F}_{\text{AM}}, \mathcal{F}_{\text{GM}}\}$ .
- The function  $\sqrt{1 - \sqrt{\mathcal{F}}}$  is a metric if  $\mathcal{F}$  is a member of  $\{\mathcal{F}_{\text{II}}, \mathcal{F}_{\text{GM}}\}$  and is still undetermined if  $\mathcal{F} = \mathcal{F}_{\text{AM}}$ .

In this paper, we consider metric properties of the functions  $\mathcal{F}_f$  on the space of nonzero positive semi-definite matrices  $\mathcal{P}$  and similarly we can also obtain such the results on any subspace of  $\mathcal{P}$ .

### 3. RESULTS

Fidelity were introduced in Jozsa [3] and is a mathematical prescription for the quantification of the degree of similarity of a pair of quantum states. The metric property of fidelity measures is an important problem in the study of fidelity. Motivated by this problem in quantum theory, in this note, we study the metric property of the functions  $\mathcal{F}$  defined on  $\mathcal{P} \times \mathcal{P}$  which should satisfy the *Jozsa's axioms*.

**Definition 3.1.** Let  $X$  be a nonempty set. A real-valued non-vanishing function  $F$  defined on  $X \times X$  is said to satisfy the *Jozsa's axioms* on  $X$  if for every  $x, y$  in  $X$ , the following conditions hold:

**J1a)**  $0 \leq F(x, y) \leq 1$ .

**J1b)**  $F(x, y) = 1$  if and only if  $x = y$ .

**J2)**  $F(x, y) = F(y, x)$ .

Note that the list of Jozsa's axioms in [1] includes some more axioms. However, in this work, we only pay attention to the ones which are useful to the metric property.

For an arbitrary positive number  $\alpha$ , if  $\mathcal{F}$  satisfies the Jozsa's axioms, then the function  $F^\alpha$  given by

$$F^\alpha(x, y) := (F(x, y))^\alpha \quad x, y \in X$$

also satisfies the Jozsa's axioms.

**3.1. Modified Bures angle and modified Bures distance.** The notations of the modified Bures angle and distance were written in [1]. Let  $\mathcal{F}$  be a function defined on  $\mathcal{P} \times \mathcal{P}$  which satisfies the Jozsa's axioms **J1a**), **J1b**), **J2**). In this subsection, we will show that the metric property of the modified Bures angle  $\arccos \mathcal{F}$  is stronger than that of the modified Bures distance  $\sqrt{1 - \mathcal{F}}$ .

**Lemma 3.2.** *Let  $d$  be a metric on  $X$  and  $f$  be a nonnegative, increasing and sub-additive function on an interval  $I = [0, m] \supset \text{Im}(d)$ , where*

$$\text{Im}(d) = \{d(x, y) \mid x, y \in X\}.$$

*Then  $\rho := f \circ d$  is a metric on  $X$  provided that  $f(t) = 0$  holds only at  $t = 0$ .*

A sub-additive function  $f$  on  $I$  we means that  $f$  satisfies  $f(a + b) \leq f(a) + f(b)$  for  $a, b \in I$ .

*Proof.* The proof the the lemma above is straightforward. □

*Remark.* If  $f$  is a concave function on  $I = [0, m]$  and  $f(0) = 0$  then  $f$  must be sub-additive.

**Corollary 3.3.** *Let  $\mathcal{F}$  be a function defined on  $\mathcal{P} \times \mathcal{P}$ . which satisfies the Jozsa's axioms **J1a**), **J1b**) **J2**). If the modified Bures angle  $\arccos \mathcal{F}$  is a metric on  $\mathcal{P}$ , so is  $\sqrt{1 - \mathcal{F}}$ .*

*Proof.* Let's consider the function  $f(t) := \sqrt{1 - \cos t}$  on  $[0, \pi/2]$ . It is straightforward to show that  $f(t)$  is nonnegative, increasing and concave on  $[0, \pi/2]$ . By the above remark and Lemma 3.2,  $\sigma_{\mathcal{F}} = f \circ d_{\mathcal{F}}$  is a metric. □

### 3.2. Metric property of the modified Bures angle.

*Remark.* Let  $F$  be a real valued function which satisfies the *Jozsa's axioms* on  $X$ . Then the *modified Bures angle*  $\arccos F$  satisfies the first two axioms of a metric, i.e.,

- (i)  $\arccos F(x, y) \geq 0$  for every  $x, y \in X$  and  $\arccos F(x, y) = 0$  if and only if  $x = y$ .
- (ii)  $\arccos F(x, y) = \arccos F(y, x)$  for every  $x, y \in X$ .

Thanks to this remark, to study the metric property of  $\arccos F(x, y)$  on  $X$ , we only consider the triangle inequality of  $\arccos F(x, y)$ , i.e.,

$$\arccos F(x, y) \leq \arccos F(x, z) + \arccos F(z, y), \quad \forall x, y, z \in X.$$

Let  $\mathcal{F}$  and  $f$  be a real valued function on  $\mathcal{P} \times \mathcal{P}$  and  $\mathbb{R}^+ \times \mathbb{R}^+$ , respectively.  $G(\mathcal{F}) = G(\mathcal{F})(A, B, C)$  and  $G_f = G_f(x, y, z)$  denote the so called *Gram-type matrices* of  $\mathcal{F}$  and  $f$ , respectively and are defined as follows.

$$G(\mathcal{F}) = \begin{pmatrix} \mathcal{F}(A, A) & \mathcal{F}(A, B) & \mathcal{F}(A, C) \\ \mathcal{F}(B, A) & \mathcal{F}(B, B) & \mathcal{F}(B, C) \\ \mathcal{F}(C, A) & \mathcal{F}(C, B) & \mathcal{F}(C, C) \end{pmatrix}, \quad G_f = \begin{pmatrix} f(x, x) & f(x, y) & f(x, z) \\ f(y, x) & f(y, y) & f(y, z) \\ f(z, x) & f(z, y) & f(z, z) \end{pmatrix}$$

for matrices  $A, B, C$  in  $\mathcal{P}$  and for real numbers  $x, y, z$  in  $\mathbb{R}^+$ . Set

$$r(\mathcal{F}) := \{(\mathcal{F}(A, B), \mathcal{F}(B, C), \mathcal{F}(C, A)) \mid A, B, C \in \mathcal{P}\} \subset \mathbb{R}^3.$$

**Proposition 3.4.** *Let  $\mathcal{F}$  be a function which satisfies the Jozsa's axioms **J1a**), **J1b**), **J2**) on  $\mathcal{P}$ . Then the following statements are equivalent.*

- (i)  $d_{\mathcal{F}} = \arccos(\mathcal{F})$  is a metric on  $\mathcal{P}$ .
- (ii) The Gram-type matrix  $G(\mathcal{F})$  of  $\mathcal{F}$  is positive semi-definite for every positive semidefinite matrices  $A, B, C \in \mathcal{P}$ .
- (iii)

$$S(x, y, z) := x^2 + y^2 + z^2 - 2xyz - 1 \leq 0, \quad \forall (x, y, z) \in r(\mathcal{F}).$$

*Proof.* The equivalence of (ii) and (iii) follows from the fact that  $S(x, y, z) = \det G(\mathcal{F})$  and the hypothesis that  $\mathcal{F}$  satisfies the axiom **J1a**).

(i)  $\Leftrightarrow$  (ii). For every positive semi-definite matrices  $A, B, C$ , in  $\mathcal{P}$ , let  $x = \mathcal{F}(A, B)$ ,  $y = \mathcal{F}(B, C)$  and  $z = \mathcal{F}(A, C)$ . We have

$$S(x, y, z) \leq 0 \Leftrightarrow z^2 - 2xyz + (y^2 + x^2 - 1) \leq 0.$$

Consider  $S(x, y, z)$  as a polynomial of degree 2 in  $z$ , the last inequality above is equivalent to

$$(3.1) \quad xy - (1-x)(1-y) \leq z \leq xy + (1-x)(1-y).$$

It turns out that this inequality is equivalent to

$$(3.2) \quad |\arccos x - \arccos y| \leq \arccos z \leq \arccos x + \arccos y.$$

This inequality is equivalent to the triangle inequality of  $d_{\mathcal{F}}$ .  $\square$

**Corollary 3.5.** *Given a function  $\mathcal{F}$  satisfying the Jozsa's axioms **J1a**), **J1b**), **J2**) on  $\mathcal{P}$ . If the modified Bures angle  $\arccos \mathcal{F}$  is a metric on  $\mathcal{P}$ , so is  $\arccos(\mathcal{F}^m)$  for every positive integer  $m$ .*

*Proof.* By Corollary 3.3, it is enough to show that  $\arccos(\mathcal{F}^m)$  is a metric. The Gram-type matrix  $G(\mathcal{F}^m)$  of  $\mathcal{F}^m$  can be decompsed as Schur product of  $G(\mathcal{F})$  :

$$G(\mathcal{F}^2) = G(\mathcal{F}) \circ G(\mathcal{F}), \quad G(\mathcal{F}^3) = G(\mathcal{F}^2) \circ G(\mathcal{F}) \circ G(\mathcal{F}), \dots$$

Hence, by Schur product Theorem,  $G(\mathcal{F}^m)$  is positive semi-definite. Then the statement follows Proposition 3.4.  $\square$

By the Cauchy Schwarz inequality (with the Frobenius inner product), we have

$$|\mathrm{Tr}(AB)| \leq \sqrt{\mathrm{Tr}(A^2)} \sqrt{\mathrm{Tr}(B^2)}$$

for every  $A, B$  in  $\mathcal{P}$ . Hence,  $0 \leq \mathcal{F}_{\mathrm{GM}}(A, B) \leq 1$ . Therefore, the function  $\arccos \mathcal{F}_{\mathrm{GM}}(A, B)$  is well-defined. The equality of the Cauchy Schwarz inequality above holds if and only if  $A = \lambda B$  for some positive number  $\lambda$ . If we assume further that  $A, B$  are density matrices, then  $\mathcal{F}_{\mathrm{GM}}(A, B) = 1$  if and only if  $A = B$ .

**Lemma 3.6.** *Let  $\mathcal{F}_{\mathrm{GM}}$  be the function defined by the formula (2.3). Then the Gram-type matrix of  $\mathcal{F}_{\mathrm{GM}}$  is positive semi-definite on  $\mathcal{P}$ . As a consequence, the modified Bures angle  $\arccos \mathcal{F}_{\mathrm{GM}}$  satisfies the triangle inequality on  $\mathcal{P}$ .*

The fidelity  $\mathcal{F}_{\mathrm{GM}}$  satisfies the axiom **J1b**) on the space of density matrices but not on  $\mathcal{P}$ . Hence, according to the above lemma,  $\arccos \mathcal{F}_{\mathrm{GM}}$  is a metric on the quantum state space, but not on  $\mathcal{P}$ . Note also that the modified Bures angle  $\arccos \sqrt{\mathcal{F}_{\mathrm{GM}}}$  is *not* a metric (it does not satisfy the triangle inequality) on the quantum state space, see [1, Table 6].

*Proof.* For any nonzero positive semi-definite matrices of the same size  $A, B, C$  and let  $v(A) = \frac{A}{\sqrt{\text{Tr}(A^2)}}$ ,  $v(B) = \frac{B}{\sqrt{\text{Tr}(B^2)}}$  and  $v(C) = \frac{C}{\sqrt{\text{Tr}(C^2)}}$  be the unit vectors in the space  $M_n$  with the Frobenius inner product  $\langle A, B \rangle = \text{Tr}(B^*A)$ . Then the Gram-type matrix of  $\mathcal{F}_{\text{GM}}$  is

$$G(\mathcal{F}_{\text{GM}}) = \begin{pmatrix} \langle v(A), v(A) \rangle & \langle v(A), v(B) \rangle & \langle v(A), v(C) \rangle \\ \langle v(B), v(A) \rangle & \langle v(B), v(B) \rangle & \langle v(B), v(C) \rangle \\ \langle v(C), v(A) \rangle & \langle v(C), v(B) \rangle & \langle v(C), v(C) \rangle \end{pmatrix}.$$

Hence,  $G(\mathcal{F}_{\text{GM}})$  is positive semi-definite. As in the proof of Proposition 3.4,  $\arccos \mathcal{F}_{\text{GM}}$  satisfies the triangle inequality on  $\mathcal{P}$ .  $\square$

**Theorem 3.7.** *Let  $f$  be a continuous function which satisfies the Jozsa's axioms **J1a**), **J1b**) and **J2**) on  $\mathbb{R}^+$ . Then the following statements hold.*

- (i) *The function  $\mathcal{F}_f(A, B)$  defined by 2.4 satisfies the Jozsas axioms **J1a**), **J1b**), **J2**) on  $\mathcal{P}$ .*
- (ii) *The modified Bures angle  $\arccos \mathcal{F}_f$  is a unitarily invariant metric on  $\mathcal{P}$  provided that the Gram-type matrix*

$$G_f = \begin{pmatrix} 1 & f(x, y) & f(x, z) \\ f(x, y) & 1 & f(y, z) \\ f(x, z) & f(y, z) & 1 \end{pmatrix}$$

*is positive semi-definite for every  $x, y, z \in (0, 1]$ .*

*Proof.* (i).

**J1a)** Combine (2.4),  $\mathcal{F}_{\text{GM}}(A, B) \in [0, 1]$  and  $f(x, y) \in [0, 1]$ , we get  $\mathcal{F}_f(A, B) \in [0, 1]$ .

**J1b)** Since  $\mathcal{F}_{\text{GM}}(A, B) \leq 1$ ,  $f(x, y) \leq 1$  and the equality (2.4), we have

$$\mathcal{F}_f(A, B) = 1 \Leftrightarrow \mathcal{F}_{\text{GM}}(A, B) = 1 \text{ and } f(\text{Tr}(A^2), \text{Tr}(B^2)) = 1.$$

Since  $f(x, y) = 1$  if and only if  $x = y$ , we get that  $\text{Tr}(A^2) = \text{Tr}(B^2)$ . In addition,  $\mathcal{F}_{\text{GM}}(A, B) = 1$  if and only if  $A = cB$  for some constant  $c > 0$ . Hence,  $A$  must be equal to  $B$ .

**J2)** The symmetry of  $\mathcal{F}_f$  follows from that of  $\mathcal{F}_{\text{GM}}$  and of  $f$ .



(ii) By Proposition 3.4, the modified Bures angle  $\arccos \mathcal{F}_f$  is a metric if and only if the Gram-type matrix  $G(\mathcal{F}_f)$  is positive semi-definite. Since

$$\mathcal{F}_f(A, B) = \mathcal{F}_{\text{GM}}(A, B)f(\text{Tr}(A^2), \text{Tr}(B^2)),$$

we can write  $G(\mathcal{F}_f)$  as the Schur product:

$$G(\mathcal{F}_f) = G(\mathcal{F}_{\text{GM}}) \circ G_f.$$

The matrix  $G(\mathcal{F}_{\text{GM}})$  is positive semi-definite by Lemma 3.6, while  $G_f$  is positive semi-definite by the hypothesis. These together with Schur's product Theorem imply that  $G(\mathcal{F}_f)$  is positive semi-definite.  $\square$

*Note:* In Theorem 3.7,  $\arccos \mathcal{F}_f$  is a metric on *the quantum state space* even when we remove the condition ' $f(x, y) = 1 \Rightarrow x = y$ ' in the hypothesis of the theorem.

*Example.* If  $f(x, y)$  is a real-valued positive definite kernel, then the Gram-type matrix  $G_f$  is positive semi-definite. In particular, if  $g(x)$  is an even nonnegative function on  $\mathbb{R}$  then  $f(x, y) = \exp(-g(x - y))$  is a positive definite kernel. Furthermore,  $f(x, y)$  satisfies the Jozsa's axioms on  $\mathbb{R}^+$  provided that 0 is the unique zero point of  $g(x)$ . By Theorem 3.7,  $\arccos \mathcal{F}_f$  is a metric on  $\mathcal{P}$  and so is  $\sqrt{1 - \mathcal{F}_f}$ . We may find more interesting examples of positive definite functions/kernels in [7, 8].

**Corollary 3.8.** *The modified Bures angle  $\arccos \mathcal{F}_{\text{II}}$  is a metric on  $\mathcal{P}$ , where  $\mathcal{F}_{\text{II}}$  is defined by (2.1).*

*Note that neither  $\arccos \sqrt{\mathcal{F}_{\text{II}}}$  nor  $\sqrt{1 - \sqrt{\mathcal{F}_{\text{II}}}}$  are metrics, see [1, Table 6].*

*Proof.* Let  $f(x, y) = \frac{\sqrt{xy}}{\max\{x, y\}}$  then  $f$  satisfies the Jozsa's axioms on  $\mathbb{R}^+$  and by Remark 2,

$$\mathcal{F}_f(A, B) = \mathcal{F}_{\text{II}}(A, B).$$

Let's consider the Gram-type matrix

$$G_f = \begin{pmatrix} 1 & f(x, y) & f(x, z) \\ f(y, x) & 1 & f(y, z) \\ f(z, x) & f(z, y) & 1 \end{pmatrix},$$

Denote by  $a = f(x, y)$ ,  $b = f(y, z)$  and  $c = f(z, x)$ . Without loss of generality, we can assume that  $0 \leq x \leq y \leq z \leq 1$ , we have

$$a = f(x, y) = \frac{\sqrt{x}}{\sqrt{y}}, \quad b = f(y, z) = \frac{\sqrt{y}}{\sqrt{z}}, \quad c = f(z, x) = \frac{\sqrt{x}}{\sqrt{z}}.$$

Then

$$\det G_f = 1 + 2abc - a^2 - b^2 - c^2 = 1 + \frac{x}{z} - \frac{x}{y} - \frac{y}{z} \geq 0,$$

since  $\frac{x}{y} \leq \frac{x+z-y}{z}$ . Therefore,  $G_f$  is positive semi-definite. By Theorem 3.7, the modified Bures angle  $\arccos \mathcal{F}_{\text{II}}$  is a metric on  $\mathcal{P}$ .  $\square$

### 3.3. Fidelity measures induced by means.

3.3.1. *Means of positive numbers.* A *mean* of positive numbers is a function  $m : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}^+$  which satisfies the following conditions:

- (i)  $m(x, x) = x$  for every positive number  $x$ .
- (ii)  $m(x, y) = m(y, x)$  for every positive numbers  $x, y$ .
- (iii) If  $x < y$  then  $x < m(x, y) < y$ .
- (iv) If  $x < x'$  and  $y < y'$  then  $m(x, y) < m(x', y')$ .
- (v)  $m(x, y)$  is continuous.

A mean is said to be *homogeneous* if

- (vi)  $m(tx, ty) = tm(x, y)$  for every positive numbers  $x, y, t$ .

See [4, 5] for more details. Thanks to the homogeneity, a two variable function  $m$  can be reduced to a single variable function  $m_1$  such that

$$m(x, y) = xm_1\left(\frac{y}{x}\right) = ym_1\left(\frac{x}{y}\right).$$

Furthermore, a homogeneous mean  $m$  above is uniquely described by such a function  $m_1$  satisfying the following properties:

- (i)'  $m_1(1) = 1$ .
- (ii)'  $tm_1(t^{-1}) = m_1(t)$ .
- (iii)'  $m_1(t) > 1$  if  $t > 1$  and  $m_1(t) < 1$  if  $0 < t < 1$ .
- (iv)'  $m_1$  is monotone increasing.
- (v)'  $m_1$  is continuous.

Conversely, each function  $f$  satisfying the properties above gives a mean  $m(x, y) = xm_1\left(\frac{y}{x}\right)$ .

The following means are the most well-known ones:

- (1) The geometric mean  $x \sharp y := \sqrt{xy}$  whose corresponding function  $\sqrt{t}$ .
- (2) The arithmetic mean  $x \nabla y := (x+y)/2$  whose corresponding function  $(t+1)/2$ .

- (3) The harmonic mean  $x!y := 2(x^{-1} + y^{-1})^{-1}$  whose corresponding function  $2t/(1+t)$ .

**Proposition 3.9.** *Let  $m \leq \sharp$  be a homogeneous mean (of two positive numbers). Denote by  $\mathcal{F}_{\frac{m}{\nabla}}$  the function defined by the formula (2.4).*

- (i) *The function  $\mathcal{F}_{\frac{m}{\nabla}}$  satisfies the Jozsa's axioms on  $\mathcal{P}$ .*  
(ii) *The modified Bures distance  $\mathcal{F}_{\frac{m}{\nabla}}$  is a metric provided that*

$$(3.3) \quad \frac{1}{4} + 4 \frac{m_1(s)}{1+s} \frac{m_1(t)}{1+t} \frac{m_1(st)}{1+st} \geq \left( \frac{m_1(s)}{1+s} \right)^2 + \left( \frac{m_1(t)}{1+t} \right)^2 + \left( \frac{m_1(st)}{1+st} \right)^2$$

*holds true for all positive numbers  $s, t$ , where  $m_1(x) = m(1, x)$ .*

*Proof.* Let  $f(x, y) = \frac{2m(x, y)}{x+y}$  be a real-valued function on  $\mathbb{R}^+ \times \mathbb{R}^+$ . Then  $\mathcal{F}_{\frac{m}{\nabla}} = \mathcal{F}_f$  defined by (2.4).

(i) Since  $m(x, y) = m(y, x)$ ,  $f(x, y)$  is a nonnegative symmetric function on  $(\mathbb{R}^+)^2$ . As  $m(x, y) \leq x\nabla y$ , we have  $0 \leq f(x, y) \leq 1$ . Clearly  $f(x, x) = 1$  because  $m(x, x) = x = x\nabla x$ . Suppose that  $f(x, y) = 1$ . Equivalently,  $m(x, y) = x\nabla y$ . Since  $m \leq \sharp$ , we have  $\sqrt{xy} = x\nabla y$ . Hence,  $x = y$ . Therefore,  $f$  satisfies the Jozsa's axioms on  $\mathbb{R}^+$ .

Thus, by Theorem 3.7,  $\mathcal{F}_{\frac{m}{\nabla}}$  is a fidelity measure satisfying **J1a**), **J1b**), **J2**).

(ii) By Theorem 3.7,  $\arccos \mathcal{F}_{\frac{m}{\nabla}}$  is a metric if the Gram-type matrix of  $f = \frac{m}{\nabla}$

$$G_f = \begin{pmatrix} 1 & f(x, y) & f(x, z) \\ f(x, y) & 1 & f(y, z) \\ f(x, z) & f(y, z) & 1 \end{pmatrix}$$

is positive semi-definite. This is equivalent to  $\det G_f \geq 0$ , i.e.,

$$(3.4) \quad 1 + 2f(x, y)f(y, z)f(z, x) \geq f^2(x, y) + f^2(y, z) + f^2(z, x), \quad \forall x, y, z \in (0, 1].$$

We have

$$f(x, y) = \frac{2m(x, y)}{x+y} = \frac{2m_1(s)}{1+s}, \quad s = \frac{x}{y}.$$

Similarly,  $f(y, z) = \frac{2m_1(t)}{1+t}$  with  $t = \frac{y}{z}$  and  $f(x, z) = \frac{2m_1(st)}{1+st}$ . Substituting these identities into the inequality (3.4), we get (3.3).  $\square$

**Corollary 3.10.** *The modified Bures angle  $\arccos \mathcal{F}_{AM}$  is a metric on  $\mathcal{P}$ , where  $\mathcal{F}_{AM}$  is defined by (2.2).*

*Proof.* Let  $f(x, y) = \frac{2\sqrt{xy}}{x+y}$  be a function on  $(\mathbb{R}^+)^2$ . By definition, we have

$$\mathcal{F}_{\text{AM}}(A, B) = \mathcal{F}_{\text{GM}}(A, B) \frac{2\sqrt{xy}}{x+y} = \mathcal{F}_f(A, B),$$

where  $x = \text{Tr}(A^2), y = \text{Tr}(B^2)$ . By Proposition 3.9, it is sufficient to show that

$$(3.5) \quad \frac{1}{4} + 4 \frac{m_1(s)}{1+s} \frac{m_1(t)}{1+t} \frac{m_1(st)}{1+st} \geq \left( \frac{m_1(s)}{1+s} \right)^2 + \left( \frac{m_1(t)}{1+t} \right)^2 + \left( \frac{m_1(st)}{1+st} \right)^2,$$

where  $m_1(x) = \sqrt{x}$ . Substitute  $m_1(x) = \sqrt{x}$  into the inequality (3.5), we get

$$1 + 2 \frac{2\sqrt{s}}{s+1} \frac{2\sqrt{t}}{t+1} \frac{2\sqrt{st}}{st+1} - 4 \left[ \frac{s}{(s+1)^2} + \frac{t}{(t+1)^2} + \frac{st}{(st+1)^2} \right] \geq 0.$$

This inequality is equivalent to

$$\begin{aligned} & s^4 t^4 + 2s^4 t^3 + 2s^3 t^4 + s^4 t^2 + 22s^3 t^3 + s^2 t^4 + 22s^3 s^2 + 22s^2 t^3 + 2s^3 t + 30s^2 t^2 \\ & + 2st^3 + 14s^2 t + 14st^2 + s^2 + t^2 + 10st - 2s - 2t + 1 \geq 0. \end{aligned}$$

This inequality holds true for all  $s \geq 0, t \geq 0$ , since

$$s^2 + t^2 + 10st - 2s - 2t + 1 = (s + t - 1)^2 + 8st \geq 0, \quad \forall s, t \geq 0.$$

□

**Corollary 3.11.** *Let  $f(x, y)$  be a symmetric function defined on  $(\mathbb{R}^+)^2$  and  $\mathcal{F}$  by*

$$\mathcal{F}(A, B) = \frac{2\text{Tr}(AB)}{\text{Tr}(A^2) + \text{Tr}(B^2)} f(\text{Tr}A^2, \text{Tr}B^2)$$

for every pair of the same size matrices  $A, B \in \mathcal{P}$ . Suppose that  $0 \leq f(x, y) \leq 1$ ,  $f(x, y) = 1$  for every positive numbers  $x, y$  and the Gram-type matrix  $G_f$  is positive definite on  $\mathbb{R}^+$ . Then  $\arccos \mathcal{F}$  is a metric on  $\mathcal{P}$ .

*Proof.* Since  $\mathcal{F}(A, B) = \mathcal{F}_{\text{AM}}(A, B) f(\text{Tr}A^2, \text{Tr}B^2)$ , and  $\mathcal{F}_{\text{AM}}$  satisfies the Jozsa's axioms **J1a**), **J1b**) and **J2**),  $\arccos \mathcal{F}(A, B)$  is nonnegative, symmetric and is equal to zero if and only if  $A = B$ . Since  $\arccos \mathcal{F}_{\text{AM}}$  is a metric on  $\mathcal{P}$  and by Theorem 3.7, the Gram-type matrix  $G(\mathcal{F}_{\text{AM}})$  is positive semi-definite. Thus,  $G(\mathcal{F}) = G(\mathcal{F}_{\text{AM}}) \circ G_f$  is positive semi-definite by the hypothesis, Corollary 3.10 and Schur product Theorem. Now, apply Theorem 3.7 again, we get the proof. □

**Corollary 3.12.** *The modified Bures angle  $\arccos \mathcal{F}_{\frac{1}{\nabla}}$  is a metric on  $\mathcal{P}$ , where  $\frac{1}{\nabla}(x, y) = 2 \frac{xy}{x+y}$  is the ratio of the harmonic and arithmetic means.*

*Proof.* By definition, we have

$$\mathcal{F}_{\frac{1}{\sqrt{xy}}}(A, B) = \mathcal{F}_{\text{AM}}(A, B) \frac{x!y}{\sqrt{xy}},$$

where  $x = \text{Tr}(A^2), y = \text{Tr}(B^2)$ . By Corollary 3.11, it suffices to show that the Gram-type matrix  $G_f$  is positive semi-definite, where  $f(x, y) = \frac{x!y}{\sqrt{xy}}$ . We can write

$$f(x, y) = \frac{x!y}{\sqrt{xy}} = \frac{2}{\sqrt{xy}(x^{-1} + y^{-1})} = \frac{2\sqrt{s}}{1+s}, \quad \text{where } s = \frac{x}{y}.$$

Similarly,

$$f(y, z) = \frac{2\sqrt{t}}{1+t}, \quad f(x, z) = \frac{2\sqrt{st}}{1+st}, \quad \text{where } t = \frac{y}{z}.$$

The fact is that  $0 < \min\{x, y\} \leq x!y \leq \sqrt{xy} \leq \max\{x, y\}$ , so  $0 < f(x, y) \leq 1$ . Hence, the Gram-type matrix  $G_f$  of  $f$  is positive semi-definite (for all positive numbers  $s, t$ ) if and only if  $\det G_f \geq 0$ . Equivalently,

$$(3.6) \quad 1 + 2 \frac{2\sqrt{s}}{s+1} \frac{2\sqrt{t}}{t+1} \frac{2\sqrt{st}}{st+1} - 4 \left[ \frac{s}{(s+1)^2} + \frac{t}{(t+1)^2} + \frac{st}{(st+1)^2} \right] \geq 0 \quad \text{for } s, t > 0.$$

As the same argument in the proof of Corollary 3.10, the inequality (3.6) holds true for all positive numbers  $s, t$ .  $\square$

If we relax the condition (iii) in the definition of mean above by

$$(iii)'' \quad \text{If } x \leq y \text{ then } x \leq m(x, y) \leq y$$

then the function  $\max, \min$  are also means of two positive numbers. Actually, Proposition 3.9 still holds true for such a relaxed mean  $m$  provided that  $m$  can be written as  $m(x, y) = xm_1(y/x) = ym_1(x/y)$ .

**Corollary 3.13.** *Let  $\mathcal{F} = \mathcal{F}_f$  be a function defined by (2.4). If  $f(x, y) = \frac{2\min\{x, y\}}{x+y}$  then  $\arccos \mathcal{F}$  is a metric on  $\mathcal{P}$ .*

*Proof.* We can write

$$\mathcal{F}(A, B) = \mathcal{F}_{\text{AM}}(A, B)g(\text{Tr}A^2, \text{Tr}B^2),$$

where  $g(x, y) = \frac{\min\{x, y\}}{\sqrt{xy}}$ . Let  $x, y, z$  be arbitrary positive numbers, without loss of generality, we can assume that  $x \leq y \leq z$ . Then

$$g(x, y) = \frac{\sqrt{x}}{\sqrt{y}}, \quad g(x, z) = \frac{\sqrt{x}}{\sqrt{z}} \quad \& \quad g(y, z) = \frac{\sqrt{y}}{\sqrt{z}}.$$

Hence the Gram-type matrix  $G_g$  is positive semi-definite (as the same argument in the proof of Corollary 3.8). By Corollary 3.11,  $\arccos \mathcal{F}$  is a metric on  $\mathcal{P}$ .  $\square$

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INSTITUTE OF MATHEMATICS (VAST), 18 HOANG QUOC VIET, 10307, HANOI, VIETNAM  
*E-mail address:* vtkhoi@math.ac.vn

INSTITUTE OF MATHEMATICS (VAST), 18 HOANG QUOC VIET, 10307, HANOI, VIETNAM  
*E-mail address:* hmtuan@math.ac.vn