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CONCAVITY OF THE FUNCTION $f(A) = \det(I - A)$ FOR DENSITY OPERATOR A

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Abstract. According to the Minkowski determinant theorem the function $f(A) = \det(I - A)^{1/n}$ is concave on the set of $n \times n$ positive contractive matrices, that is, $0 \leqslant A \leqslant I$. When $n > 1$ the exponent $1/n$ can not be removed. On the other hand $\det(I - A)$ has meaning even for a trace-class Hilbert space operator A. In this paper we will prove that the function $f(A) = \det(I - A)$ is concave on the set of density operators, that is, $0 \leqslant A$ with $\mathrm{tr}(A) = 1$.

1. Introduction

The study on operator inequalities and convex operator functions is an interesting subject for many researchers ([1–3]). Moreover, many operator inequalities have been applied to the research of quantum information and other fields ([3, 6]). According to the Minkowski determinant theorem ([6, P. 54]), the function $f(A) = \det(I - A)^{1/n}$ is concave if A is a positive contractive matrix of order n. An example given at the end of this note will show the exponent $1/n$ can not be removed when $n > 1$. On the other hand, based on the importance of trace-class operators on a Hilbert space to quantum information theory and quantum computation, we shall investigate the concavity of density operators function $f(A) = \det(I - A)$, where A is a density operator.For a trace-class operator A, $\det(I - A)$ is also usually called the Fredholm determinant. As an application, the gap of the proof [5, Theorem 1] can be made up.

We shall adopt the following conventions and notations. Let $\mathscr{H}$ be an n-dimension Hilbert space and $\mathscr{S}(\mathscr{H})$ be the set of all quantum states on the quantum system $\mathscr{H}$. That is $\rho \in \mathscr{S}(\mathscr{H})$ if and only if $\rho \geqslant 0$ and $\mathrm{tr}(\rho) = 1$. For an n by n matrix $A = [a_{ij}]$, the trace of A is defined by $tr(A) = \sum_{i=1}^{n} a_{ii}$. As usual, $\lambda(\rho)$ is used to denote the eigenvalues of ρ with the non-increasing order.

Let $x, y \in \mathscr{D} \subset \mathbb{R}^n$, where $\mathscr{D} = \{(z_1, z_2, \cdots, z_n) : z_1 \geqslant z_2 \geqslant \cdots \geqslant z_n\}$. We say that x is majorised by y, in symbols $x \prec y$, if

$$\sum_{i=1}^{k} x_i \leqslant \sum_{i=1}^{k} y_i, \text{ for } k = 1, 2, \cdots, n-1; \text{ and } \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

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Majorization is a powerful and flexible mathematical tool which could be applied to a variety of problems in quantum mechanics. Another definition, which is closely related to majorization is Schur-convexity. A real-valued function Φ define on a set $\mathscr{A} \subset \mathbb{R}^n$ is said to be Schur-convex(Schur-concave) on $\mathscr{A}$ if

$$x \prec y \; on \; \mathscr{A} \Rightarrow \Phi(x) \leqslant \Phi(y) \, (\Phi(x) \geqslant \Phi(y)).$$

2. Concavity of operators function $f(A) = \det(\mathrm{I} - \mathrm{A})$

Let $\mathscr{C} \subseteq \mathbb{R}^n$ be a convex set. A function $f : \mathscr{C} \to \mathbb{R}$ is said to be concave provided that the inequality $f((1-\lambda)x + \lambda y) \geqslant (1-\lambda)f(x) + \lambda f(y)$ holds for every $x, y \in \mathscr{C}$ and every $0 \leqslant \lambda \leqslant 1$. Also, f is called convex if and only if $-f$ is concave. To prove the main result, we first show the following lemma.

LEMMA 2.1. *The function*

$$f(x) := \{\sum_{i=1}^{n} x_i\} \cdot \{\prod_{j=1}^{n}(1 - x_j)\} \quad for \; x = (x_1, \ldots, x_n) \in \mathbb{R}^n$$

is concave on the convex set

$$P := \Big\{ x = (x_1, \ldots, x_n) \mid \sum_{i=1}^{n} x_i \leqslant 1, \; 0 \leqslant x_i \leqslant 1 \; (i = 1, \ldots, n) \Big\}.$$

Proof. When $n = 1$, concavity in question is nothing but the concavity of the function $x(1-x)$ for $0 \leqslant x \leqslant 1$.

Now let $n \geqslant 2$. By a well-known fact (see [7, Theorem 4.5]) concavity in question is equivalent to the negative definiteness of the Hessian (matrix) $H_f(x) := [\frac{\partial^2}{\partial x_i \partial x_j} f(x)]_{i,j=1}^{n}$ on $\mathrm{int}(P)$, the interior of P. Notice that

$$\mathrm{int}(P) = \Big\{ (x_1, \ldots, x_n) | \sum_{i=1}^{n} x_i < 1, 0 < x_i < 1 \; (i = 1, 2, \ldots, n) \Big\}.$$

To get an explicit form of $H_f(x)$, write

$$s(x) := \sum_{i=1}^{n} x_i \quad \text{and} \quad t(x) := \prod_{i=1}^{n}(1 - x_i).$$

Notice that both $s(x)$ and $t(x)$ are positive on $\mathrm{int}(P)$. By a direct calculation the explicit form of $H_f(x) := [h_{j,j}(x)]_{i,j=1}^{n}$ is given by

$$h_{i,i}(x) = \frac{-2t(x)}{1 - x_i} \quad \text{and} \quad h_{i,j}(x) = \frac{\{s(x) + x_i + x_j - 2\}t(x)}{(1 - x_i)(1 - x_j)} \; for \; i \neq j \; (i, j = 1, 2, \ldots, n).$$

When $n = 2$, we have

$$\frac{-H_f(x)}{2} = \begin{pmatrix} 1 - x_2 & 1 - x_1 - x_2 \\ 1 - x_1 - x_2 & 1 - x_1 \end{pmatrix}.$$

Since both diagonal entries of the matrix on the right hand side are positive and its determinant is positive on $\operatorname{int}(P)$; in fact

$$(1-x_2)(1-x_1)-(1-x_1-x_2)^2 = (1-x_1-x_2)(x_1+x_2)+x_1x_2 > 0$$

we can conclude that $H_f(x)$ is negative definite on $\operatorname{int}(P)$.

Now let $n \geqslant 3$ and let $Q_1(x) := \operatorname{diag}(1-x_1,\dots,1-x_n)$. Notice that

$$Q_1^T(x)\cdot H_f(x)\cdot Q_1(x) = t(x)\Big\{-s(x)I+(s(x)-2)J+\Big(x_i+x_j\Big)_{i,j=1}^{n}\Big\}$$

where J is the matrix with all entries equal to 1, and that

$$J = e^T e \quad \text{and} \quad (x_i+x_j)_{i,j=1}^n = e^T x + x^T e$$

where $e := (1,1,\dots,1)$.

To diagonalize the real symmetric matrix $H_f(x)$ via *-congruence, let us use the matrix units $E_{i,j}$ $(i,j = 1,2,\dots,n)$ in the space of $n\times n$ complex matrices $\mathbb{M}_n$; the (i,j)-entry of $E_{i,j}$ is 1 and other entries are 0.

Let

$$Q_2 := \sum_{j=1}^{n-1}\frac{1}{j}\Big\{\sum_{i=1}^{j}E_{i,j}\Big\} - \sum_{i=1}^{n-1}E_{i+1,i} + E_{n,n}.$$

For instance, in the case $n = 4$,

$$Q_2 = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} & 0 \\ -1 & \frac{1}{2} & \frac{1}{3} & 0 \\ 0 & -1 & \frac{1}{3} & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}.$$

Notice that $\det(Q_2) = 1$.

It is immediate to see that

$$Q_2^T Q_2 = \begin{pmatrix} D & -f^T \\ -f & 1 \end{pmatrix}$$

where

$$\mathbb{M}_{n-1} \ni D = \operatorname{diag}(\frac{2}{1},\frac{3}{2},\dots,\frac{n}{n-1}) \quad \text{and} \quad \mathbb{R}^{n-1} \ni f = (0,\dots,0,1).$$

Further we can see that for $x = (x_1,\dots,x_n) \in \mathbb{R}^n$,

$$xQ_2 = (g_1(x),\dots,g_{n-1}(x),x_n)$$

where

$$g_i(x) = \frac{1}{i}\sum_{j=1}^{i}x_j - x_{i+1} \quad (i = 1,\dots,n-1).$$

In particular, $eQ_2 = (0,\dots,0,1)$. Write for $x = (x_1,\dots,x_n) \in \mathbb{R}^n$,

$$\mathbb{R}^{n-1} \ni g(x) := (g_1(x),\dots,g_{n-1}(x)).$$

Now

$$\begin{aligned}
&Q_2^T Q_1^T(x)\cdot H_f(x)\cdot Q_1(x)Q_2\\
&= t(x)\Big\{-s(x)Q_2^TQ_2 + (s(x)-2)(eQ_2)^T\cdot(eQ_2) + (eQ_2)^T\cdot(xQ_2) + (xQ_2)^T\cdot(eQ_2)\Big\}\\
&= t(x)\Big\{-s(x)\begin{pmatrix} D & -f^T\\ -f & 1\end{pmatrix} + (s(x)-2)\begin{pmatrix} O & 0\\ 0 & 1\end{pmatrix} + \begin{pmatrix} O & g(x)^T\\ g(x) & 2x_n\end{pmatrix}\Big\}\\
&= t(x)\begin{pmatrix} -s(x)D & s(x)f^T + g(x)^T\\ s(x)f + g(x) & 2(x_n-1)\end{pmatrix}.
\end{aligned}$$

Since $s(x) > 0$ and D is invertible, with help of the matrix

$$Q_3(x) := \begin{pmatrix} I_{n-1} & \frac{1}{s(x)}D^{-1}\{s(x)f^T + g(x)^T\}\\ 0 & 1\end{pmatrix}$$

we can see

$$Q_3^T(x)Q_2^TQ_1^T(x)\cdot H_f(x)\cdot Q_1(x)Q_2Q_3(x) = t(x)\begin{pmatrix} -s(x)D & 0\\ 0 & h(x)\end{pmatrix}$$

where

$$\begin{aligned}
h(x) &= \frac{1}{s(x)}\{s(x)f + g(x)\}D^{-1}\{s(x)f+g(x)\}^T + 2(x_n-1)\\
&= \frac{1}{s(x)}\Big\{\sum_{i=1}^{n-2}\frac{i}{i+1}g_i^2(x) + \frac{n-1}{n}\{g_{n-1}(x)+s(x)\}^2\Big\} + 2(x_n-1).
\end{aligned}$$

Since $-s(x)D$ is negative definite, $H_f(x)$ is negative definite on $\operatorname{int}(P)$ if and only if $h(x) < 0$ on $\operatorname{int}(P)$. Obviously this is also equivalent to $s(x)h(x) < 0$.

To see that $s(x)h(x) < 0$ on $\operatorname{int}(P)$, it suffices to prove that, with fixed $0 < x_n^{(0)} < 1$,

$$l(x_1,\dots,x_{n-1}) := (\sum_{i=1}^{n-1} x_i + x_n^{(0)})\cdot h(x_1,\dots,x_{n-1},x_n^{(0)}) < 0$$

on the convex set

$$\tilde{P} := \Big\{(x_1,\dots,x_{n-1}) \in \mathbb{R}^{n-1}\Big|\sum_{i=1}^{n-1} x_i \leqslant 1 - x_n^{(0)},\ x_i \geqslant 0\ (i = 1,2,\dots,n-1)\Big\}.$$

Since

$$\begin{aligned} l(x_1,\dots,x_{n-1}) = &\sum_{i=1}^{n-2} \frac{i}{i+1} g_i^2(x_1,\dots,x_{n-1},x_n^{(0)}) \\ &+\frac{n-1}{n}\{g_{n-1}(x_1,\dots,x_{n-1},x_n^{(0)}) \\ &+s(x_1,\dots,x_{n-1},x_n^{(0)})\}^2 + s(x_1,\dots,x_{n-1},x_n^{(0)})(2x_n^{(0)}-2) \end{aligned}$$

and all $g_i(x_1,\dots,x_{n-1},x_n^{(0)})$ $(i=1,2,\dots,n-1)$ and $s(x_1,\dots,x_{n-1},x_n^{(0)})$ are affine functions of $x_1,\dots,x_{n-1}$, we can see that $l(x_1,\dots,x_{n-1})$ is a convex function of $(x_1,\dots,x_{n-1})$. Therefore, $l(x_1,\dots,x_{n-1})$ attains its maximum on $\tilde{P}$ at some of vertices of $\tilde{P}$.

The vertices of $\tilde{P}$ are exactly $v_0, v_1, \dots$ and v_{n-1}, where

$$v_0 = (0,\dots,0) \quad \text{and} \quad v_k = (0,\dots,0,\overbrace{1-x_n^{(0)}}^{(k)},0,\dots,0) \quad (k=1,2,\dots,n-1).$$

For $x = (0,\dots,0,x_n^{(0)}) \in \mathbb{R}^n$, it is easy to see that

$$s(x) = x_n^{(0)},\ g_i(x) = 0\ (i=1,2,\dots,n-2) \quad \text{and} \quad g_{n-1}(x)+s(x) = -x_n^{(0)} + x_n^{(0)} = 0.$$

Therefore

$$l(v_0) = 2x_n^{(0)}(x_n^{(0)}-1) < 0.$$

For $x = (0,\dots,0,\overbrace{1-x_n^{(0)}}^{(k)},0,\dots,0,x_n^{(0)})$, it is easy to see that $s(x) = 1$ and

$$\begin{aligned} &g_i(x) = 0\ (i=1,\dots,k-2), \quad g_{k-1}(x) = -(1-x_n^{(0)}) \\ &g_i(x) = \frac{1}{i}(1-x_n^{(0)})\ (i=k,\dots,n-2) \quad \text{and} \quad g_{n-1}(x)+s(x) = \frac{n}{n-1}(1-x_n^{(0)}). \end{aligned}$$

Then calculation will show

$$l(v_k) = \sum_{i=1}^{n-2} \frac{i}{i+1} g_i^2(x) + \frac{n-1}{n}\{g_{n-1}(x)+s(x)\}^2 + s(x)(2x_n^{(0)}-2) = 2x_n^{(0)}(x_n^{(0)}-1) < 0.$$

This completes the proof. □

To show the main result, we also need the following consequence of Ky Fan maximum principle.

LEMMA 2.2. ([2, 6]) *Let A,B be $n \times n$ Hermitian matrices, $\lambda(A), \lambda(B)$, and $\lambda(A+B)$ are the vectors of eigenvalues of A,B, and $A+B$ with non-increasing order, respectively. Then $\lambda(A+B) \prec \lambda(A)+\lambda(B)$.*

LEMMA 2.3. ([2, 6]) *The product function $f(x) := \prod_{i=1}^n x_i$ is Schur-concave in region of $\mathscr{C} := \{(x_1,x_2,\cdots x_n) : x_i \geqslant 0 \text{ for all } i\}$.*

THEOREM 2.4. *The function* $f(A) = \operatorname{tr}(A) \cdot \det(I - A)$ *is concave on the set of positive trace-class operators* A *with* $\operatorname{tr}(A) \leqslant 1$ *on a Hilbert space* $\mathscr{H}$.

As a consequence, the function $f(A) = \det(I - A)$ *is concave on the set of density operators, that is,* $0 \leqslant A$ *and* $\operatorname{tr}(A) = 1$.

Proof. First suppose that $\dim(\mathscr{H}) = n < \infty$. We have to show that for $0 \leqslant A$, B in $\mathbb{M}_n$ with $\operatorname{tr}(A), \operatorname{tr}(B) \leqslant 1$ and for $0 < \lambda < 1$,

$$\begin{aligned} &\operatorname{tr}\Big(\lambda A + (1-\lambda)B\Big) \cdot \det\Big(I - \lambda A - (1-\lambda)B\Big) \\ &\qquad \geqslant \quad \lambda \operatorname{tr}(A) \cdot \det(I - A) + (1-\lambda)\operatorname{tr}(B) \cdot \det(I - B). \end{aligned}$$

Let $x_1 \geqslant \ldots \geqslant x_n (\geqslant 0)$ be the eigenvalues of A and let $y_1 \geqslant \ldots \geqslant y_n (\geqslant 0)$ be the eigenvalues of B. Then by Lemma 2.1,

$$\begin{aligned} \lambda \operatorname{tr}(A) \cdot \det(I - A) + (1-\lambda)\operatorname{tr}(B) \cdot \det(I - B) &= \lambda s(x) \cdot t(x) + (1-\lambda) s(y) \cdot t(y) \\ &\leqslant s\Big(\lambda x + (1-\lambda)y\Big) \cdot t\Big(\lambda x + (1-\lambda)y\Big) \end{aligned}$$

where $s(x) = \sum_{i=1}^n x_i$ and $t(x) = \prod_{i=1}^n (1 - x_i)$ as before.

Let $z = (z_1, \ldots, z_n)$ be the vector of the eigenvalues of $\lambda A + (1-\lambda)B$. Notice that $s(z) = s(\lambda x + (1-\lambda)y)$ and $1 - z$ is majorized by $1 - (\lambda x + (1-\lambda)y)$. Then by Lemma 2.3

$$\begin{aligned} \operatorname{tr}\Big(\lambda A + (1-\lambda)B\Big) \cdot \det\Big(I - \lambda A - (1-\lambda)B\Big) &= s(z) \cdot t(z) = s(\lambda x + (1-\lambda)y) \cdot t(z) \\ \geqslant s\Big(\lambda x + (1-\lambda)y\Big) \cdot t\Big(\lambda x + (1-\lambda)y\Big) & \\ \geqslant \lambda \operatorname{tr}(A) \cdot \det(I - A) + (1-\lambda)\operatorname{tr}(B) \cdot \det(I - B). & \end{aligned}$$

Next, when $\dim(\mathscr{H}) = \infty$, take an increasing sequence of orthoprojections of finite rank P_n converging strongly to the identity. Then the functions $\operatorname{tr}(P_n A P_n) \cdot \det(I - P_n A P_n)$ $(n = 1, 2, \ldots)$ are concave on the set of $A \geqslant 0$ with $\operatorname{tr}(A) \leqslant 1$ and

$$\operatorname{tr}(A) \cdot \det(I - A) = \lim_{n \to \infty} \operatorname{tr}(P_n A P_n) \cdot \det(I - P_n A P_n).$$

Thus, the function $f(A) = \operatorname{tr}(A) \cdot \det(I - A)$ is concave on the set of $A \geqslant 0$ with $\operatorname{tr}(A) \leqslant 1$. $\square$

COROLLARY 2.5. *Let* $a_i, b_i \geqslant 0$ *for* $i = 1, \ldots, n$ *with* $\sum_{i=1}^n a_i = m$ *and* $\sum_{i=1}^n b_i = m$, *where* $m > 0$. *Then*

$$\prod_{i=1}^n \Big(m - \frac{a_i + b_i}{2}\Big) \geqslant \frac{1}{2}\Big(\prod_{i=1}^n (m - a_i) + \prod_{i=1}^n (m - b_i)\Big).$$

Proof. It is clear that $\sum_{i=1}^n \frac{a_i}{m} = 1$ and $\sum_{i=1}^n \frac{b_i}{m} = 1$, then by Lemma 2.1,

$$\prod_{i=1}^n \Big(1 - \frac{a_i + b_i}{2m}\Big) \geqslant \frac{1}{2}\Big(\prod_{i=1}^n \Big(1 - \frac{a_i}{m}\Big) + \prod_{i=1}^n \Big(1 - \frac{b_i}{m}\Big)\Big),$$

so

$$\prod_{i=1}^{n}\left(m - \frac{a_i + b_i}{2}\right) \geqslant \frac{1}{2}\left(\prod_{i=1}^{n}(m - a_i) + \prod_{i=1}^{n}(m - b_i)\right). \quad \square$$

REMARK. Although it is obtained in [4] that

$$\det(A + B) \geqslant \det(A) + \det(B), \tag{1}$$

for all positive semi-definite matrices A and B, however in general for $0 \leqslant \lambda \leqslant 1$,

$$\det[\lambda A + (1 - \lambda)B] \geqslant \lambda \det(A) + (1 - \lambda) \det(B) \tag{2}$$

does not hold.

A simple example is the following.

$$A = \mathrm{diag}(1, 1) \text{ and } B = \mathrm{diag}\left(\frac{1}{2}, \frac{1}{2}\right).$$

Then

$$\det\left[\frac{1}{2}A + \frac{1}{2}B\right] = \frac{9}{16} < \frac{5}{8} = \frac{1}{2}\det(A) + \frac{1}{2}\det(B).$$

Our Theorem shows that for quantum states $A_i \in \mathscr{S}(\mathscr{H})$ and $0 \leqslant \lambda_i$ with $\sum_i \lambda_i = 1$,

$$\det(I - \sum_i \lambda_i A_i) \geqslant \sum_i \lambda_i \det(I - A_i).$$

Thus the gap of proof [5, Theorem 1], which used the inequality (2.2), has been made up.

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