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AN EXTENDED MATRIX EXPONENTIAL FORMULA

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Abstract. In this paper we present matrix exponential formulae for the geometric and spectral geometric means of positive definite matrices using a conjectured exponential formula that solved by Wasin So [Linear Algebra Appl. 379 (2004)].

1. Introduction

A conjectured matrix exponential formula has recently been proved by Wasin So [10, 11]: For Hermitian n by n matrices X and Y, there exist unitary matrices U and V such that

$$e^{X/2}e^{Y}e^{X/2} = e^{UXU^{*}+VYV^{*}} \tag{1.1}$$

or equivalently $e^{X+VYV^{*}} = U(e^{X/2}e^{Y}e^{X/2})U^{*}$. In other words, the Hermitian matrix $\log(e^{X/2}e^{Y}e^{X/2})$ belongs to the sum of the unitary orbits of X and Y

$$\log(e^{X/2}e^{Y}e^{X/2}) \in \mathrm{U}(n)\cdot X + \mathrm{U}(n)\cdot Y = \{UXU^{*}+VYV^{*} : U, V \in \mathrm{U}(n)\}.$$

We note that positive definite matrices of the form $e^{X/2}e^{Y}e^{X/2}$ appear in an extended Lie-Trotter formula as infinitesimal generators [3]

$$e^{X+Y} = \lim_{n\to\infty}(e^{X/2n}e^{Y/n}e^{X/2n})^{n}.$$

The exponential formula leads to a trace equality; $\mathrm{Tr}e^{X+VYV^{*}} = \mathrm{Tr}(e^{X/2}e^{Y}e^{X/2}) = \mathrm{Tr}e^{X}e^{Y}$ for some unitary matrix V, in comparison with the well-known Golden-Thompson trace inequality $\mathrm{Tr}e^{X+Y} \leqslant \mathrm{Tr}e^{X}e^{Y}$ [6, 12].

The main purpose of this paper is to derive matrix exponential formulae for the geometric and spectral geometric means that also appeared in extended Lie-Trotter formulae as infinitesimal generators and in the study of logarithmic trace inequalities complementing the Golden-Thompson trace inequality. The geometric and spectral means of positive definite matrices A and B are defined by

$$A\#B = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}, \quad A\natural B = (A^{-1}\#B)^{1/2}A(A^{-1}\#B)^{1/2}.$$

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If A and B commute then $A\#B = A\natural B = A^{1/2}B^{1/2} = (AB)^{1/2}$. The geometric mean $A\#B$ is realized as a unique midpoint (geodesic middle) of A and B for a congruence transformation invariant Riemannian metric on the open convex cone of positive definite matrices [4, 8, 9]. The spectral geometric mean $A\natural B$ is introduced and studied in detail by Fiedler and V. Pták [5]. Extended Lie-Trotter formulae via the geometric and spectral geometric means appear in [7, 1]

$$\lim_{n\to\infty}\left(e^{2X/n}\#e^{2Y/n}\right)^n = e^{X+Y} = \lim_{n\to\infty}\left(e^{2X/n}\natural e^{2Y/n}\right)^n.$$

More generally, $e^{X+Y} = \lim_{n\to\infty}\gamma(1/n)^n$ for any differentiable curve γ defined on $(-\epsilon,\epsilon)$ to the open convex cone of positive definite matrices with $\gamma(0) = I$ and $\gamma'(0) = X+Y$. See [1] for a proof.

We state the main result of this paper.

THEOREM 1.1. *For Hermitian matrices X and Y, there exist unitary matrices U_i and V_i such that*

$$e^{2X}\#e^{2Y} = e^{U_1XU_1^*+V_1YV_1^*} \text{ and } e^{2X}\natural e^{2Y} = e^{U_2XU_2^*+V_2YV_2^*}. \tag{1.2}$$

In particular for $p>0$,

$$Tr\, e^{X+UYU^*} = Tr\,(e^{pX}\#e^{pY})^{2/p} \leqslant Tr\, e^{X+Y} \leqslant Tr(e^{pX}\natural e^{pY})^{2/p} = Tr\, e^{X+VYV^*} \tag{1.3}$$

for some unitary matrices U and V, depending on p and X,Y.

2. Geometric and spectral means

Throughout this paper all matrices are assumed to be complex $n\times n$ matrices. Let $\mathrm{H}(n)$ be the space of Hermitian matrices and let $\mathrm{U}(n)$ be the group of unitary matrices.

The following Riccati lemma is useful for our purpose. See [2, 9] for a proof.

LEMMA 2.1. (Riccati Lemma) *For positive definite matrices A and B, the geometric mean $A\#B$ is a unique positive definite solution of the Riccati equation $XA^{-1}X = B$.*

The following properties of the geometric and spectral mean operations are well-known [2, 5, 9].

PROPOSITION 2.2. *Let A and B be positive definite matrices. Then*

(i) $A\#A = A\natural A = A$;

(ii) $A\#B = B\#A, A\natural B = B\natural A$;

(iii) $(A\#B)^{-1} = A^{-1}\#B^{-1}, (A\natural B)^{-1} = (A^{-1})\natural(B^{-1})$;

(iv) $A\#B = A\natural B$ *if and only if A and B commute; and*

(vi) $(MAM^*)\#(MBM^*) = M(A\#B)M^*$ *and* $(UAU^*)\natural(UBU^*) = U(A\natural B)U^*$ *for any invertible matrix M and $U\in U(n)$.*

PROPOSITION 2.3. *Let A and B be positive definite matrices. Then*

$$A\natural B = U(A^{1/2}BA^{1/2})^{1/2}U^* \tag{2.1}$$

for some unitary matrix U.

Proof. Note that X^*X and XX^* are unitarily similar for any invertible matrix X. Setting $X = A^{1/2}(A^{-1}\#B)^{1/2}$, there exists a unitary matrix U such that

$$A\natural B = X^*X = UXX^*U^* = UA^{1/2}(A^{-1}\#B)^{1/2}\cdot(A^{-1}\#B)^{1/2}A^{1/2}U^* = U(A^{1/2}BA^{1/2})U^*.$$

□

3. Proof and related results

Proof of Theorem 1.1. We consider the matrix exponential equations of the geometric and spectral geometric means: $e^{2X}\#e^{2Y} = e^Z$ and $e^{2X}\natural e^{2Y} = e^W$. By Riccati Lemma, $e^Ze^{-2X}e^Z = e^{2Y}$ and by (1.1) there exist unitary matrices U and V such that $e^Ze^{-2X}e^Z = e^{2Z/2}e^{-2X}e^{2Z/2} = e^{2UZU^*-2VXV^*}$. Since the exponential map on the space of Hermitian matrices is bijective onto the convex cone of positive definite matrices, we have $2UZU^* - 2VXV^* = 2Y$ and hence $UZU^* = VXV^* + Y$ or $Z = WXW^* + U^*YU$ where $W = U^*V$.

For the spectral geometric mean, we apply Proposition 2.3:

$$e^W = e^{2X}\natural e^{2Y} = U(e^Xe^{2Y}e^X)^{1/2}U^*$$

for some unitary U. Then by (1.1), $e^W = Ue^{V_1XV_1^*+V_2YV_2^*}U^* = e^{U_1XU_1^*+U_2YU_2^*}$ for some unitary V_1, V_2 and therefore $W = U_1XU_1^* + U_2YU_2^*$.

Finally we prove (1.3): The first and last equalities follow from (1.2). By Theorem 3.4 and Theorem 1.1 of [7],

$$\mathrm{Tr}\,(e^{pX}\#e^{pY})^{2/p} \leqslant \mathrm{Tr}\,e^{X+Y} \leqslant \mathrm{Tr}(e^{pX/2}e^{pY}e^{pX/2})^{1/p}.$$

Since $e^{pX}\natural e^{pY}$ is similar to $(e^{pX/2}e^{pY}e^{pX/2})^{1/2}$, $(e^{pX}\natural e^{pY})^{2/p}$ is similar to $(e^{pX/2}e^{pY}e^{pX/2})^{1/p}$. Therefore $\mathrm{Tr}(e^{pX/2}e^{pY}e^{pX/2})^{1/p} = \mathrm{Tr}(e^{pX}\natural e^{pY})^{2/p}$ for every $p > 0$. This shows the inequalities of (1.3).

DEFINITION 3.1. Define differentiable maps $p, g, s : \mathrm{H}(n)\times\mathrm{H}(n) \to \mathrm{H}(n)$ by

$$e^{X/2}e^Ye^{X/2} = e^{p(X,Y)},\ \ e^{2X}\#e^{2Y} = e^{g(X,Y)},\ \ e^{2X}\natural e^{2Y} = e^{s(X,Y)}.$$

PROPOSITION 3.2. *Let $X, Y \in H(n)$.*

(1) If X and Y commute then $X + Y = p(X,Y) = g(X,Y) = s(X,Y)$.

(2) $g(X,Y) = g(Y,X)$, $s(X,Y) = s(Y,X)$, $p(-X,-Y) = -p(X,Y)$, $g(-X,-Y) = -g(X,Y)$, $s(-X,-Y) = -s(X,Y)$.

(3) $p(X,Y) = Up(Y,X)U^*, s(X,Y) = \frac{1}{2}Vp(2X,2Y)V^*$ for some unitary matrices U, V depending on X and Y.

(4) $g(-Y/2, p(X,Y)/2) = X/2$, $g(X,Y) = p(2X, \frac{1}{2}p(-2X,2Y))$, and $p(-2X, g(X,Y)) = \frac{1}{2}p(-2X,2Y)$.

(5) $p(2g(X,Y),-2X) = 2Y$, $p(X,Y) = \frac{1}{2}p(X,p(2Y,X))$, and $p(2X,Y) = p(X,p(X,Y))$.

Proof. (1) Straightforward.

(2) This follows from the commutative and inversion property of the geometric and spectral means (Proposition 2.2).

(3) This follows from (2.1) and (1.1) and the fact that $A^{1/2}BA^{1/2}$ and $B^{1/2}AB^{1/2}$ are unitarily similar for any positive definite matrices A and B.

(4) By Riccati Lemma, $e^{X/2}e^{Y}e^{X/2} = e^{p(X,Y)}$ implies that $e^{X/2} = e^{-Y}\#e^{p(X,Y)} = e^{g(-Y/2,p(X,Y)/2)}$. From

$$e^{g(X,Y)} = e^{2X}\#e^{2Y} = e^{X}\left(e^{-X}e^{2Y}e^{-X}\right)^{1/2}e^{X} = e^{X}e^{\frac{1}{2}p(-2X,2Y)}e^{X} = e^{p(2X,\frac{1}{2}p(-2X,2Y))},$$

we have $g(X,Y) = p(2X,\frac{1}{2}p(-2X,2Y))$ and $e^{\frac{1}{2}p(-2X,2Y)} = e^{-X}e^{g(X,Y)}e^{-X} = e^{p(-2X,g(X,Y))}$.

(5) By Riccati Lemma, $e^{g(X,Y)} = e^{2X}\#e^{2Y}$ implies that $e^{g(X,Y)}e^{-2X}e^{g(X,Y)} = e^{2Y}$ and hence $2Y = p(2g(X,Y),-2Y)$. The remaining parts are immediate. □

REMARK 3.3. For fixed $X,Y \in \mathrm{H}(n)$, we consider the sum of two unitary orbits

$$\mathrm{U}(X,Y) := \{UXU^* + VYV^* : U,V \in \mathrm{U}(n)\}.$$

The previous results imply that $p(X,Y), g(X,Y)$ and $s(X,Y)$ lie in the compact subset $\mathrm{U}(X,Y)$. Now, we consider weighted geometric and spectral means and associated Lie-Trotter formulae. For any real number t, the t-weighted geometric and spectral means are naturally defined by

$$A\#_tB := A^{1/2}(A^{-1/2}BA^{-1/2})^tA^{1/2},\ \ A\natural_tB := (A^{-1}\#B)^tA(A^{-1}\#B)^t.$$

We note that the line $t \mapsto A\#_tB$ is the unique geodesic line passing A and B on the Riemannian symmetric space of positive definite matrices [8, 9]. It is shown ([1]) that

$$e^{(1-t)X+tY} = \lim_{n\to\infty}\left(e^{(1-t)X/2n}e^{tY/n}e^{(1-t)X/2n}\right)^n = \lim_{n\to\infty}\left(e^{X/n}\#_te^{Y/n}\right)^n = \lim_{n\to\infty}\left(e^{X/n}\natural_te^{Y/n}\right)^n.$$

Moving to Hermitian matrices, we get $p_t, g_t, s_t : \mathrm{H}(n)\times\mathrm{H}(n) \to \mathrm{H}(n)$ defined by

$$e^{p_t(X,Y)} = e^{(1-t)X/2}e^{tY}e^{(1-t)X/2},\quad e^{g_t(X,Y)} = e^{X}\#_te^{Y},\quad e^{s_t(X,Y)} = e^{X}\natural_te^{Y}.$$

From (1.1) we have that $p_t(X,Y) \in \mathrm{U}_t(X,Y) := \mathrm{U}((1-t)X,tY)$, the t-weighted sum of the unitary orbits.

We remark in closing that higher-order exponential formulae are immediate from induction and So's result. For Hermitian matrices $X_1, X_2, \ldots, X_m$,

$$\begin{aligned} e^{X_1/2}e^{X_2/2}\cdots e^{X_{m-1}/2}e^{X_m}e^{X_{m-1}/2}\cdots e^{X_2/2}e^{X_1/2} &= e^{\sum_{i=1}^m U_iX_iU_i^*} \\ e^{2X_1}\#e^{4X_2}\#\cdots\#e^{2^{m-1}X_{n-1}}\#e^{2^{m-1}X_m} &= e^{\sum_{i=1}^m V_iX_iV_i^*} \\ e^{2X_1}\natural e^{4X_2}\natural\cdots\natural e^{2^{m-1}X_{m-1}}\natural e^{2^{m-1}X_m} &= e^{\sum_{i=1}^m W_iX_iW_i^*} \end{aligned}$$

for some unitary matrices U_i, V_i and $W_i, i = 1,2,\ldots,m$. Here we used the notation $A_1\#A_2\#\cdots\#A_{n-1}\#A_n$ in the usual way:

$$A_1\#A_2\#\cdots\#A_{n-1}\#A_n = A_1\#\left(A_2\#\cdots\#A_{n-1}\#A_n\right)$$

although the geometric mean operation is not associative. Similarly for spectral geometric means.

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