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Operator Means of Lower Triangular Matrices

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Abstract. We show that every Kubo-Ando operator mean of positive definite operators exists on the solvable Lie group of lower triangular matrices with positive diagonal entries. In particular, we show that the operator geometric mean of such lower triangular matrices appears as the common limit of the iteration process of the arithmetic and harmonic means. We further show that the iteration terminates in the finite number $\lceil \log_2 m \rceil$ of iterations for $m \times m$ lower unitriangular matrices and present its entrywise closed form for $m \leq 4$.

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1. Introduction

To the best of our knowledge, this paper is the first to study operator means of Kubo and Ando theory [11] on non-additive matrix Lie groups, especially the operator geometric mean that lies at the heart of Kubo and Ando theory of Hermitian positive definite operators.

The operator mean $\mu_f(A,B) := A^{1/2} f(A^{-1/2}BA^{-1/2})A^{1/2}$ of positive definite matrices (operators) for an operator monotone function $f : (0,\infty) \to (0,\infty)$ with $f(1) = 1$ has the following integral representation

$$\mu_f(A,B) = aA + bB + \int_0^\infty \frac{1+t}{t} \left[t^{-1}A^{-1} + B^{-1}\right]^{-1} dm(t), \tag{1}$$

where $a, b \geq 0$ and the probability measure m on $[0,\infty]$ are uniquely determined by the operator monotone function f. Conversely every operator mean arises in this way. This is a major result of F. Kubo and T. Ando [11] in the theory of operator means on positive definite operators on a Hilbert space.

The operator geometric mean of positive definite Hermitian matrices A and B of fixed size is explicitly given by

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

whose integral expression is given by [9, 11]:

$$A\#B = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{t}} \left[A^{-1} + tB^{-1}\right]^{-1} dt. \tag{3}$$

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A fast algorithm for computing the geometric mean is the iteration process of arithmetic and harmonic means [2, 6, 7, 11, 12]

$$A\#B = \lim_{k\to\infty} A_k = \lim_{k\to\infty} B_k, \tag{4}$$

where $$A_0 := A,\ B_0 := B,\ A_{k+1} := \frac{A_k + B_k}{2},\ B_{k+1} := \left[\frac{A_k^{-1} + B_k^{-1}}{2}\right]^{-1}. \tag{5}$$

In this paper we consider the solvable Lie group $\mathcal{L}_m$ of $m \times m$ lower triangular matrices with positive diagonal entries and study operator means on $\mathcal{L}_m$ based on (1) and particularly the geometric means (2), (3), and (4). The sequences in the arithmetic and harmonic mean iteration (5) of lower triangular matrices with positive diagonal entries are well defined and belong to $\mathcal{L}_m$, and henceforth their convergence to a common limit arises naturally.

The main result of this paper is the following.

Theorem 1.1. *Every operator mean* (1) *exists on the Lie group* $\mathcal{L}_m$ *and the three means* $(2)-(4)$ *are well-defined on* $\mathcal{L}_m$ *and are all equal. Moreover, for lower unitriangular matrices* A *and* B,

$$A_k = B_k, \qquad k \geq \lceil \log_2 m \rceil. \tag{6}$$

The geometric mean, denoted by $A\#B$, of lower triangular matrices defined independently via (2)-(4) is new in matrix analysis and matrix Lie groups and of interest in operator means of *nonpositive* matrices. It is shown that $X = A\#B$ is a unique solution in $\mathcal{L}_m$ of the Ricatti equation

$$XA^{-1}X = B \tag{7}$$

and satisfies commutativity $A\#B = B\#A$, self-duality $(A\#B)^{-1} = A^{-1}\#B^{-1}$, the group invariance

$$(XAX)\#(XBX) = X(A\#B)X, \qquad X \in \mathcal{L}_m,$$

and $$\left[\frac{A^{-1} + B^{-1}}{2}\right]^{-1} \# \left[\frac{A+B}{2}\right] = A\#B.$$

The paper is organized as follows. In Section 2, we handle the problem on the nilpotent Lie group $\mathcal{N}_m$ of $m \times m$ lower unitriangular matrices with $m \leq 4$ and present an entrywise closed form for the geometric mean (4). It is shown that the geometric means (3) and (4) are equal by using the integral formula

$$\frac{1}{\pi}\int_0^\infty \frac{t^m}{\sqrt{t}(1+t)^n}dt = \frac{(2m-1)!!(2n-2m-3)!!}{2^{n-1}(n-1)!}.$$

In Section 3, we prove the main theorem. We first prove the main theorem for the nilpotent Lie group $\mathcal{N}_m$ and then for $\mathcal{L}_m$ with the same method (Remark 3.3 and Remark 3.5). We show that the Lie group $\mathcal{N}_m$ is uniquely 2-divisible where the unique square root is given by

$$A^{1/2} = \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}} A(tI + A)^{-1} dt \tag{8}$$

and the integrand is absolutely convergent and $A^{1/2}$ defined in (8) is indeed lower unitriangular for every $A \in \mathcal{N}_m$. We then show that the operator geometric mean (3) is well-defined and belongs to $\mathcal{N}_m$, and is a unique lower unitriangular solution of the Ricatti equation (7), from which the means (2) and (3) are equal. Using basic properties of strictly lower triangular (nilpotent) matrices, we prove that the iteration (5) stops in the finite step $\lceil \log_2 m \rceil$. The group invariance (1) for both geometric means (3) and (4) ensures the reduction to $B = I$. Then we apply the Newton's square root algorithm to show that these means are equal. It is noted in Remark 3.3 that the integrand in (1) is well-defined on $\mathcal{L}_m$ in a similar way and (1) belongs to $\mathcal{L}_m$. In Section 5, we extend the results on the operator geometric mean to the general setting of simply connected nilpotent Lie groups.

2. Examples

We will provide a closed form for the geometric mean (4) of lower unitriangular matrices A and B, denoted by $A\natural B$, when $m = 2, 3, 4$. It is direct to see that for $m = 2$,

$$\left[\frac{A^{-1} + B^{-1}}{2}\right]^{-1} = \frac{A + B}{2} = A\natural B. \tag{9}$$

Suppose that $m = 3$. Let

$$A = \begin{bmatrix} 1 & 0 & 0 \\ a_1 & 1 & 0 \\ a_3 & a_2 & 1 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 & 0 \\ b_1 & 1 & 0 \\ b_3 & b_2 & 1 \end{bmatrix}.$$

Using

$$A^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -a_1 & 1 & 0 \\ a_1a_2 - a_3 & -a_2 & 1 \end{bmatrix}, \qquad B^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ -b_1 & 1 & 0 \\ b_1b_2 - b_3 & -b_2 & 1 \end{bmatrix}$$

we have that

$$B_1 = \left[\frac{A^{-1} + B^{-1}}{2}\right]^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 \\ \frac{a_3+b_3}{2} - \frac{(a_1-b_1)(a_2-b_2)}{4} & \frac{a_2+b_2}{2} & 1 \end{bmatrix}.$$

By direct computation,

$$A_2 = \frac{A_1+B_1}{2} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 \\ \frac{a_3+b_3}{2} - \frac{(a_1-b_1)(a_2-b_2)}{8} & \frac{a_2+b_2}{2} & 1 \end{bmatrix} = \left[\frac{A_1^{-1}+B_1^{-1}}{2}\right]^{-1} = B_2, \tag{10}$$

from which we obtain $A\natural B = A_2 = B_2$.

Suppose that $m = 4$. In this case,

$$A\natural B = A_2 = B_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 & 0 \\ \frac{a_4+b_4}{2} - u & \frac{a_2+b_2}{2} & 1 & 0 \\ \frac{a_6+b_6}{2} - w & \frac{a_5+b_5}{2} - v & \frac{a_3+b_3}{2} & 1 \end{bmatrix} \tag{11}$$

where $$u=\frac{(a_1-b_1)(a_2-b_2)}{8},\quad v=\frac{(a_2-b_2)(a_3-b_3)}{8},$$

$$w=-\frac{(a_1-b_1)(a_5-b_5)+(a_3-b_3)(a_4-b_4)}{8}+\frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)}{16}.$$

A detailed proof of (11) is in Appendix A for the convenience of the reader.

Remark 2.1. By similar computations one can show that $X=A\natural B$ for $m=2,3,4$, is a unique lower unitriangular solution of the Riccati equation

$$XA^{-1}X=B.$$

For $m=2$, $$\frac{A+B}{2}A^{-1}\frac{A+B}{2}=\frac{A+2B+B^2A^{-1}}{4}=B.$$

It is quite nontrivial to show that for general $m\geq 5$.

Definition 2.2. For $A,B\in\mathcal{N}_m$, the nilpotent Lie group of lower unitriangular matrices, define $l_m(A,B):=\min\{k\geq 0: A_k=B_k\}$ if $A_k=B_k$ for some $k\in\mathbb{N}$.

We saw in the preceding examples that $l_2(A,B)\leq 1$ and $l_3(A,B)$, $l_4(A,B)\leq 2$.
By Theorem 1.1, $l_m(A,B)\leq\lceil\log_2 m\rceil$, $\forall A,B\in\mathcal{N}_m$.
For instance, $l_5(A,B)$, $l_6(A,B)$, $l_7(A,B)$, $l_8(A,B)\leq 3$ and

$$l_9(A,B),\cdots,l_{16}(A,B)\leq 4,\qquad l_{17}(A,B),\cdots,l_{32}(A,B)\leq 5.$$

Next, we consider the mean (3) for lower unitriangular matrices A and B, denoted by $A\#B$. We will show that $A\#B=A\natural B$ for $m\leq 4$. Note from (3) that

$$\int_0^\infty\frac{1}{\sqrt{t}(1+t)}dt=\pi.\tag{12}$$

Generally $$\frac{1}{\pi}\int_0^\infty\frac{t^m}{\sqrt{t}(1+t)^n}dt=\frac{(2m-1)!!(2n-2m-3)!!}{2^{n-1}(n-1)!}.\tag{13}$$

The above integral is in fact the beta function. Recall that the beta function $B(\alpha,\beta)$ is a function of two complex variables α, β, defined by

$$B(\alpha,\beta)=\int_0^1 x^{\alpha-1}(1-x)^{\beta-1}dx,$$

provided that $\Re(\alpha)>0$, $\Re(\beta)>0$. The beta function can be rewritten as

$$B(\alpha,\beta)=\int_0^\infty\frac{t^{\alpha-1}}{(1+t)^{\alpha+\beta}}dt.$$

The beta function can also be expressed as the gamma function Γ.

$$B(\alpha,\beta)=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}.$$

Note that for a nonnegative integer m

$$\Gamma(m) = (m-1)! \quad \text{and} \quad \Gamma(m+\frac{1}{2}) = \frac{(2m-1)!!}{2^m}\sqrt{\pi}.$$

Then it follows that

$$\int_0^\infty \frac{t^m}{\sqrt{t}(1+t)^n}dt = \int_0^\infty \frac{t^{m-\frac{1}{2}}}{(1+t)^n}dt = B\left(m+\frac{1}{2}, n-m-\frac{1}{2}\right)$$

$$= \frac{\Gamma(m+\frac{1}{2})\Gamma(n-m-\frac{1}{2})}{\Gamma(n)} = \frac{(2m-1)!!(2n-2m-3)!!}{2^{n-1}(n-1)!}\pi.$$

For $A = \begin{bmatrix} 1 & 0 \\ a & 1 \end{bmatrix}$, $B = \begin{bmatrix} 1 & 0 \\ b & 1 \end{bmatrix}$ one can see from (12) that

$$A\#B = \begin{bmatrix} 1 & 0 \\ & 1 \end{bmatrix}, \quad \text{where } * = \frac{1}{\pi}\int_0^\infty \frac{a+tb}{\sqrt{t}(1+t)^2}dt.$$

By (13), $$* = \frac{a-b}{\pi}\int_0^\infty \frac{1}{\sqrt{t}(1+t)^2}dt + \frac{b}{\pi}\int_0^\infty \frac{1}{\sqrt{t}(1+t)}dt$$

$$= \frac{a-b}{2} + b = \frac{a+b}{2}.$$

This together with (9) ensures that $A\#B = \frac{A+B}{2} = A\natural B$.

Suppose that $m = 3$.

Let $$A = \begin{bmatrix} 1 & 0 & 0 \\ a_1 & 1 & 0 \\ a_3 & a_2 & 1 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 & 0 \\ b_1 & 1 & 0 \\ b_3 & b_2 & 1 \end{bmatrix}.$$

Then $$A\#B = \begin{bmatrix} 1 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 \\ & \frac{a_2+b_2}{2} & 1 \end{bmatrix},$$

where $$* = \frac{a_3+b_3}{2} - \frac{(a_1-b_1)(a_2-b_2)}{\pi}\int_0^\infty \frac{t}{\sqrt{t}(1+t)^3}dt$$

$$= \frac{a_3+b_3}{2} - \frac{(a_1-b_1)(a_2-b_2)}{8}.$$

We conclude from (10) and (13) that $A\#B = A\natural B$.

For $m = 4$, let $$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ a_1 & 1 & 0 & 0 \\ a_4 & a_2 & 1 & 0 \\ a_6 & a_5 & a_3 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ b_1 & 1 & 0 & 0 \\ b_4 & b_2 & 1 & 0 \\ b_6 & b_5 & b_3 & 1 \end{bmatrix}.$$

Then $$A\#B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 & 0 \\ * & \frac{a_2+b_2}{2} & 1 & 0 \\ *** & ** & \frac{a_3+b_3}{2} & 1 \end{bmatrix},$$

where
$$\begin{aligned} * &= \frac{1}{\pi}\int_0^\infty \frac{(a_4+tb_4)(1+t)-(a_1-b_1)(a_2-b_2)t}{\sqrt{t}(1+t)^3}dt \\ &= \frac{1}{\pi}\int_0^\infty \frac{a_4+tb_4}{\sqrt{t}(1+t)^2}dt - \frac{1}{\pi}\int_0^\infty \frac{(a_1-b_1)(a_2-b_2)t}{\sqrt{t}(1+t)^3}dt \\ &= \frac{a_4+b_4}{2} - \frac{(a_1-b_1)(a_2-b_2)}{8}, \end{aligned}$$

$$\begin{aligned} ** &= \frac{1}{\pi}\int_0^\infty \frac{(a_5+tb_5)(1+t)-(a_2-b_2)(a_3-b_3)t}{\sqrt{t}(1+t)^3}dt \\ &= \frac{1}{\pi}\int_0^\infty \frac{a_5+tb_5}{\sqrt{t}(1+t)^2}dt - \frac{1}{\pi}\int_0^\infty \frac{(a_2-b_2)(a_3-b_3)t}{\sqrt{t}(1+t)^3}dt \\ &= \frac{a_5+b_5}{2} - \frac{(a_2-b_2)(a_3-b_3)}{8}, \end{aligned}$$

$$\begin{aligned} *** &= \frac{1}{\pi}\int_0^\infty \frac{(a_6+tb_6)(1+t)^2}{\sqrt{t}(1+t)^4}dt \\ &\quad - \frac{(a_3-b_3)(a_4-b_4)+(a_1-b_1)(a_5-b_5)}{\pi}\int_0^\infty \frac{(1+t)t}{\sqrt{t}(1+t)^4}dt \\ &\quad + \frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)}{\pi}\int_0^\infty \frac{t}{\sqrt{t}(1+t)^4}dt \\ &= \frac{a_6+b_6}{2} - \frac{(a_3-b_3)(a_4-b_4)+(a_1-b_1)(a_5-b_5)}{8} \\ &\quad + \frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)}{16}. \end{aligned}$$

We conclude that $A\#B$ is well-defined on $\mathcal{N}_4$ and is equal to $A\natural B$.

3. Proof of the main theorem

We recall that if A is a complex square matrix and $\sigma(A)$, the set of eigenvalues of A, lies in $\mathbb{C}\setminus(-\infty,0]$, then A has a unique square root, called the principal square root, whose spectrum lies in the open right half plane and is given by

$$A^{1/2} = \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}A(tI+A)^{-1}dt. \tag{14}$$

Generally, $$A^p = \frac{\sin p\pi}{\pi}\int_0^\infty t^{1-p}A(tI+A)^{-1}dt, \qquad 0<p<1. \tag{15}$$

See [4, 8, 9] for details.

Let $A\in\mathcal{N}_m$. Obviously $\sigma(A)=\{1\}\subset\mathbb{C}\setminus(-\infty,0]$. The diagonal entries of

$$\frac{1}{\sqrt{t}}A(tI+A)^{-1} = \frac{1}{\sqrt{t}}(I+tA^{-1})^{-1}$$

are all $\dfrac{1}{\sqrt{t}(1+t)}$ and hence by (12): $\qquad A^{1/2}\in\mathcal{N}_m. \qquad (16)$

This implies that the Lie group $\mathcal{N}_m$ is uniquely 2-divisible. This together with the group property of $\mathcal{N}_m$ implies that

$$A^{-1/2}BA^{-1/2} \in \mathcal{N}_m$$

for all $A, B \in \mathcal{N}_m$. In particular,

$$A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2} \in \mathcal{N}_m, \qquad \forall A, B \in \mathcal{N}_m. \tag{17}$$

Remark 3.1. Let $\mathfrak{n}_m$ be the Lie algebra of $\mathcal{N}_m$, the space of lower triangular matrices with vanishing diagonal entries. The exponential map $\exp : \mathfrak{n}_m \to \mathcal{N}_m$ is bijective. Its inverse is given by

$$\log A = \int_0^\infty \left[(1+t)^{-1}I - (tI + A)^{-1}\right] dt. \tag{18}$$

We then have $$A^{1/2} = e^{(1/2)\log A}, \quad \forall A \in \mathcal{N}_m.$$

The integral formula (18) holds for every A with $\sigma(A) \subset \mathbb{C} \setminus (-\infty, 0]$ and hence the preceding results holds on the Lie group $\mathcal{L}_m$, whose Lie algebra is the space of lower triangular matrices with real diagonal entries.

Let $A, B \in \mathcal{N}_m$. It is direct to see from $A^{1/2}B^{-1}A^{1/2} \in \mathcal{N}_m$ that

$$I + tA^{1/2}B^{-1}A^{1/2}$$

is invertible for all $t \geq 0$ (indeed, all of its diagonal entries are positive) and hence

$$(tA) : B = tA^{1/2}\left[I + tA^{1/2}B^{-1}A^{1/2}\right]^{-1}A^{1/2}$$

is well-defined, where $A : B = (A^{-1} + B^{-1})^{-1}$ is the parallel addition of invertible matrices A and B. One can see that

$$\frac{t+1}{t}||(tA) : B|| \leq \frac{(t+1)||A^{1/2}||^2}{1 - t||A^{1/2}B^{-1}A^{1/2}||}$$

and the right had side is bounded for sufficiently small $t > 0$. Similarly

$$(tA) : B = \left[(tA)^{-1} + B^{-1}\right]^{-1} = B^{1/2}\left[I + t^{-1}B^{1/2}A^{-1}B^{1/2}\right]^{-1}B^{1/2}$$

and $$\frac{t+1}{t}||(tA) : B|| \leq \frac{(t+1)||B^{1/2}||^2}{t - ||B^{1/2}A^{-1}B^{1/2}||}.$$

(We have used the Neumann formula $(I - A)^{-1} = \sum_{k=0}^{\infty} A^k$ for $||A|| < 1$). The right had side is bounded for sufficiently large $t > 0$.

We conclude that $A\#B$, the integrand (3) of lower unitriangular matrices A and B, is absolutely convergent and hence is well defined. By (16) and (17),

$$\begin{aligned} A\#B &= A^{1/2}\left[\frac{1}{\pi}\int_0^\infty \frac{\left(I + t(A^{-1/2}BA^{-1/2})^{-1}\right)^{-1}}{\sqrt{t}}dt\right]A^{1/2} \\ &= A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2} \in \mathcal{N}_m. \end{aligned} \tag{19}$$

An immediate consequence of the preceding result is

Proposition 3.2. *Let $A, B \in \mathcal{N}_m$. For $X \in \mathcal{N}_m$, $X = A\#B$ if and only if $XA^{-1}X = B$. Moreover, $A\#B = B\#A$, $(XAX)\#(XBX) = X(A\#B)X$ and $(A\#B)^{-1} = A^{-1}\#B^{-1}$ for every $X \in \mathcal{N}_m$.*

Remark 3.3. In [8], F. Hiai established a multi-dimensional version of Löwner theorem for dissipative operators; every operator mean of positive definite operators on a Hilbert space admits an analytic continuation on the space of dissipative operators, the Siegel upper half plane. His elegant idea that we have taken here for the operator geometric mean on Lie group $\mathcal{N}_m$ is available for any operator mean on the Lie group of lower triangular matrices with diagonal matrices. In fact, the absolute convergence of the integral in (1) for every operator monotone function f holds for matrices in $\mathcal{L}_m$ in a similar way and hence the operator mean (1) is well-defined and belongs to $\mathcal{L}_m$. The properties in the above holds true for the operator geometric means on $\mathcal{L}_m$.

Next, we consider the iteration (4) for lower unitriangular matrices and will show that the iteration always terminates after the finite number of steps $k = \lceil \log_2 m \rceil$. For $A \in \mathcal{N}_m$, we decompose $A = I + N_A$, where $N_A \in \mathfrak{n} := \mathfrak{n}_m$, the set of all $m \times m$ lower triangular nilpotent matrices. Then the inverse of $A = I + N_A$ is

$$A^{-1} = (I + N_A)^{-1} = I + \sum_{k=1}^{m-1} (-1)^k N_A^k. \tag{20}$$

We are greatly indebted to Professor Fumio Hiai for suggesting the following nice lemma.

Lemma 3.4. *For $A, B \in \mathcal{N}_m$,*

$$\left[\frac{A^{-1} + B^{-1}}{2}\right]^{-1} = \frac{A+B}{2} - \left[\frac{N_A - N_B}{2}\right]\left[I + \frac{N_A + N_B}{2}\right]^{-1}\left[\frac{N_A - N_B}{2}\right].$$

Proof. It suffices to show that

$$\left[\frac{A^{-1} + B^{-1}}{2}\right]^{-1} = \frac{A+B}{2} - \left[\frac{A-B}{2}\right]\left[\frac{A+B}{2}\right]^{-1}\left[\frac{A-B}{2}\right].$$

Letting $X := A^{-1/2}BA^{-1/2}$ we have

$$A^{-1/2}(LHS)A^{-1/2} = \left[\frac{I + X^{-1}}{2}\right]^{-1} = 2X(I+X)^{-1}$$

and

$$\begin{aligned} A^{-1/2}(RHS)A^{-1/2} &= \frac{I+X}{2} - \left[\frac{I-X}{2}\right]\left[\frac{I+X}{2}\right]^{-1}\left[\frac{I-X}{2}\right] \\ &= \frac{I+X}{2} - \frac{(I-X)^2(I+X)^{-1}}{2} \\ &= \frac{(I+X)^{-1}\left[(I+X)^2 - (I-X)^2\right]}{2} = 2X(I+X)^{-1}. \qquad \blacksquare \end{aligned}$$

Define subspaces $\mathfrak{n}^{(k)}$ of $\mathfrak{n}$

$$\{0\} = \mathfrak{n}^{(m+l)} = \mathfrak{n}^{(m)} \subset \mathfrak{n}^{(m-1)} \subset \cdots \subset \mathfrak{n}^{(1)} = \mathfrak{n}$$

where $l \in \mathbb{N}$ and $\mathfrak{n}^{(k)}$ for $1 < k < m$ consists of lower triangular nilpotent matrices having vanishing entries along the j-th subdiagonal, $1 \le j \le k$. For instance, $\mathfrak{n}^{(2)}$ consists of strictly lower triangular matrices with the following form:

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & \vdots \\ * & 0 & 0 & \cdots & \vdots \\ \vdots & \ddots & & & \\ * & * & * & \cdots & 0 \end{bmatrix}.$$

It is direct to check that $\mathfrak{n}^{(k)}\mathfrak{n}^{(l)} \subset \mathfrak{n}^{(k+l)}$ for all k, l.

Let $A, B \in \mathcal{N}_m$ and consider the sequences A_k and B_k of the iteration precess from the given $A, B \in \mathcal{N}_m$. We shall show that $A_k = I + N_{A_k} = I + N_{B_k} = B_k$ for all $k \ge \lceil \log_2 m \rceil$. That is, $N_{A_k} - N_{B_k} = 0$ for $2^k > m$. It suffices to show that

$$N_{A_k} - N_{B_k} \in \mathfrak{n}^{(2^k)}, \qquad \forall k \ge 0. \tag{21}$$

It is easy to check that N_{A_0}, $N_{B_0} \in \mathfrak{n}^{(1)}$. Suppose that $N_{A_k} - N_{B_k} \in \mathfrak{n}^{(2^k)}$. By Lemma 3.4 and (20),

$$\begin{aligned} N_{A_{k+1}} - N_{B_{k+1}} = A_{k+1} - B_{k+1} &= \frac{A_k + B_k}{2} - \left[\frac{A_k^{-1} + B_k^{-1}}{2}\right]^{-1} \\ &= \left[\frac{N_{A_k} - N_{B_k}}{2}\right]\left[I + \frac{N_{A_k} + N_{B_k}}{2}\right]^{-1}\left[\frac{N_{A_k} - N_{B_k}}{2}\right] \\ &= \left[\frac{N_{A_k} - N_{B_k}}{2}\right]\left[I + \sum_{j=1}^{m-1}(-1)^j\left(\frac{N_{A_k} + N_{B_k}}{2}\right)^j\right]\left[\frac{N_{A_k} - N_{B_k}}{2}\right] \\ &= \sum_{j=1}^{m-1}(-1)^j\left[\frac{N_{A_k} - N_{B_k}}{2}\right]\left(\frac{N_{A_k} + N_{B_k}}{2}\right)^j\left[\frac{N_{A_k} - N_{B_k}}{2}\right] \\ &\quad + \left[\frac{N_{A_k} - N_{B_k}}{2}\right]^2 \in \mathfrak{n}^{(2^{k+1})}. \end{aligned}$$

By induction, we complete the proof of (21). We let $A\natural B$ the common limit of the iteration process from A and B.

Finally we shall show that $A\#B = A\natural B$ for all $A, B \in \mathcal{N}_m$. It is straightforward to see that the geometric mean $A\natural B$, the common limit of the iteration, satisfies the group invariance (1). Also, the mean $A\#B$ satisfies this property:

$$\begin{aligned} (XAX)\#(XBX) &= \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}}\left[(XAX)^{-1} + t(XBX)^{-1}\right]^{-1} dt \\ &= \frac{1}{\pi}\int_0^\infty \frac{1}{\sqrt{t}} X\left[A^{-1} + tB^{-1}\right]^{-1} X\, dt \\ &= X(A\#B)X. \end{aligned}$$

Then we may assume that $B = I$. In this case, the sequence A_k in the iteration process (4) defining $A\natural I$ coincides with the Newton's iteration

$$X_{k+1} = \frac{X_k + X_k^{-1}A}{2}, \qquad X_0 = I. \tag{22}$$

Indeed,
$$X_1 = \frac{I + A}{2} = A_1, \qquad B_1 = A_1^{-1}A = AA_1^{-1} \tag{23}$$

and then $X_k = A_k$ and $B_k = A_k^{-1}A = AA_k^{-1}$ for all $k \geq 0$, by induction. This implies that the limit $X_\infty := \lim A_k = A\natural I$ satisfies $X^2 = A$. By Proposition 3.2,

$$X_\infty = A\natural I = A^{1/2} = A\#I.$$

Remark 3.5. For $A, B \in \mathcal{L}_m$, the iteration process of the arithmetic and harmonic means converges to the common limit $A\#B$ by the reduction $B = I$ and Iannazzo's result [10] on the convergence of the Newton's algorithm (22) for any matrix A with $\sigma(A) \subset \mathbb{C} \setminus (-\infty, 0]$.

Remark 3.6. For every $A = [a_{ij}] \in \mathcal{L}_m$ can be written uniquely as $A = A'D_A$, where $D_A = \operatorname{diag}(a_{11}, \ldots, a_{mm})$ is the diagonal part of A and $A' \in \mathcal{N}_m$. Then for $A, B \in \mathcal{L}_m$, we have

$$A\#B = (A\#B)'D_{A\#B}.$$

By (2), $D_{A\#B} = \sqrt{D_{AB}}$ and hence $A'\#B' = (A\#B)\sqrt{D_{A^{-1}B^{-1}}}$. One may expect that $(A\#B)' = A'\#B'$. It probably fails.

4. Simply connected nilpotent Lie groups

Let G be a (uniquely) 2-divisible subgroup of $\mathcal{N}_m$. Then

$$A\#B := A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2} \in G, \qquad \forall A, B \in G.$$

By Theorem 1.1, it has the integral expression (3) and also the finite iteration algorithm (4), although the subgroup G is not closed under the arithmetic and harmonic means, in general. Such 2-divisible subgroups arise commonly from finite dimensional simply connected nilpotent Lie groups.

Let G be a finite dimensional simply connected nilpotent Lie group and let $\mathfrak{g}$ be its Lie algebra. Since $\exp : \mathfrak{g} \to G$ is diffeomorphic, G is uniquely 2-divisible. By Lie-Kolchin Theorem (cf. Theorem 3.6.6 of [16]), G has a faithful representation $\rho : G \to \mathcal{N}_m$ and hence $\rho(G)$ is a 2-divisible subgroup of $\mathcal{N}_m$. It is well known that the group G is isomorphic to $(\mathfrak{g}, *)$, where $x * y$ is the Baker-Campbell-Hausdorff multiplication and satisfies $\exp(x * y) = \exp(x)\exp(y)$. Note that $0 \in \mathfrak{g}$ acts as the identity element and $x \mapsto -x$ is inversion on the group $(\mathfrak{g}, *)$. Also, $x * x = 2x$ for all $x \in \mathfrak{g}$ and hence $(1/2)x$ is a unique square root of x. Define

$$x\#y := \frac{x}{2} * \frac{\left(\frac{-x}{2} * y * \frac{-x}{2}\right)}{2} * \frac{x}{2}, \qquad x, y \in \mathfrak{g}.$$

Then $\exp(x\#y) = \exp(x)\#\exp(y)$, where $a\#b = a^{1/2}(a^{-1/2}ba^{-1/2})^{1/2}a^{1/2}$ for $a, b \in G$. The integral representation and finite iteration algorithm for $x\#y$ exist by appealing on the Lie algebras $\mathfrak{g} \leq \mathfrak{n}_m$ and the faithful representation of G.

5. Final remarks

Every group G is a Loos symmetric space equipped with the binary operation $x \bullet y := xy^{-1}x$. If G is uniquely 2-divisible, then the equation $x \bullet a = b$ has a unique solution $x \in X$, called the *midpoint* or *mean* of a and b, and denoted by $a\#b$. One can directly see that $a\#b = a^{1/2}(a^{-1/2}ba^{-1/2})^{1/2}a^{1/2}$ ([13, 14]). The Lie group $\mathcal{L}_m$ is uniquely 2-divisible and hence $A\#B := A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$ appears in this context. In this paper, we have obtained its integral representation and the iteration algorithm (4) on $\mathcal{L}_m$.

We have shown that the operator means $\mu_f(A,B) := A^{1/2}f(A^{-1/2}BA^{-1/2})A^{1/2}$ over operator monotone functions $f > 0$ with $f(1) = 1$ are well defined on $\mathcal{L}_m$. For instance, the weighted geometric means $A\#_pB := A^{1/2}(A^{-1/2}BA^{-1/2})^pA^{1/2}$, $0 \le p \le 1$, exist on $\mathcal{L}_m$. It is of interest to study operator means on general uniquely 2-divisible matrix Lie groups, where the geometric mean

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

already exists.

The geometric mean $A\natural B$ from the iteration process of arithmetic and harmonic means of lower unitriangular matrices is natural in the context of the matrix geometric means. Finding a closed form for $A\natural B$ in terms of the entries of A and B for general $m \ge 5$, like (10) and (11), is attractive for further work.

The geometric mean $A\#B$ of positive definite matrices arises as the unique midpoint between A and B for the Riemannian trace metric δ on the open convex cone $\mathbb{P}_m$ of $m \times m$ Hermitian positive definite matrices, where $\delta(A,B) = \|\log A^{-1/2}BA^{-1/2}\|_2$ (see [12]). It is unknown to us whether the operator geometric mean $A\#B$ of lower unitriangular matrices can be realized as a metric midpoint on the Lie group $\mathcal{N}_m$ or not. Since $\log(A^{-1/2}BA^{-1/2})$ is in the Lie algebra of $\mathcal{N}_m$, the notion of $\delta(A,B) := ||\log A^{-1/2}BA^{-1/2}||_2$ on $\mathcal{N}_m$ seems natural to consider as one of desired metrics. But we do not know whether it is indeed a metric on the Lie group $\mathcal{N}_m$, and also whether $\delta(A,B) = (1/2)\delta(A, A\#B)$ for all $A, B \in \mathcal{N}_m$ or not.

The original motivation of this paper was the LDL^* decomposition (square-root-free Cholesky factorization) of positive definite matrices $A = LDL^*$, where L is a lower unitriangular matrix and D is a diagonal matrix with positive diagonal entries. A closed form for the LDL^* decomposition of the geometric mean $A\#B$ of positive definite matrices is unknown [15]. It is then natural to see how our geometric mean on $\mathcal{N}_m$ is closely related to this decomposition and the Lie group action $\mathcal{N}_m \times \mathbb{P}_m \to \mathbb{P}_m$ defined by $(A, P = LDL^*) \mapsto ALDL^*A^*$. In general, for the LDL^* factorization of two positive definite matrices $X = ADA^*$ and $Y = BFB^*$,

$$X\#Y = (ADA^*)\#(BDB^*) \neq (A\#B)\sqrt{DF}(A\#B)^*.$$

This gives an alternative new binary operation $X{*}Y := (A\#B)\sqrt{DF}(A\#B)^*$ on $\mathbb{P}_m$.

Finally, one can see that for lower triangular nilpotent matrices X and Y, the curve $\gamma(t) = e^{tX}\#e^{tY}$ is smooth with $\gamma(0) = I$ and $\gamma'(0) = (1/2)(X+Y)$ using the Riccati equation. Then we obtain an alternative Lie-Trotter formula

$$e^{\frac{X+Y}{2}} = \lim_{t\to 0}\left(e^{tX}\#e^{tY}\right)^{\frac{1}{t}}.$$

This is well known for Hermitian matrices (cf. [1]). We expect various results from the operator geometric mean on $\mathcal{N}_m$ and also on $\mathcal{L}_m$ that are well known on

Hermitian matrices and positive definite matrices through the exponential map. For instance, the (resp. finite step) convergence of the iteration of arithmetic and geometric means on $\mathcal{L}_m$ (resp. on $\mathcal{N}_m$).

6. Appendix: Proof of (11)

Let
$$A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ a_1 & 1 & 0 & 0 \\ a_4 & a_2 & 1 & 0 \\ a_6 & a_5 & a_3 & 1 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ b_1 & 1 & 0 & 0 \\ b_4 & b_2 & 1 & 0 \\ b_6 & b_5 & b_3 & 1 \end{bmatrix}$$

be 4×4 lower unitriangular matrices. Then

$$A^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -a_1 & 1 & 0 & 0 \\ a_1a_2 - a_4 & -a_2 & 1 & 0 \\ a_1a_5 + a_3a_4 - (a_1a_2a_3 + a_6) & a_2a_3 - a_5 & -a_3 & 1 \end{bmatrix}, \tag{24}$$

$$B^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -b_1 & 1 & 0 & 0 \\ b_1b_2 - b_4 & -b_2 & 1 & 0 \\ b_1b_5 + b_3b_4 - (b_1b_2b_3 + b_6) & b_2b_3 - b_5 & -b_3 & 1 \end{bmatrix} \tag{25}$$

and

$$A_1 = \frac{A+B}{2} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 & 0 \\ \frac{a_4+b_4}{2} & \frac{a_2+b_2}{2} & 1 & 0 \\ \frac{a_6+b_6}{2} & \frac{a_5+b_5}{2} & \frac{a_3+b_3}{2} & 1 \end{bmatrix}, \tag{26}$$

$$B_1^{-1} = \frac{A^{-1}+B^{-1}}{2} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{a_1+b_1}{2} & 1 & 0 & 0 \\ x & -\frac{a_2+b_2}{2} & 1 & 0 \\ z & y & -\frac{a_3+b_3}{2} & 1 \end{bmatrix}, \tag{27}$$

where

$$x = \frac{a_1a_2 - a_4 + b_1b_2 - b_4}{2}, \quad y = \frac{a_2a_3 - a_5 + b_2b_3 - b_5}{2},$$

$$z = \frac{a_1a_5 + a_3a_4 - (a_1a_2a_3 + a_6) + b_1b_5 + b_3b_4 - (b_1b_2b_3 + b_6)}{2}.$$

By (24) and (25),

$$B_1 = \left[\frac{A^{-1}+B^{-1}}{2}\right]^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \frac{a_1+b_1}{2} & 1 & 0 & 0 \\ x' & \frac{a_2+b_2}{2} & 1 & 0 \\ z' & y' & \frac{a_3+b_3}{2} & 1 \end{bmatrix}, \tag{28}$$

where

$$\begin{aligned}
x' &= \frac{(a_1+b_1)(a_1+b_2)}{4} - x = \frac{(a_1+b_1)(a_1+b_2)}{4} - \frac{a_1a_2 - a_4 + b_1b_2 - b_4}{2} \\
&= \frac{a_4+b_4}{2} - \frac{1}{4}(a_1-b_1)(a_2-b_2), \\
y' &= \frac{(a_2+b_2)(a_3+b_3)}{4} - y = \frac{(a_2+b_2)(a_3+b_3)}{4} - \frac{a_2a_3 - a_5 + b_2b_3 - b_5}{2} \\
&= \frac{a_5+b_5}{2} - \frac{1}{4}(a_2-b_2)(a_3-b_3), \\
z' &= -\frac{(a_1+b_1)y}{2} - \frac{(a_3+b_3)x}{2} - \left[-\frac{(a_1+b_1)(a_2+b_2)(a_3+b_3)}{8} + z\right] \\
&= \frac{a_6+b_6}{2} - \frac{(a_1-b_1)(a_5-b_5)+(a_3-b_3)(a_4-b_4)}{4} + \frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)}{8},
\end{aligned}$$

and

$$A_1^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{a_1+b_1}{2} & 1 & 0 & 0 \\ x'' & -\frac{a_2+b_2}{2} & 1 & 0 \\ z'' & y'' & -\frac{a_3+b_3}{2} & 1 \end{bmatrix}, \tag{29}$$

where

$$\begin{aligned}
x'' &= \frac{(a_1+b_1)(a_2+b_2)}{4} - \frac{a_4+b_4}{2}, \quad y'' = \frac{(a_2+b_2)(a_3+b_3)}{4} - \frac{a_5+b_5}{2}, \\
z'' &= \frac{(a_1+b_1)(a_5+b_5)+(a_3+b_3)(a_4+b_4)}{4} \\
&\quad -\frac{(a_1+b_1)(a_2+b_2)(a_3+b_3)}{8} - \frac{a_6+b_6}{2}.
\end{aligned}$$

Note that

$$x' + x'' - x = \frac{a_4+b_4}{2}, \qquad y' + y'' - y = \frac{a_5+b_5}{2}, \tag{30}$$

and

$$\begin{aligned}
z' + z'' + z = {} & \frac{a_6+b_6}{2} - \frac{(a_1-b_1)(a_5-b_5)+(a_3-b_3)(a_4-b_4)}{4} \\
&+ \frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)}{8} + \frac{(a_1+b_1)(a_5+b_5)+(a_3+b_3)(a_4+b_4)}{4} \\
&- \frac{(a_1+b_1)(a_2+b_2)(a_3+b_3)}{8} - \frac{a_6+b_6}{2} \\
&+ \frac{a_1a_5 + a_3a_4 - (a_1a_2a_3 + a_6) + b_1b_5 + b_3b_4 - (b_1b_2b_3 + b_6)}{2} \\
= {} & -\frac{a_6+b_6}{2} + \frac{a_1a_5 + a_3a_4 + b_1b_5 + b_3b_4}{2} \\
&+ \frac{(a_1+b_1)(a_5+b_5) - (a_1-b_1)(a_5-b_5)}{4} \\
&+ \frac{(a_3+b_3)(a_4+b_4) - (a_3-b_3)(a_4-b_4)}{4}
\end{aligned}$$

$$
\begin{aligned}
&+\frac{(a_1-b_1)(a_3-b_3)(a_2+b_2)-(a_1+b_1)(a_2+b_2)(a_3+b_3)}{8}\\
&-\frac{a_1a_2a_3+b_1b_2b_3}{2}\\
=&-\frac{a_6+b_6}{2}+\frac{1}{2}(a_1a_5+a_3a_4+b_1b_5+b_3b_4+a_1b_5+a_5b_1+a_3b_4+a_4b_3)\\
&-\frac{1}{4}(2a_1a_2a_3+2b_1b_2b_3+a_1a_2b_3+a_1b_2b_3+a_2a_3b_1+a_3b_1b_2)\\
=&-\frac{a_6+b_6}{2}+\frac{(a_1+b_1)(a_5+b_5)+(a_3+b_3)(a_4+b_4)}{2}-*,
\end{aligned}
$$

where $\quad * := \frac{1}{4}(2a_1a_2a_3+2b_1b_2b_3+a_1a_2b_3+a_1b_2b_3+a_2a_3b_1+a_3b_1b_2).$

We claim that $A_2 = B_2$, equivalently, $I = A_2B_2^{-1}$. Since

$$
A_2 = \frac{A_1+B_1}{2}, \qquad B_2^{-1} = \frac{A_1^{-1}+B_1^{-1}}{2},
$$

it suffices to show that $(A_1+B_1)(A_1^{-1}+B_1^{-1}) = 4I$, that is,

$$
A_1B_1^{-1} + B_1A_1^{-1} = 2I.
$$

By (27) and (29),

$$
\begin{aligned}
A_1B_1^{-1} &= \begin{bmatrix} 1 & 0 & 0 & 0\\ \frac{a_1+b_1}{2} & 1 & 0 & 0\\ \frac{a_4+b_4}{2} & \frac{a_2+b_2}{2} & 1 & 0\\ \frac{a_6+b_6}{2} & \frac{a_5+b_5}{2} & \frac{a_3+b_3}{2} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0\\ -\frac{a_1+b_1}{2} & 1 & 0 & 0\\ x & -\frac{a_2+b_2}{2} & 1 & 0\\ z & y & -\frac{a_3+b_3}{2} & 1 \end{bmatrix},\\
B_1A_1^{-1} &= \begin{bmatrix} 1 & 0 & 0 & 0\\ \frac{a_1+b_1}{2} & 1 & 0 & 0\\ x' & \frac{a_2+b_2}{2} & 1 & 0\\ z' & y' & \frac{a_3+b_3}{2} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0\\ -\frac{a_1+b_1}{2} & 1 & 0 & 0\\ x'' & -\frac{a_2+b_2}{2} & 1 & 0\\ z'' & y'' & -\frac{a_3+b_3}{2} & 1 \end{bmatrix}.
\end{aligned}
$$

Using (30), the sum of $(3,1)$ (resp. $(4,2)$) entries of $A_1B_1^{-1}$ and $B_1A_1^{-1}$ is zero. The sum of $(4,1)$ entries of $A_1B_1^{-1}$ and $B_1A_1^{-1}$ is

$$
\begin{gathered}
\frac{a_6+b_6}{2} - \frac{(a_1+b_1)(a_5+b_5)}{4} + \frac{a_3+b_3}{2}x + z\\
+z' - \frac{a_1+b_1}{2}y' + \frac{a_3+b_3}{2}x'' + z'',
\end{gathered}
$$

and is equal to zero if and only if

$$
\begin{aligned}
z'+z''+z &= -\left[\frac{a_6+b_6}{2} - \frac{(a_1+b_1)(a_5+b_5)}{4} + \frac{a_3+b_3}{2}x - \frac{a_1+b_1}{2}y' + \frac{a_3+b_3}{2}x''\right]\\
&= -\frac{a_6+b_6}{2} + \frac{a_1+b_1}{2}\left[\frac{a_5+b_5}{2}+y'\right] - \frac{a_3+b_3}{2}(x+x'')\\
&= -\frac{a_6+b_6}{2} + \frac{a_1+b_1}{2}\left[a_5+b_5-\frac{1}{4}(a_2-b_2)(a_3-b_3)\right]\\
&\quad -\frac{a_3+b_3}{2}\left[-(a_4+b_4)+\frac{1}{4}(3a_1a_2+3b_1b_2+a_1b_2+a_2b_1)\right]\\
&= -\frac{a_6+b_6}{2} + \frac{(a_1+b_1)(a_5+b_5)+(a_3+b_3)(a_4+b_4)}{2} - \star,
\end{aligned}
$$

where

$$\star = \frac{1}{8}\left[(a_1+b_1)(a_2-b_2)(a_3-b_3)+(a_3+b_3)(3a_1a_2+3b_1b_2+a_1b_2+a_2b_1)\right].$$

One can check that $\star = *$ and hence the equality in above holds true. We have shown that $A\natural B = A_2 = B_2$.

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