Constructing matrix geometric means

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Abstract

In this paper, we analyze the process of "assembling" new matrix geometric means from existing ones, and show what new means can be found, and what cannot be done because of group-theoretical obstructions. We show that for $n = 4$ a new matrix mean exists which is simpler to compute than the existing ones. Moreover, we show that for $n > 4$ the existing strategies of composing matrix means and taking limits of iterations cannot provide a mean computationally simpler than the existing ones.

Keywords. matrix geometric mean; positive definite matrix; invariance properties; groups of permutations
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1 Introduction

Several papers [1, 2, 3, 4, 6, 7] are devoted to defining a proper way to generalize the concept of geometric mean to $n \geq 3$ symmetric, positive definite $m \times m$ matrices. Ando, Li and Mathias [1], Lim [6], and Bini, Meini and Poloni [4] proposed different definitions of a geometric mean; their definitions are recursively based on limit processes and functions assembled by composing other matrix geometric means of $n' < n$ matrices.

In this paper, we aim to analyze in more detail the process of "assembling" new matrix means from existing ones, and show what new means can be found, and what cannot be done because of group-theoretical obstructions related to the symmetry properties of matrix means. We are interested only in those symmetries that can be deduced from the symmetry properties of the starting mean. For example, if the map $(X, Y) \mapsto X \# Y$

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is symmetric (i.e., $X \# Y = Y \# X$ for all $X, Y \in \mathbb{C}^{m\times m}$), then the map $(A_1, A_2, A_3, A_4) \mapsto (A_1 \# A_2) \#(A_3 \# A_4)$ is invariant for some permutations σ of $\{A_1, A_2, A_3, A_4\}$, for instance $(A_1, A_2, A_3, A_4) \mapsto (A_4, A_3, A_1, A_2)$, but not for some others, for instance $(A_1, A_2, A_3, A_4) \mapsto (A_3, A_2, A_1, A_4)$.

Of course, for special choices of the map # further unexpected symmetries may appear; e.g., if $X, Y \in \mathbb{C}^{m\times m}$, and $X \# Y$ is replaced by the addition $X+Y$, then the above map is invariant for *all* permutations of its arguments. However, for other choices of #, e.g. $X \# Y := (XY + YX)$, only the invariance properties that can be formally deduced from the symmetries of the "building blocks" are in effect. For matrix geometric means, except for the trivial case $m = 1$, no such additional properties seem to hold, so all attempts to define matrix geometric means with invariance properties appearing in literature are based on formal symmetries.

In the present paper, by means of a group-theoretical analysis, we will show that for $n = 4$ a new matrix mean exists which is simpler to compute than the existing ones; numerical experiments show that the new definition leads to a significant computational advantage. Moreover, we will show that for $n > 4$ the existing strategies of composing matrix means and taking limits cannot provide a mean which is computationally simpler than the existing ones.

2 Matrix geometric means

Notations Let us denote by $\mathbb{P}_m$ the space of symmetric positive-definite $m \times m$ matrices. For each $A, B \in \mathbb{P}_m$, we shall say that $A < B$ ($A \leq B$) if $B - A$ is positive definite (semidefinite). With A^* we denote the conjugate transpose of A. We shall say that $\underline{A} = (A_i)_{i=1}^n \in (\mathbb{P}_m)^n$ is a *scalar* n-tuple of matrices if $A_1 = A_2 = \cdots = A_n$. We shall use the convention that both $Q(\underline{A})$ and $Q(A_1, \dots, A_n)$ denote the application of the map $Q : (\mathbb{P}_m)^n \to \mathbb{P}_m$ to the n-tuple $\underline{A}$.

ALM axioms Ando, Li and Mathias [1] introduced ten axioms that define when a map $G : (\mathbb{P}_m)^n \to \mathbb{P}_m$ is called a *geometric mean*. Following their paper, we report here the axioms for $n = 3$ only, for the sake of simplicity; the generalization to different values of n is straightforward.

P1 Consistency with scalars. If A, B, C commute then $G(A, B, C) = (ABC)^{1/3}$.

P1' This implies $G(A, A, A) = A$.

P2 Joint homogeneity. $G(\alpha A, \beta B, \gamma C) = (\alpha\beta\gamma)^{1/3} G(A, B, C)$, for each $\alpha, \beta, \gamma > 0$.

P2' This implies $G(\alpha A, \alpha B, \alpha C) = \alpha G(A, B, C)$.

P3 Permutation invariance. $G(A, B, C) = G(\pi(A, B, C))$ for any permutation $\pi(A, B, C)$ of A, B, C.

P4 Monotonicity. $G(A, B, C) \geq G(A', B', C')$ whenever $A \geq A'$, $B \geq B'$, $C \geq C'$.

P5 Continuity from above. If A_n, B_n, C_n are monotonic decreasing sequences converging to A, B, C, respectively, then $G(A_n, B_n, C_n)$ converges to $G(A, B, C)$.

P6 Congruence invariance. $G(S^*AS, S^*BS, S^*CS) = S^*G(A, B, C)S$ for any nonsingular S.

P7 Joint concavity. If $A = \lambda A_1 + (1-\lambda)A_2$, $B = \lambda B_1 + (1-\lambda)B_2$, $C = \lambda C_1 + (1-\lambda)C_2$, then $G(A, B, C) \geq \lambda G(A_1, B_1, C_1) + (1-\lambda)G(A_2, B_2, C_2)$.

P8 Self-duality. $G(A, B, C)^{-1} = G(A^{-1}, B^{-1}, C^{-1})$.

P9 Determinant identity. $\det G(A, B, C) = (\det A \det B \det C)^{1/3}$.

P10 Arithmetic–geometric–harmonic mean inequality:

$$\frac{A+B+C}{3} \geq G(A, B, C) \geq \left(\frac{A^{-1}+B^{-1}+C^{-1}}{3}\right)^{-1}.$$

The matrix geometric mean for $n = 2$ For $n = 2$, the ALM axioms uniquely define a matrix geometric mean which can be expressed explicitly as

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

This is a particular case of the more general map

$$A \#_t B := A(A^{-1}B)^t, \quad t \in \mathbb{R}, \tag{2}$$

which has a geometrical interpretation as the parametrization of the geodesic joining A and B for a certain Riemannian geometry on $\mathbb{P}_m$ [2].

The ALM and BMP means Ando, Li and Mathias [1] recursively define a matrix geometric mean in this way. The mean G_2^{ALM} of two matrices coincides with (1); for $n \geq 3$, suppose the mean of $n-1$ matrices G_{n-1}^{ALM} is already defined. Given $A_1, \dots, A_n$, compute for each $j = 1, 2, \dots$

$$A_i^{(j+1)} = G_{n-1}^{ALM}(A_1^{(j)}, A_2^{(j)}, \dots A_{i-1}^{(j)}, A_{i+1}^{(j)}, \dots A_n^{(j)}) \quad i = 1, \dots, n, \tag{3}$$

where $A_i^{(0)} = A_i$, $i = 1, \dots n$. The sequences $(A_i^{(j)})_{j=1}^{\infty}$ converge to a common (not depending on i) matrix, and this matrix is a geometric mean of $A_1^{(0)}, \dots, A_n^{(0)}$.

The mean proposed by Bini, Meini and Poloni [4] is defined in the same way, but with (3) replaced by

$$A_i^{(j+1)} = G_{n-1}^{BMP}(A_1^{(j)}, A_2^{(j)}, \dots A_{i-1}^{(j)}, A_{i+1}^{(j)}, \dots A_n^{(j)}) \#_{1/n} A_i \quad i = 1, \dots, n. \tag{4}$$

Though both maps satisfy the ALM axioms, matrices A, B, C exist for which $G^{ALM}(A, B, C) \neq G^{BMP}(A, B, C)$.

While the former iteration converges linearly, the latter converges cubically, and thus allows one to compute a matrix geometric mean with a lower number of iterations. In fact, if we call p_k the average number of iterations that the process giving a mean of k matrices takes to converge (which may vary significantly depending on the starting matrices), the total computational cost of the ALM and BMP means can be expressed as $O(n! p_3 p_4 \dots p_n m^3)$. The only difference between the two complexity bounds lies in the expected magnitude of the values p_k. The presence of a factorial and of an exponential expression is undesirable, since it means that the problem scales very badly with n. In fact, already with $n = 7, 8$ and moderate values of m, a large CPU time is generally needed to compute a matrix geometric mean [4].

In the next sections, we shall address the problem whether the existing "tools" allow one to construct a matrix geometric mean which scales more nicely to large values of n.

3 Means obtained by map composition

Quasi-means Let us introduce the following variants to some of the Ando–Li–Mathias axioms.

P1" Weak consistency with scalars. There are $\alpha, \beta, \gamma \in \mathbb{R}$ such that if A, B, C commute, then $G(A, B, C) = A^{\alpha} B^{\beta} C^{\gamma}$.

P2” Weak homogeneity. There are $\alpha, \beta, \gamma \in \mathbb{R}$ such that for each $r, s, t > 0$, $G(rA, sB, tC) = r^\alpha s^\beta t^\gamma G(A, B, C)$. Notice that if P1” holds as well, these must be the same α, β, γ (proof: substitute scalar values in P1”).

P9’ Weak determinant identity. For all $d > 0$, if $\det A = \det B = \det C = d$, then $\det G(A, B, C) = d$.

We shall call a *quasi-mean* a function $Q : (\mathbb{P}_m)^n \to (\mathbb{P}_m)$ that satisfies P1”,P2”, P4, P6, P7, P8, P9’. This models expressions which are built starting from basic matrix means but are not symmetric, e.g. $A \# G(B, C, D)$.

Theorem 1. *If a quasi-mean Q satisfies P3, then it is a geometric mean.*

Proof. From P2” and P3, it follows that $\alpha = \beta = \gamma$. From P9’, it follows that if $\det A = \det B = \det C = 1$,

$$2 = \det(2A, 2B, 2C) = 2^{\alpha+\beta+\gamma} \det(A, B, C) = 2^{\alpha+\beta+\gamma},$$

thus $\alpha + \beta + \gamma = 1$. The two relations combined together yield $\alpha = \beta = \gamma = 1/3$. Finally, it is proved in Ando, Li and Mathias [1] that P5 and P10 are implied by the other eight properties P1–P4 and P6–P9. □

Isotropy groups of quasi-means

Group theory notations The notation $H \leq G$ ($H < G$) means that H is a subgroup (proper subgroup) of G. Let us denote by $\mathfrak{S}_n$ the symmetric group on n elements, i.e., the group of all permutations of the set $\{1, 2, \dots, n\}$. As usual, the symbol $(a_1 a_2 a_3 \dots a_k)$ stands for the permutation (“cycle”) that maps $a_1 \mapsto a_2$, $a_2 \mapsto a_3$, $\dots a_{k-1} \mapsto a_k$, $a_k \mapsto a_1$ and leaves the other elements of $\{1, 2, \dots n\}$ unchanged. Different symbols in the above form can be chained to denote the group operation of function composition; for instance, $\sigma = (13)(24)$ is the permutation $(1, 2, 3, 4) \mapsto (3, 4, 1, 2)$. We shall denote by $\mathfrak{A}_n$ the alternating group on n elements, i.e., the only subgroup of index 2 of $\mathfrak{S}_n$, and by $\mathfrak{D}_n$ the dihedral group over n elements, with cardinality $2n$. The latter is identified with the subgroup of $\mathfrak{S}_n$ generated by the rotation $(1, 2, \dots, n)$ and the mirror symmetry $(2, n-1)(3, n-2) \dots$.

We may define an action of $\mathfrak{S}_n$ on the set of quasi-means of n matrices as

$$\sigma Q(A_1, \dots, A_n) = Q(A_{\sigma^{-1}(1)}, \dots, A_{\sigma^{-1}(n)}),$$

in the usual contravariant manner. When Q is a quasi-mean of r matrices and $R_1, R_2, \dots R_r$ are quasi-means of n matrices, let us define $Q \circ (R_1, R_2, \dots R_r)$ as the map

$$(Q \circ (R_1, R_2, \dots R_r))\,(\underline{A}) := Q(R_1(\underline{A}), R_2(\underline{A}), \dots, R_r(\underline{A})). \qquad (5)$$

Theorem 2. *Let $Q(A_1, \dots, A_r)$ and $R_j(A_1, \dots A_n)$ (for $j = 1, \dots, n$) be quasi-means. Then,*

1. *For all $\sigma \in \mathfrak{S}_r$, σQ is a quasi-mean.*
2. *$(A_1, \dots, A_n, A_{r+1}) \mapsto Q(A_1, \dots, A_r)$ is a quasi-mean.*
3. *$Q \circ (R_1, R_2, \dots R_r)$ is a quasi-mean.*

Proof. All properties follows directly from the monotonicity (P4) and from the corresponding properties for the means Q and R_j. ☐

We may then define the *isotropy group*, or *stabilizer* of a quasi-mean Q

$$\mathrm{Stab}(Q) := \{\sigma \in \mathfrak{S}^n : \sigma Q = Q\}. \tag{6}$$

The following result shows that when examining function composition we may restrict to studying quasi-means whose arguments are in a special form.

Theorem 3. *Let Q be a quasi-mean of $r + s$ matrices, and $R_1, R_2, \dots, R_r$, $S_1, S_2, \dots, S_s$ be quasi-means of n matrices such that $R_i(\underline{A}) \neq \sigma S_j(\underline{A})$ for all $i, j, \underline{A}$ and every $\sigma \in \mathfrak{S}_n$. Then, in the generic case,*

$$\begin{aligned}\mathrm{Stab}(Q \circ (R_1, R_2, \dots, R_r, S_1, S_2, \dots, S_s)) \\ \subseteq \mathrm{Stab}(Q \circ (R_1, \dots, R_r, R_1, R_1, \dots, R_1)).\end{aligned} \tag{7}$$

Proof. Let σ be an element of $\mathrm{Stab}(Q \circ (R_1, R_2, \dots, R_r, S_1, S_2, \dots S_s))$; since the only invariance properties that we may assume on Q are those predicted by its invariance group, it must be the case that for each $\underline{A}$

$$(\sigma R_1(\underline{A}), \sigma R_2(\underline{A}), \dots, \sigma R_r(\underline{A}), \sigma S_1(\underline{A}), \sigma S_2(\underline{A}), \dots \sigma S_s(\underline{A}))$$

is a permutation of $(R_1(\underline{A}), R_2(\underline{A}), \dots, R_r(\underline{A}), S_1(\underline{A}), S_2(\underline{A}), \dots S_s(\underline{A}))$ belonging to $\mathrm{Stab}(Q)$. Since $R_i(\underline{A}) \neq \sigma S_j(\underline{A})$, this permutation must map the sets $\{R_1(\underline{A}), R_2(\underline{A}), \dots, R_r(\underline{A})\}$ and $\{S_1(\underline{A}), S_2(\underline{A}), \dots S_s(\underline{A})\}$ to themselves. Therefore, the same permutation maps

$$(R_1(\underline{A}), R_2(\underline{A}), \dots, R_r(\underline{A}), R_1(\underline{A}), R_1(\underline{A}), \dots R_1(\underline{A}))$$

to

$$(\sigma R_1(\underline{A}), \sigma R_2(\underline{A}), \dots, \sigma R_r(\underline{A}), \sigma R_1(\underline{A}), \sigma R_1(\underline{A}), \dots \sigma R_1(\underline{A})).$$

This implies that

$$\begin{aligned}Q(R_1(\underline{A}), R_2(\underline{A}), \dots, R_r(\underline{A}), R_1(\underline{A}), R_1(\underline{A}), \dots R_1(\underline{A})) \\ = Q(\sigma R_1(\underline{A}), \sigma R_2(\underline{A}), \dots, \sigma R_r(\underline{A}), \sigma R_1(\underline{A}), \sigma R_1(\underline{A}), \dots \sigma R_1(\underline{A}))\end{aligned}$$

as requested. ☐

Coset transversals Let now $H \leq \mathfrak{S}_n$, and let $\{\sigma_1, \ldots, \sigma_r\} \subset \mathfrak{S}_n$ be a transversal for the left cosets σH, i.e., a set of maximal cardinality $r = n!/|H|$ such that $\sigma_j^{-1}\sigma_i \notin H$ for all $i \neq j$. The group $\mathfrak{S}_n$ acts by permutation over the cosets $(\sigma_1 H, \ldots, \sigma_r H)$, i.e., there is a permutation $\tau = \rho_H(\sigma)$ such that

$$(\sigma\sigma_1 H, \ldots, \sigma\sigma_r H) = (\sigma_{\tau(1)} H, \ldots, \sigma_{\tau(r)} H)$$

Notice that if H is a normal subgroup of $\mathfrak{S}_n$, then the action of $\mathfrak{S}_n$ over the coset space is represented by the quotient group $\mathfrak{S}_n/H$, and the kernel of ρ_H is H.

If $H = \mathrm{Stab}(R)$, quasi-means in the form σR are uniquely determined by the coset to which σ belongs; therefore, by combining equal arguments and introducing dummy arguments if needed, we may assume that all function compositions take the form

$$Q \circ (\sigma_1 R, \sigma_2 R, \ldots \sigma_r R), \tag{8}$$

which we may briefly denote with $Q \circ R$, assuming a standard choice of the transversal for H. Notice that $Q \circ R$ depends on the ordering of the cosets $\sigma_1 H, \ldots, \sigma_r H$, but not on the choice of the coset representative σ_i, since $\sigma_i h Q(\underline{A}) = \sigma_i Q(\underline{A})$ for each $\underline{A}$ and $h \in H$.

Example 1. The quasi-mean $(A, B, C) \mapsto (A \# B) \# (B \# C)$ is $Q \circ Q$, where $Q(X, Y, Z) = X \# Y$, $H = \{(12)\}$, and the transversal is $\{e, (13), (23)\}$.

Example 2. The quasi-mean $(A, B, C) \mapsto (A \# B) \# C$ is not in the form (8), but in view of Theorem 3, its isotropy group is a subgroup of that of $(A, B, C) \mapsto (A \# B) \# (A \# B)$.

Theorem 4. *Let $G, H \leq \mathfrak{S}_n$, R be a quasi-mean of n matrices such that* $\mathrm{Stab}\, R \leq H$ *and Q be a quasi-mean of $r = n!/|H|$ matrices such that* $\rho_H(G) \leq \mathrm{Stab}(Q)$. *Then, the isotropy group of $Q \circ R$ contains G.*

Proof. Let $g \in G$ and $\tau = \rho_H(g)$; we have

$$\begin{aligned} g(Q \circ R)(\underline{A}) &= gQ\big(\sigma_1 R(\underline{A}), \sigma_2 R(\underline{A}), \ldots, \sigma_r R(\underline{A})\big) \\ &= Q\big(\sigma_1 R(g^{-1}\underline{A}), \sigma_2 R(g^{-1}\underline{A}), \ldots, \sigma_r R(g^{-1}\underline{A})\big) \\ &= Q\big(g\sigma_1 R(\underline{A}), g\sigma_2 R(\underline{A}), \ldots, g\sigma_r R(\underline{A})\big) \\ &= Q\big(\sigma_{\tau(1)} R(\underline{A}), \sigma_{\tau(2)} Q(\underline{A}), \ldots, \sigma_{\tau(r)} R(\underline{A})\big) \\ &= Q\big(\sigma_1 R(\underline{A}), \sigma_2 R(\underline{A}), \ldots, \sigma_r R(\underline{A})\big), \end{aligned}$$

where the last equality holds because $\tau \in \mathrm{Stab}(Q)$. □

Example 3. Let $Q(A,B,C,D) = (A \# C) \# (B \# D)$. Its isotropy group is the dihedral group $\mathfrak{D}_4$, of order 8. Its coset space has size $4!/8 = 3$, and we have $\rho_H(\mathfrak{S}_4) \cong \mathfrak{S}_3$. Thus $G_3 \circ Q$, where G_3 is any geometric mean of three elements, has isotropy group $\mathfrak{S}_4$ by Theorem 4, and therefore is a geometric mean.

It is important to notice that with the previous example we obtain a geometric mean of four matrices by means of a single limit process. This is more efficient than the existing definitions, which compute a mean of four matrices via several means of three matrices, each of which requires a limit process in its computation. We will return to this topic in Section 5.

Above four elements Is the technique of Theorem 4 of any help for $n > 4$? We will now see why the answer is no.

Theorem 5. *Suppose Theorem 4 holds with* $G \geq \mathfrak{A}_n$ *and* $n > 4$. *Then* $\mathfrak{A}_n \leq \operatorname{Stab}(Q)$ *or* $\mathfrak{A}_n \leq \operatorname{Stab}(R)$.

Proof. Let us consider $K = \ker \rho_H$. It is a normal subgroup of $\mathfrak{S}_n$, but for $n > 4$ the only normal subgroups of $\mathfrak{S}_n$ are the the trivial group $\{e\}$, $\mathfrak{A}_n$ and $\mathfrak{S}_n$ [5]. Let us consider the three cases separately.

1. $K = \{e\}$. In this case, $\rho_H(G) \cong G$, and thus $G \leq \operatorname{Stab} Q$.

2. $K = \mathfrak{S}_n$. In this case, $\rho_H(\mathfrak{S}_n)$ is the trivial group. But the action of $\mathfrak{S}_n$ over the coset space is transitive, since $\sigma_j \sigma_i^{-1}$ sends the coset $\sigma_i H$ to the coset $\sigma_j H$. So the only possibility is that there is a single coset in the coset space, i.e., $H = \mathfrak{S}_n$.

3. $K = \mathfrak{A}_n$. As in the above case, since the action is transitive, it must be the case that there are at most two cosets in the coset space, and thus $H = \mathfrak{S}_n$ or $H = \mathfrak{A}_n$. □

Thus it is impossible to apply Theorem 4 to obtain a quasi-mean with isotropy group containing $\mathfrak{A}_n$, unless one of the two starting quasi-means has an isotropy group already containing $\mathfrak{A}_n$.

4 Means obtained as limits

An algebraic setting for limit means We shall now describe a unifying algebraic setting in terms of isotropy groups for the known means defined by limit processes, such as the ALM-mean and the mean of Bini *et al.*

Let $S : (\mathbb{P}_m)^n \to (\mathbb{P}_m)^n$ be a map; we shall say that S *preserves* a subgroup $H < \mathfrak{S}_n$ if there is a map $\tau : H \to H$ such that $hS(\underline{A}) = S(h^{-1}\underline{A})$ is equal to $\tau(h)\left(S(\underline{A})\right)$ for all $\underline{A} \in \mathbb{P}_m$. In this case, τ must be a group homomorphism.

Theorem 6. *Let $S : (\mathbb{P}_m)^n \to (\mathbb{P}_m)^n$ be a map and $H < \mathfrak{S}_n$ be a permutation group such that*

1. *$(\underline{A}) \to \left(S(\underline{A})\right)_i$ is a quasi-mean for all $i = 1, \dots, n$,*
2. *S preserves H,*
3. *for all $\underline{A} \in (\mathbb{P}_m)^n$, $\lim_{k\to\infty} S^k(\underline{A})$ is a scalar n-tuple*[1]*,*

and let us denote by $S^\infty(\underline{A})$ the common value of all entries of the scalar n-tuple $\lim_{k\to\infty} S^k(\underline{A})$. Then, $S^\infty(\underline{A})$ is a quasi-mean with isotropy group H.

Proof. The fact that S^∞ is a quasi-mean follows from Theorem 2. Let us take $h \in H$. It is easy to prove by induction on k that $hS^k(\underline{A}) = \tau^k(h)\left(S^k(\underline{A})\right)$. Now, choose a matrix norm inducing the usual topology on $\mathbb{P}_m$; let $\varepsilon > 0$ be fixed, and let us take K such that for all $k > K$ and for all $i = 1, \dots, n$ the following inequalities hold:

- $\left\|\left(S^k(\underline{A})\right)_i - S^\infty(\underline{A})\right\| < \varepsilon,$
- $\left\|\left(S^k(h^{-1}\underline{A})\right)_i - S^\infty(h^{-1}\underline{A})\right\| < \varepsilon.$

We know that $\left(S^k(h^{-1}\underline{A})\right)_i = \left(\tau^k(h)S^k(\underline{A})\right)_i = \left(S^k(\underline{A})\right)_{\tau^k(h)(i)}$, therefore

$$\left\|S^\infty(\underline{A}) - S^\infty(h^{-1}\underline{A})\right\| \le \left\|\left(S^k(\underline{A})\right)_{\tau^k(h)(i)} - S^\infty(\underline{A})\right\| + \left\|\left(S^k(h^{-1}\underline{A})\right)_i - S^\infty(h^{-1}\underline{A})\right\| < 2\varepsilon.$$

Since ε is arbitrary, the two limits must coincide.This holds for each $h \in H$, therefore $H \le \operatorname{Stab} S^\infty$. ∎

Example 4. Let the map S be

$$\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} \mapsto \begin{pmatrix} A \# B \\ B \# C \\ C \# D \\ D \# A \end{pmatrix}.$$

S preserves the dihedral group $\mathfrak{D}_4$. Therefore, provided the iteration process converges to a scalar n-tuple, S^∞ is a quasi-mean with isotropy group $\mathfrak{D}_4$.

[1]Here S^k denotes function iteration: $S^1 = S$ and $S^{k+1}(\underline{A}) = S(S^k(\underline{A}))$ for all k.

Efficiency of the limit process

Theorem 7. *Let $S : (\mathbb{P}_m)^n \to (\mathbb{P}_m)^n$ preserve a group H. Then, the invariance group of each of its components S_i, $i = 1, \dots, n$, is a subgroup of H of index at most n.*

Proof. Let i be fixed, and set $I_k := \{h \in H : \tau(h)(i) = k\}$. The sets I_k are mutually disjoint and their union is H, so the largest one has cardinality at least $|H|/n$, let us call it $I_{\bar{k}}$.

From the hypothesis that S preserves H, we get $S_i h^{-1}(\underline{A}) = S_{\bar{k}}(\underline{A})$ for each $\underline{A}$ and each $h \in I_k$; therefore the invariance group of S_i contains $I_{\bar{k}}$. □

Moreover, the following result holds [5, page 147].

Theorem 8. *For $n > 4$, the only subgroups of $\mathfrak{S}_n$ with index at most n are:*

- *the alternating group $\mathfrak{A}_n$,*
- *the n groups $T_k = \{\sigma : \sigma(k) = k\}$, $k = 1, \dots, n$, all of which are isomorphic to $\mathfrak{S}_{n-1}$,*
- *for $n = 6$ only, there is another conjugacy class of 6 subgroups of index 6 isomorphic to $\mathfrak{S}_5$.*

This shows that whenever we try to construct a geometric mean of n matrices by taking a limit processes, such as in the Ando–Li–Mathias approach, the starting means cannot be "simpler" (in the sense of the invariance group) than a mean of $n - 1$ elements.

5 Computational issues and numerical experiments

A faster mean of four matrices While the results we have exposed up to now are impossibility results, it turns out that for $n = 4$, since $\mathfrak{A}_n$ is not a simple group, there is the possibility of obtaining a mean that is computationally simpler than the ones in use. Such a mean is the one we described in Example 3. Let us take any mean of three elements (we shall use G_3^{BMP} here since it is the one with the best computational results); the new mean is therefore defined as

$$G_4^{NEW}(A, B, C, D) := G_3^{BMP}\left((A \# B) \#(C \# D), (A \# C) \#(B \# D), (A \# D) \#(B \# C)\right). \quad (9)$$

Data set (number of matrices)	BMP mean	New mean
$NaClO_3$ (5)	1.3E+00	3.1E-01
Ammonium dihydrogen phosphate (4)	3.5E-01	3.9E-02
Potassium dihydrogen phosphate (4)	3.5E-01	3.9E-02
Quartz (6)	2.9E+01	6.7E+00
Rochelle salt (4)	6.0E-01	5.5E-02

Table 1: CPU times for the elasticity data sets

Notice that only one limit process is needed in order to compute the mean; conversely, when computing G_4^{ALM} or G_4^{BMP} we are performing an iteration whose elements are computed by doing four additional limit processes; thus we may expect a large saving in the overall computational cost.

We may extend the definition recursively to $n > 4$ elements using the construction described in (4), but with G^{NEW} instead of G^{BMP}. The total computational cost, computed in the same fashion as for the ALM and BMP means, is $O(n! p_3 p_5 p_6 \dots p_n m^3)$. Thus the undesirable dependence from $n!$ does not disappear; the new mean should only yield a saving measured by a multiplicative constant in the complexity bound.

Benchmarks We have implemented the original BMP algorithm and the new one described in the above section with Matlab® and run some tests on the same set of examples used by Moakher [7] and Bini *et al.* [4]. It is an example deriving from physical experiments on elasticity. It consists of five sets of matrices to average, with n varying from 4 to 6, and 6×6 matrices split into smaller diagonal blocks.

For each of the five data sets, we have computed both the BMP and the new matrix mean. The CPU times are reported in Table 1. As a stopping criterion for the iterations, we used

$$\max_{i,j,k} \left| (A_i^{(h)})_{jk} - (A_i^{(h+1)})_{jk} \right| < 10^{-13}.$$

As we expected, our mean provides a substantial reduction of the CPU time which is roughly by an order of magnitude.

Following Bini *et al.* [4], we then focused on the second data set (ammonium dihydrogen phosphate) for a deeper analysis; we report in Table 5 the number of iterations and matrix roots needed in both computations.

The examples in these data sets are mainly composed of matrices very close to each other; we shall consider here instead an example of mean of

	BMP mean		New mean
Outer iterations ($n = 4$)		3	none
Inner iterations ($n = 3$)	4×2.0 (avg.)	per outer iteration	2
Matrix square roots (`sqrtm`)		72	15
Matrix p-th roots (`rootm`)		84	6

Table 2: Number of inner and outer iterations needed, and number of matrix roots needed (ammonium dihydrogen phosphate)

	BMP mean		New mean
Outer iterations ($n = 4$)		4	none
Inner iterations ($n = 3$)	4×2.5 (avg.)	per outer iteration	3
Matrix square roots (`sqrtm`)		120	18
Matrix p-th roots (`rootm`)		136	9

Table 3: Number of inner and outer iterations needed, and number of matrix roots needed

four matrices whose mutual distances are larger:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 100 \end{pmatrix},$$
$$C = \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}, \quad D = \begin{pmatrix} 20 & 0 & -10 \\ 0 & 20 & 0 \\ -10 & 0 & 20 \end{pmatrix}.$$

The results regarding these matrices are reported in Table 3.

Accuracy To check whether the computed means are accurate, we have computed $G(A^4, I, I, I) - A$, which should yield zero in exact arithmetic. The results for both means are shown in Table 4. Here A is taken as the first matrix of the second data set on elasticity. The results are well within the errors permitted by the stopping criterion, and show that both algorithms can reach a satisfying precision.

Operation	Result
$\left\Vert G^{BMP}(A^4, I, I, I) - A \right\Vert_2$	2.0E-14
$\left\Vert G^{NEW}(A^4, I, I, I) - A \right\Vert_2$	5.0E-14

Table 4: Accuracy tests

6 Conclusions

Research lines The results of this paper show that, by combining existing matrix means, it is possible to create a new mean which is faster to compute than the existing ones. Moreover, we show that using only function compositions and limit processes it is not possible to achieve any further significant improvement with respect to the existing algorithms. In particular, the dependency from $n!$ cannot be removed. New attempts should focus on other aspects, such as:

- proving new "unexpected" algebraic relations involving the existing matrix means.
- proving that the mean called $\mathrm{ls}(\cdot)$ in Bhatia and Holbrook [3] is a matrix mean in the sense of Ando–Li–Mathias (currently P4 is an open problem), and/or providing faster and reliable algorithms to compute it.
- introducing new kinds of matrix geometric means or quasi-means.

It is an interesting question whether it is possible to construct a quasi-mean whose isotropy group is exactly $\mathfrak{A}_n$.

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