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Geometric modeling approach to the means of positive definite symmetric metrices

US Negi and Manoj Singh Bisht

Abstract
In this paper, we have defined and studied the geometric modeling approach to the means of positive definite symmetric metrices. In our space usual arithmetic mean is related with Euclidean metric and geometric mean is related with Riemannian metric. Also we have studied properties of Euclidean mean and invariance properties of Riemannian mean and some tools to present a classification of Riemannian metric.

Keywords: Means, positive-definite matrices, symmetric matrices, riemannian metric, MSC 2010: 15A48, 15A57, 26E60, 47A64

Introduction
Initially arithmetic, geometric and harmonic means defined for two positive numbers and then defined for a finite set of positive numbers. So for a set of m positive numbers, $\{x_k\}, 1 \leq k \leq m$, the arithmetic mean(always positive) is given as

$$\bar{x} = \frac{1}{m} \sum_{k=1}^{m} x_k.$$

For given points x_k arithmetic mean has a property that is minimizes the sum of the squared distances.

$$x_k = \underset{x>0}{\arg min} \sum_{k=1}^{m} d_e(x, x_k)^2, \quad (1.1)$$

Where $d_e(x, y) = |x - y|$ is the usual Euclidean distance in real number system R. Geometric mean of$\{x_k\}, 1 \leq k \leq m$, given by $\tilde{x} = \sqrt[m]{x_1 x_2 \dots x_m}$, also it has a property that it minimizes the sum of the squared hyperbolic distances.

$$\tilde{x} = \underset{x>0}{\arg min} \sum_{k=1}^{m} d_h(x_k, x)^2, \quad (1.2)$$

Where hyperbolic distance between x and y is given by $d_h(x, y) = |logx - logy|$. As we know that harmonic mean is the inverse of the arithmetic mean of their inverses, for$\{x_k\}, 1 \leq k \leq m$harmonic mean $\hat{x} = [\frac{1}{m} \sum_{k=1}^{m} (x_k)^{-1}]^{-1}$, and it has variational property as well.

Review of Literature
For regular elements of linear Euclidean spaces we generally use arithmetic mean. Arithmetic mean for application purpose referred to as the center of mass and the average. On the other hand, the geometric mean has been used only to positive numbers and positive integrable functions. In Hilbert space the geometric and harmonic means for a pair of positive operators were introduced by Anderson and Trapp, and Pusz and Woronowicz in 1975 [17]. It has been previously observed that geometric mean of two positive-definite operators holds many of the properties of geometric mean of two positive numbers. The geometric mean of positive operators has been primarily used as a binary operation.

[Trapp, G.E. (1984)] [17] have studied and investigated that, how to define the geometric mean of more than two Hermitian semi-definite matrices and used iterative method for it but it work only when matrices commute with each other. [Alice M. *et al*. (1997)] [1], have given a definition for the geometric mean of a finite set of operators however, this definition was not invariant under recording of the matrices. [Moakher, M. (2002)] [15], have studied about means of a finite number of 3-Dimensional rotational matrices and conclude that there is a close relation between the geometric mean of two Hermitian definite matrices and the Riemannian mean of two rotations.

We assemble each the necessary background from applied differential geometry and optimization theory on manifolds that will be used in the result. Furthermore information on this reduced material as Manifolds, Curves, and Surfaces, Convex Functions, Matrix groups and Optimization Techniques on Riemannian Manifolds have been established by [Curtis, M.L.(1979); Berger, M. and Gostiaux, B.(1998); Eblerlein, P.B.(1989); Terras, A.(1988)] [7, 3, 8, 19]. Again, we have studied Riemannian-metric based concept of mean for two positive-definite matrices. For Riemannian mean, We have studied its invariance properties and proved that when two matrices are to be averaged, then Riemannian mean coincides with geometric mean.

Geometric modeling approach to Riemannian metric based concept of mean for positive-definite matrices

Now we include circumstances, if we have Riemannian manifold μ with metric $d\ (x, y)$. then by equations (1.1) and (1.2), we define mean with respect to $d\ (x, y)$ for m points in μ as:

$$\mathfrak{m}(x_1, \dots, x_k) = \underset{x \in \mu}{\arg min} \sum_{k=1}^{m} d(x_k, x)^2. \tag{3.1}$$

As we know for the set of positive real numbers at the same time, a Lie group and an open convex cone, different concept of mean can be correlated with different matrices. This follows that we will generalize these metric-based means to the cone positive-definite transformations. The techniques and concepts used in this paper carry over to the complex complement of the space considered here, i.e., convex cone of Hermitian definite transformations. We here focus on the real space just for simplicity but not for any elementary reason.

Let μ(n) denotes set of $n \times n$ real matrices and we consider its subset of all non-singular matrices denoted by GL(n). GL(n) is a group (Lie group), i.e., a group which is a differenatiable manifold and for which the operators (operations) of the group multiplication and inverse are totally valid. Lie algebra denoted by gl(n) is the tangent space at the identity. This is the space of all linear transformations in $R^n, i.e.,$ μ(n). In μ(n), we use the Euclidean (Frobenius) inner product defined by $\langle A, B\rangle_F = tr(A^T B)$, where tr denotes the trace and the superscript T stands for the transpose. The connected norm$\|A\|_F = \langle A, A\rangle_F^{1/2}$, is used to describe the Euclidean distance on μ(n).

$$d_F(A, B) = \|A - B\|_F. \tag{3.2}$$

The exponential of a particular matrix in $gl(n)$ is given by the convergent series as:

$$\text{Exp}\, A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k. \tag{3.3}$$

We state that $Exp(A.B) = \text{Exp}(A + B)$, only when $A\ and\ B$ commutes with each other. In $GL(n)$ solutions of the equations $\text{Exp}\, X = A$ are Logarithms of A. When have eigenvalues in the (open) positive real line, there exists a unique principal logarithms, denoted by $Log\ A$, whose range lies in the infinite strip $\{z \in C: -\pi < Im(z) < \pi\}$ of the Complex plane. Furthermore, for any given matrix norm$\|.\|$,$\|A - I\| < 1$, where I be the identity transformation in R^n, then the series $-\sum_{k=1}^{\infty} \frac{(I-A)^k}{k}$ converges to $Log\ A$ and consequently we can write

$$Log\ A = -\sum_{k=1}^{\infty} \frac{(I-A)^k}{k} \tag{3.4}$$

We denote that in general $Log(AB) \neq LogA + LogB$. We here recollect the important fact by [Curtis, M.L. (1979)] [7].

$$Log(A^{-1}BA) = A^{-1}(LogB)A. \tag{3.5}$$

This result is also correct when Log in the above equation (3.5) is replaced by an analytic matrix function. So, we give the following essential theorem in the progress of our study.

Theorem 3.1: Let $X(t)$ denotes a real matrix-valued function of real variable *t*. We suppose that, for each *t* in its domain, $X(t)$ Is an invertible matrix which have eigenvalues on the open positive real line. Then

$$\frac{d}{dt}\ tr\ [Log^2 X(t)] = 2tr\ [Log X(t)\ X^{-1}(t)\ \frac{d}{dt} X(t)].$$

Proof: We recollect the following fats:

(1) $tr(AB) = tr(BA)$.

(2) $tr\left(\int_a^b M(s)ds\right) = \int_a^b tr\big(M(s)\big)ds.$

(3) $Log\ A\ commute\ with\ [(A-I)+I]^{-1}$.

(4) $\int_0^1 [(A-I)s+I]^{-2} ds = (A-I)^{-1} | [(A-I)s+I]^{-1} |_0^1 = A^{-1}$.

(5) $\frac{d}{dt} Log\ X(t) = \int_0^1 [(A-I)s+I]^{-1} \frac{d}{dt} X(t) [(X(t)-I)s+I]^{-1} ds$.

The facts (1), (2), (3), (4), (5) are easily verified.
Using the above we have

$$\frac{d}{dt}\ tr\ ([Log\ X(t)]^2) = 2\ tr(Log\ X(t)) \frac{d}{dt} Log\ X(t)$$

$$= 2tr\left(Log\ X(t) \int_0^1 [(X(t)-I)s+I]^{-1} \frac{d}{dt} X(t)\ [(X(t)-I)s+I]^{-1} ds\right), \text{ from (v)}$$

$$= 2tr\left(\int_0^1 Log\ X(t)[(X(t)-I)s+I]^{-1} \frac{d}{dt} X(t)\ [(X(t)-I)s+I]^{-1} ds\right)$$

$$= 2\int_0^1 tr(Log\ X(t)[(X(t)-I)s+I]^{-1} \frac{d}{dt} X(t)\ [(X(t)-I)s+I]^{-1}) ds, \text{ from (ii)}$$

$$= 2\int_0^1 tr([(X(t)-I)s+I]^{-1} Log\ X(t)\ [(X(t)-I)s+I]^{-1} \frac{d}{dt} X(t)) ds, \text{ from (i)}$$

$$= 2\int_0^1 tr(Log\ X(t)\ [(X(t)-I)s+I]^{-2} \frac{d}{dt} X(t)) ds, \text{ from (iii)}$$

$$= 2tr(Log\ X(t) \int_0^1 [(X(t)-I)s+I]^{-2} ds \frac{d}{dt} X(t))$$

$$= 2tr\left(LogX(t) X^{-1}(t) \frac{d}{dt} X(t)\right).$$

For any real valued function f(x) (defined on a Riemannian manifold μ), the gradient ∇f is the unique tangent vector u at x such that

$$\langle u, \nabla f \rangle = \frac{d}{dt} f(\gamma(t))\Big]_{t=0}, \quad (3.6)$$

Where $\langle u, \nabla f \rangle$, is the Riemannian inner product(R.I.P.) on the tangent space and $\gamma(t)$ is a geodesic emanating from x in direction of u.

A subset Â of μ(a Riemannian manifold) is convex if the shortest curve (geodesic) between any two points x and y is unique in μ and lies in Â. A function (real valued) defined on a convex subset Â of μ is convex of its limitations to any geodesic path is convex, i.e., $if\ t \to f(t) \equiv f(exp_x(tu))$ is convex over its domain for all$x \in \mu$, is the exponential map at x.

We prepared the space of all $n \times n$ symmetric matrices denoted by $S(n) = \{A \in \mu(n),\ A^T = A\}$, and The set of all $n \times n$ positive-definite matrices by $\mathrm{P}(n) = \{A \in S(n), A > 0\}$. Here $A > 0$ means that matrix A is positive definite or the quadratic form $x^T Ax > 0$ for every $x \in R^n/0$. It is well-known that $\mathrm{P}(n)$ is an open convex cone or if $P\ and\ Q$ are in $\mathrm{P}(n)$, so is $P + tQ$ for any $t > 0$.

We remind that the exponential map from $S(n)$ to $\mathrm{P}(n)$ is bijective (one-to-one and onto). In other words, positive-definite symmetric matrix is the exponential of symmetric matrix and the inverse of the exponential (i.e., the principal logarithms) for any positive-definite symmetric matrix is a symmetric matrix. $\mathrm{P}(n)$ is an open subset of $S(n)$, for every $P \in \mathrm{P}(n)$, I classify the set T_p of tangent vectors to $\mathrm{P}(n)$ at P with $S(n)$, on the Tangent Space at P, we define the positive-definite inner product and its corresponding norm as

$$\langle A, B \rangle_P = tr(P^{-1}AP^{-1}B), \|A\|_P = \langle A, A \rangle_P^{1/2}, \quad (3.7)$$

which depends on the points P. The positive definiteness is a outcome of the positive definiteness of the Euclidean inner product for:

$$\langle A, A \rangle_P = tr\left(P^{-1/2}\ AP^{-1/2}\ P^{-1/2}\ AP^{-1/2}\right) = \langle P^{-1/2}\ AP^{-1/2},\ P^{-1/2}\ AP^{-1/2} \rangle.$$

Suppose [a, b] is a closed interval in R & $\Gamma: [a, b] \to \mathrm{P}(n)$ be a sufficiently continuous curve in $\mathrm{P}(n)$. we describe the lengths of Γ by

$$\mathcal{L}(\Gamma) = \int_a^b \sqrt{\langle \dot{\Gamma}(t), \dot{\Gamma}(t) \rangle_{\Gamma(t)}} dt = \int_a^b \sqrt{tr\Gamma(t)^{-1}\Gamma(t)^2}\, dt. \quad (3.8)$$

We indicate that the length $\mathcal{L}(\Gamma)$ is invariant under congruent transformation, $\Gamma \mapsto C\Gamma C^T$,, for some fixed element C of $\epsilon GL(n)$. As $\frac{d}{dt}\Gamma^{-1} = -\Gamma^{-1}\dot{\Gamma}\Gamma^{-1}$, which implies that this length is also invariant under inversion.
In $\mathrm{P}(n)$, the distance between two matrices A and B (considered as a differentiable manifold) is the infimum of lengths of curves joining them

$$d_{\mathrm{P}(n)}(A,B) = \inf \{\mathcal{L}(\Gamma) | \Gamma: [\,a,b] \to \mathrm{P}(n)\; with\; \Gamma(a) = A, \Gamma(b) = B\}. \quad (3.9)$$

This metric implies that $\mathrm{P}(n)$ a Riemannian manifold of dimension $\frac{1}{2}n(n+1)$ and the geodesic emanating from I to S, given explicitly by e^{tS} [Maab, H. (1971)] [14], is a (symmetric) matrix in the Tangent Space. Using invariance under congruent transformations, $\mathrm{P}(0) = P$ and $\dot{P}(0) = S$, the geodesic $\mathrm{P}(n)$ is given by

$$\mathrm{P}(t) = P^{1/2}\, e^{tP^{-1/2}}\, S\, P^{-1/2}\, P^{1/2}.$$

It implies that the Riemannian metric of P_1 and P_2 in $\mathrm{P}(n)$ is given by

$$d_{\mathrm{P}(n)}(P_1, P_2) = \|Log(P_1^{-1}P_2)\|_F = [\textstyle\sum_{i=1}^{n} l\, n^2 \lambda_i]^{1/2}, \quad (3.10)$$

Where$\lambda_i, 1 \le i \le n$, are real and positive n eigenvalues of $P_1^{-1}P_2$. whereas in general $P_1^{-1}P_2$ is not symmetric. This shows that $P_1^{-1}P_2$ is similar to the positive-definite symmetric matrix $P_2^{1/2}\, P_1^{-1}\, P_2^{1/2}$. It is essential to note that any real-valued function defined on $\mathrm{P}(n)$by $P \mapsto d_{\mathrm{P}(n)}(P,S)$, where $S \in \mathrm{P}(n)$ is fixed, is (geodesically) convex [Mostow, G.D. (1973)] [16].
We know that $\mathrm{P}(n)$ is a homogeneous space of the Lie group $GL(n)$ (where $\mathrm{P}(n)$ given by the quotient$\frac{GL(n)}{O(n)}$. It is also a non compact type symmetric space. [Terras, A. (1988)] [19]. We will also take the symmetric space of some special positive matrices: $SP(n) = \{A \in \mathrm{P}(n), detA = 1\}$.
This submanifold of $\mathrm{P}(n)$can also be written with the quotient$\frac{SL(n)}{O(n)}$. Here $SL(n)$ is the special linear group of all matrices from$GL(n)$, whose determinant is one. We conclude that $SP(n)$ is a completely geodesic submanifold of $P(n)$ [Maab, H. (1971)] [14]. Now since $P(n) = SP(n) \times IR^+$, $P(n)$ can be considered as a foliated manifold whose dimension minus (-) one leaves are isomorphic to H^p (the hyperbolic space), where$p = \frac{1}{2}n(n+1) - 1$.

Geometric modeling approach to the Means of Positive-Definite Symmetric Matrices.
Taking the definition (3.1) with the two metric function (3.2) and (3.10) we establish the two different concept of mean in $P(n)$.

Definition 4.1: The Euclidean mean, i.e., associated with the distance function (3.2), of m given positive-definite Symmetric Matrices $P_1, P_2, \dots, P_m$ is defined as

$$\mathfrak{U}(P_1, P_2, \dots, P_m) = \underset{P \in P(n)}{\arg min} \textstyle\sum_{k=1}^{n} \|P_k - P\|_F^2. \quad (4.1)$$

Definition 4.2: The Riemannian mean, i.e., associated with the distance function (3.10), of m given Positive-Definite Symmetric Matrices $P_1, P_2, \dots, P_m$ is defined as

$$\mathfrak{S}\,(P_1, P_2, \dots, P_m) = \underset{P \in P(n)}{\arg min} \textstyle\sum_{k=1}^{n} \|LogP_k^{-1}P\|_F^2. \quad (4.2)$$

After this, we can say that these two means satisfy the following properties:

1. For any permutation σ of a numbers 1,…, m, re-ordering is invariant, i.e., we have $m(P_1, P_2, \dots, P_m) = m(P_{\sigma(1)}, P_{\sigma(2)}, \dots, P_{\sigma(m)})$.
2. Congruent transformations is also invariant: If P is Positive-Definite Symmetric mean of P_k,$1 \le k \le m$, then CPC^T is the Positive-Definite Symmetric mean of $\{\, CP_kC^T\}$, $1 \le k \le m$, for each $C \in GL(n)$. Special case, when C belongs to the full orthogonal group$O(n)$, we conclude the invariance under Orthogonal transformations.
3. Inversion is also invariant, i.e., If P is the Mean of P_k,$1 \le k \le m$, then P^{-1} is the Mean of $\{P_k^{-1}\}$, $1 \le k \le$m.

The Euclidean mean satisfy many other properties but they are not relevant for the space of Positive-definite Symmetric matrices. In addition, the solution of the problem (4.1) is simply usual arithmetic mean given by$P = \frac{1}{m}\sum_{k=1}^{m} P_k$, which is minimized. Therefore, the Euclidean mean will not be considered any more.
The Riemannian mean of $P_1, P_2, \dots, P_m$ may be called as the Riemannian barycenter of matrices$P_1, P_2, \dots, P_m$, which concept was introduced by [Grove, Karcher and Ruh (1974)]. [Karcher, H. (1977)] [10, 12] proved that for manifolds with Non-Positive sectional curvature, the Riemannian mean (barycenter) is unique. We will give a property of the Riemannian barycenter in the following theorem.

Theorem 4.1: The Riemannian barycenter of a given m symmetric Positive- Definite matrices $P_1, P_2, \ldots, P_m$ is the unique symmetric Positive-Definite solution of the nonlinear matrix equation

$$\sum_{k=1}^{m} Log(P_k^{-1}P) = 0. \quad (4.3)$$

Proof: First of all, we will find the derivative of the real-valued function
$H(S(t)) = \frac{1}{2}\|\log(W^{-1}S(t))\|_F^2$ w. r. t. t, where $S(t) = P^{1/2}\exp(tA)P^{1/2}$ is the Geodesic emanating from P towards $\Delta = \dot{S}(0) = P^{1/2}AP^{1/2}$, and $W \in P(n)$, is a constant matrix.
Using equation (3.5) and few properties of the trace of a matrix, we have:

$$H(S(t)) = \frac{1}{2}\left\|Log(W^{-1/2}S(t)W^{-1/2})\right\|_F^2,$$

because $Log(W^{-1/2}\, S(t)\, W^{-1/2}$ is symmetric.
We have

$$\frac{d}{dt}\, H(S(t))\Big]_{t=0} = \frac{1}{2}\frac{d}{dt} tr \left|Log(W^{-1/2}\, S(t)\, W^{-1/2}{}^2\right|_{t=0}.$$

So, the result of Theorem 4.1, applied to the above gives

$$\frac{d}{dt}H(S(t))\Big]_{t=0} = tr[Log(W^{-1}P)P^{-1}\Delta] = tr[\Delta Log(W^{-1}P)P^{-1}],$$

Hence, ∇H (the gradient of H) is given by

$$\nabla H = Log(W^{-1}P)P^{-1} = P^{-1}Log(PW^{-1}), \quad (4.4)$$

This is certainly in the tangent space, i.e. in $S(n)$.
Let G be the objective function for the minimization problem (4.2), i.e.,

$$G(P) = \sum_{k=1}^{m}\|Log(P_k^{-1}P\|_F^2. \quad (4.5)$$

Using equation (4.5), the gradient of G becomes

$$\nabla G = P\sum_{k=1}^{m} Log(P_k^{-1}P). \quad (4.6)$$

$G(P)$ in equation (4.5) is the sum of convex functions implies that the necessary and sufficient condition for P to be the least amount of (4.5) is the vanishing of the gradient ∇G given in equation (4.6), or,

$$\sum_{k=1}^{m} Log(P_k^{-1}P) = 0.$$

This value noting that, the classification for the mean in Riemannian sense given in equation (4.3) is like to the classification

$$\sum_{k=1}^{m} ln(x_k^{-1}x) = 0. \quad (4.7)$$

of the geometric mean of positive numbers given in equation (1.2). Furthermore, unlike the case of positive numbers where equation (4.7) gives to an explicit expression of the above geometric mean, in general, due to the asymmetric nature of $p(n)$, (4.3) can't be solved in closed from.

Conclusion

Above all properties are related to the geodesic reversing isometry in the symmetric space here taken by us. Hence, the concept of geometric mean, which is completely based on the Riemannian metric, can be used to describe the geometric mean on other symmetric spaces. Also various other properties of arithmetic mean, geometric mean, harmonic mean can be obtained for future work.

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