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MEANS AND AVERAGING IN THE GROUP OF ROTATIONS*

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Abstract. In this paper we give precise definitions of different, properly invariant notions of mean or average rotation. Each mean is associated with a metric in $SO(3)$. The metric induced from the Frobenius inner product gives rise to a mean rotation that is given by the closest special orthogonal matrix to the usual arithmetic mean of the given rotation matrices. The mean rotation associated with the intrinsic metric on $SO(3)$ is the Riemannian center of mass of the given rotation matrices. We show that the Riemannian mean rotation shares many common features with the geometric mean of positive numbers and the geometric mean of positive Hermitian operators. We give some examples with closed-form solutions of both notions of mean.

Key words. Special orthogonal group, Rotation, Geodesics, Operator means, Averaging

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1. Introduction.

In many applications, such as the study of plate tectonics [22] or sequence-dependent continuum modeling of DNA [19], experimental data are given as a sequence of three-dimensional orientation data that usually contain a substantial amount of noise. A common problem is to remove or reduce the noise by processing the raw data, for example by the construction of a suitable filter, in order to obtain appropriately smooth data.

Three-dimensional orientation data are elements of the group of rotations that generally are given as a sequence of proper orthogonal matrices, or a sequence of Euler angles, or a sequence of unit quaternions, etc. As the group of rotations is not an Euclidean space, but rather a differentiable manifold, the notion of mean or average is not obvious so that appropriate filters are similarly not obvious. One might choose some local coordinate representation of the group, for instance a set of Euler angles, then apply the usual averaging and smoothing techniques of Euclidean spaces. Although this approach is simple to implement, it is not properly invariant under the action of rigid transformations. In this article alternative approaches will be discussed.

There has been an extensive literature on the statistics of circular and spherical data, see [20, 27, 9, 8] and the references therein. In a more general context, Downs [4], Khatri and Mardia [18], and Jupp and Mardia [15], developed statistical methods for data in the Stiefel manifold, i.e., the Riemannian space $V_{n,p},\ 1 \le p \le n$, of $n \times p$ orthogonal matrices, (the hypersphere S^n and the special orthogonal group $SO(n)$ are examples of such manifolds). The general approach of these statistical studies is to embed the given data into an Euclidean space of dimension larger than the dimension of the manifold (circle, sphere, hypersphere, etc.), then to pursue standard statistical approaches in this linear space, and finally to project the result onto the manifold. Prentice [22] used the parameterization of the group of rotations by four-dimensional axes (unsigned unit quaternions) and a slight modification of the algorithm of smoothing directional data on S^2 proposed in [16] to fit smooth spline paths to three-dimensional rotation data.

In this paper we are mainly concerned with a general mathematical theory of

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different possible notions of mean in the group of three-dimensional rotations rather than a statistical theory based on a specific notion of mean. In analogy with mean in Euclidean space, we define the mean rotation of a given sequence of rotations to be the minimizer of the sum of squared distances from the given rotations. The *projected arithmetic mean* is obtained when one uses the inherent Euclidean distance of the ambient space. We show that this is the orthogonal projection of the usual arithmetic mean in the space of 3×3 matrices onto the rotation group. It is the same as the directional mean of the statistics literatures mentioned above. The *geometric mean* arises when one uses the Riemannian metric intrinsic to the group of rotations. We find close similarities between this mean and the geometric mean of positive numbers, as well as the geometric mean of positive Hermitian operators. We show that these two notions of mean are properly invariant under a change of frame and share many common properties with means of elements of Euclidean spaces.

To the best of our knowledge, the geometric mean rotation has not been discussed previously. In this paper, we show that the geometric mean and the Euclidean mean rotation, which we call the projected arithmetic mean, each arise from a least-square error approach, but with different metrics. We also give some properties of the Euclidean mean rotation that have not been discussed in the literature, as well as its connection with the geometric mean.

The remainder of this paper is organized as follows. In § 2 we gather all the necessary background from Lie group theory, differential geometry and optimization on manifolds that will be used in the sequel. Further information on this condensed material can be found in [3, 1, 23, 21, 26, 13]. In § 3 we introduce two bi-invariant notions of mean rotation: the projected arithmetic mean and the geometric mean. We give the characterization and main features of these two notions of mean rotation. Examples of closed-form calculations of mean rotations are given in § 4. Finally, weighted means and power means of rotations are presented in § 5.

2. Geometry of the rotation group.

Let $\mathcal{M}(3)$ be the set of 3-by-3 real matrices and $GL(3)$ be its subset containing only non-singular matrices. The group of rotations in $\mathbb{R}^3$, denoted by $SO(3)$, is the Lie group of special orthogonal transformations in $\mathbb{R}^3$

$$SO(3) = \left\{ \boldsymbol{R} \in GL(3) \mid \boldsymbol{R}^T\boldsymbol{R} = \boldsymbol{I} \text{ and } \det \boldsymbol{R} = 1 \right\}, \tag{2.1}$$

where $\boldsymbol{I}$ is the identity transformation in $\mathbb{R}^3$ and the superscript ^{T} denotes the transpose. The corresponding Lie algebra, denoted by $\mathfrak{so}(3)$, is the space of skew-symmetric matrices

$$\mathfrak{so}(3) = \left\{ \boldsymbol{A} \in \mathfrak{gl}(3) \mid \boldsymbol{A}^T = -\boldsymbol{A} \right\} \tag{2.2}$$

where $\mathfrak{gl}(3)$, the space of linear transformations in $\mathbb{R}^3$, is the Lie algebra corresponding to Lie group $GL(3)$.

2.1. Exponential and logarithm.

The exponential of a matrix $\boldsymbol{X}$ in $GL(3)$ is denoted $\exp \boldsymbol{X}$ and is given by the limit of the convergent series $\exp \boldsymbol{X} = \sum_{k=0}^{\infty} \frac{1}{k!}\boldsymbol{X}^k$. When a matrix $\boldsymbol{Y}$ in $GL(3)$ does not have eigenvalues in the (closed) negative real line, there exists a unique real logarithm, called the principal logarithm, denoted by $\operatorname{Log} \boldsymbol{Y}$, whose spectrum lies in the infinite strip $\{z \in \mathbb{C} \ : \ -\pi < \operatorname{Im}(z) < \pi\}$ of the complex plane [3]. Furthermore, for any given matrix norm $\|\cdot\|$, if $\|\boldsymbol{I}-\boldsymbol{Y}\|<1$ then the series $-\sum_{k=1}^{\infty}\frac{(\boldsymbol{I}-\boldsymbol{Y})^k}{k}$ converges and hence one can write $\operatorname{Log}\boldsymbol{Y}=-\sum_{k=1}^{\infty}\frac{(\boldsymbol{I}-\boldsymbol{Y})^k}{k}$. However, as we will describe, the infinite series representations of the exponential of matrices in $\mathfrak{so}(3)$ and the logarithm of matrices in $SO(3)$ can be given as closed-form expressions.

The exponential of a skew-symmetric matrix $\boldsymbol{A}$ such that, $a=\sqrt{\frac{1}{2}\operatorname{tr}(\boldsymbol{A}^T\boldsymbol{A})}$ is in $[0,\pi)$, is the proper orthogonal matrix given by Rodrigues' formula

$$\exp\boldsymbol{A}=\begin{cases}\boldsymbol{I}, & \text{if } a=0,\\ \boldsymbol{I}+\frac{\sin a}{a}\boldsymbol{A}+\frac{1-\cos a}{a^2}\boldsymbol{A}^2, & \text{if } a\neq 0,\end{cases} \tag{2.3}$$

The principal logarithm for a matrix $\boldsymbol{R}$ in $SO(3)$ is the matrix in $\mathfrak{so}(3)$ given by

$$\operatorname{Log}\boldsymbol{R}=\begin{cases}\boldsymbol{0}, & \text{if } \theta=0,\\ \frac{\theta}{2\sin\theta}(\boldsymbol{R}-\boldsymbol{R}^T), & \text{if } \theta\neq 0,\end{cases} \tag{2.4}$$

where θ satisfies $\operatorname{tr}\boldsymbol{R}=1+2\cos\theta$ and $|\theta|<\pi$ (this formula breaks down when $\theta=\pm\pi$). An alternative expression for the logarithm of a matrix in $SO(3)$, where the parameter θ does not appear, is given in [14].

Solutions in $SO(3)$ of the matrix equation $\boldsymbol{Q}^k=\boldsymbol{R}$ with k a positive integer will be called kth roots of $\boldsymbol{R}$. These kth roots are given by

$$\exp\left(\frac{1}{k}\left(1+\frac{2l\pi}{\theta}\right)\operatorname{Log}\boldsymbol{R}\right),\ l=0,\dots,k-1,$$

where θ is the angle of rotation of $\boldsymbol{R}$. The kth root $\exp(\frac{1}{k}\operatorname{Log}\boldsymbol{R})$ is the one for which the eigenvalues have the largest positive real part, and is the only one we denote by $\boldsymbol{R}^{1/k}$. In the case $k=2$, it is the only square root with positive real part.

2.2. Metrics in $SO(3)$. A straightforward way to define a distance function in $SO(3)$ is to use the Euclidean distance of the ambient space $\mathcal{M}(3)$, i.e., if $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are two rotation matrices then

$$\mathrm{d}_F(\boldsymbol{R}_1,\boldsymbol{R}_2)=\|\boldsymbol{R}_1-\boldsymbol{R}_2\|_F, \tag{2.5}$$

where $\|\cdot\|_F$ is the Frobenius norm which is induced by the Euclidean inner product, known as the Frobenius inner product, defined by $\langle\boldsymbol{R}_1,\boldsymbol{R}_2\rangle_F=\operatorname{tr}(\boldsymbol{R}_1^T\boldsymbol{R}_2)$. It is easy to see that this distance is bi-invariant in $SO(3)$, i.e., $\mathrm{d}_F(\boldsymbol{P}\boldsymbol{R}_1\boldsymbol{Q},\boldsymbol{P}\boldsymbol{R}_2\boldsymbol{Q})=\mathrm{d}_F(\boldsymbol{R}_1,\boldsymbol{R}_2)$ for all $\boldsymbol{P},\boldsymbol{Q}$ in $SO(3)$.

Another way to define a distance function in $SO(3)$ is to use its Riemannian structure. The Riemannian distance between two rotations $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ is given by

$$\mathrm{d}_R(\boldsymbol{R}_1,\boldsymbol{R}_2)=\frac{1}{\sqrt{2}}\|\operatorname{Log}(\boldsymbol{R}_1^T\boldsymbol{R}_2)\|_F. \tag{2.6}$$

It is the length of the shortest geodesic curve that connects $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ given by

$$\boldsymbol{Q}(t)=\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^t=\boldsymbol{R}_1\exp(t\operatorname{Log}(\boldsymbol{R}_1^T\boldsymbol{R}_2)),\quad 0\le t\le 1. \tag{2.7}$$

Note that the geodesic curve of minimal length may not be unique. If $\boldsymbol{R}_1^T\boldsymbol{R}_2$ is an involution, in other words if $(\boldsymbol{R}_1^T\boldsymbol{R}_2)^2 = \boldsymbol{I}$, i.e., a rotation through an angle π, then $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ can be connected by two curves of equal length. In such a case, the rotations $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are said to be antipodal points in $SO(3)$ and $\boldsymbol{R}_2$ is said to be the cut point of $\boldsymbol{R}_1$ and *vice versa*.

The Riemannian distance (2.6) is also bi-invariant in $SO(3)$. Indeed, using the fact $\operatorname{Log}(\boldsymbol{Q}^{-1}\boldsymbol{R}\boldsymbol{Q}) = \boldsymbol{Q}^{-1}(\operatorname{Log}\boldsymbol{R})\boldsymbol{Q}$ [3], we can show that $\mathrm{d}_R(\boldsymbol{P}\boldsymbol{R}_1\boldsymbol{Q}, \boldsymbol{P}\boldsymbol{R}_2\boldsymbol{Q}) = \mathrm{d}_R(\boldsymbol{R}_1, \boldsymbol{R}_2)$ for all $\boldsymbol{P}, \boldsymbol{Q}$ in $SO(3)$.

REMARK 2.1. *The Euclidean distance (2.5) represents the chordal distance between $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, i.e., the length of the Euclidean line segment in the space of $\mathcal{M}(3)$ (except for the end points $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, this line segment does not lie in $SO(3)$), whereas the Riemannian distance (2.6) represents the arc-length of the shortest geodesic curve (great-circle arc), which lies entirely in $SO(3)$, passing through $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$.*

REMARK 2.2. *If θ denotes the angle of rotation of $\boldsymbol{R}_1^T\boldsymbol{R}_2$ then $\mathrm{d}_F(\boldsymbol{R}_1, \boldsymbol{R}_2) = 2\sqrt{2}|\sin\frac{\theta}{2}|$ and $\mathrm{d}_R(\boldsymbol{R}_1, \boldsymbol{R}_2) = |\theta|$. Therefore, when the rotations $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are sufficiently close, i.e., θ is small, we have $\mathrm{d}_F(\boldsymbol{R}_1, \boldsymbol{R}_2) \approx \sqrt{2}\,\mathrm{d}_R(\boldsymbol{R}_1, \boldsymbol{R}_2)$.*

2.3. Covariant derivative and Hessian. We recall that the tangent space at a point $\boldsymbol{R}$ of $SO(3)$ is the space of all matrices $\boldsymbol{\Delta}$ such that $\boldsymbol{R}^T\boldsymbol{\Delta}$ is skew symmetric and that the normal space (associated with the Frobenius inner product) at $\boldsymbol{R}$ consists of all matrices $\boldsymbol{N}$ such that $\boldsymbol{R}^T\boldsymbol{N}$ is symmetric [5].

For a real-valued function $f(\boldsymbol{R})$ defined on $SO(3)$, the covariant derivative ∇f is the unique tangent vector at $\boldsymbol{R}$ such that

$$\operatorname{tr}(\boldsymbol{\Delta}^T\nabla f) = \frac{d}{dt}f(\boldsymbol{Q}(t))\Big|_{t=0}, \tag{2.8}$$

where $\boldsymbol{Q}(t)$ is a geodesic emanating from $\boldsymbol{R}$ in the direction of $\boldsymbol{\Delta}$, i.e., $\boldsymbol{Q}(t) = \boldsymbol{R}\exp(t\boldsymbol{A})$ and $\boldsymbol{R}^T\boldsymbol{\Delta} = \boldsymbol{A}$ is skew symmetric.

The Hessian of $f(\boldsymbol{R})$ is given by the quadratic form

$$\operatorname{Hess} f(\boldsymbol{\Delta}, \boldsymbol{\Delta}) = \frac{d^2}{dt^2}f(\boldsymbol{Q}(t))\Big|_{t=0} \tag{2.9}$$

where $\boldsymbol{Q}(t)$ is a geodesic and $\boldsymbol{\Delta}$ is in the tangent space at $\boldsymbol{R}$ as above.

2.4. Geodesic convexity. We recall that a subset A of a Riemannian manifold M is said to be convex if the shortest geodesic curve between any two points x and y in A is unique in M and lies in A. A real-valued function defined on a convex subset A of M is said to be convex if its restriction to any geodesic path is convex, i.e., if $t \mapsto \hat{f}(t) \equiv f(\exp_x(tu))$ is convex over its domain for all $x \in M$ and $u \in T_x(M)$, where $\exp_x$ is the exponential map at x.

With these definitions, one can readily see that any geodesic ball $B_r(\boldsymbol{Q})$ in $SO(3)$ of radius r less than $\frac{\pi}{2}$ around $\boldsymbol{Q}$ is convex and that the real-valued function f defined on $B_r(\boldsymbol{Q})$ by $f(\boldsymbol{R}) = \|\operatorname{Log}(\boldsymbol{Q}^T\boldsymbol{R})\|_F$ is convex when r is less than $\frac{\pi}{2}$. Geodesic balls with radius greater or equal than $\frac{\pi}{2}$ are not convex.

3. Mean rotation. For a given set of N points $\boldsymbol{x}_n$, $n = 1, \dots, N$ in $\mathbb{R}^d$ the arithmetic mean $\bar{\boldsymbol{x}}$ is given by the barycenter $\bar{\boldsymbol{x}} = \frac{1}{N}\sum_{n=1}^N \boldsymbol{x}_n$ of the N points. The arithmetic mean also has a variational property; it minimizes the sum of the squared distances to the given points $\boldsymbol{x}_n$,

$$\bar{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}\in\mathbb{R}^d} \sum_{n=1}^{N} \mathrm{d}_e(\boldsymbol{x}, \boldsymbol{x}_n)^2, \tag{3.1}$$

where here $\mathrm{d}_e(\cdot,\cdot)$ represents the usual Euclidean distance in $\mathbb{R}^d$.

One can also use the arithmetic mean to average N positive real numbers $x_n > 0$, $n = 1, \ldots, N$, and the mean is itself a positive number. In many applications, however, it is more appropriate to use the geometric mean to average positive numbers, which is possible because positive numbers form a multiplicative group. The geometric mean $\tilde{x} = x_1^{1/N} \cdots x_N^{1/N}$ also has a variational property; it minimizes the sum of the squared *hyperbolic distances* to the given data

$$\tilde{x} = \operatorname*{arg\,min}_{x>0} \sum_{n=1}^{N} \mathrm{d}_h(x_n, x)^2, \tag{3.2}$$

where $\mathrm{d}_h(x, y) = |\log x - \log y|$ is the hyperbolic distance[1] between x and y.

As we have seen, for the set of positive real numbers different notions of mean can be associated with different metrics. In what follows, we will extend these notions of mean to the group of proper orthogonal matrices.

By analogy with $\mathbb{R}^d$, a plausible definition of the mean of N rotation matrices $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N$ is that it is the minimizer in $SO(3)$ of the sum of the squared distances from that rotation matrix to the given rotation matrices $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N$, i.e., $\mathfrak{M}(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N) = \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \sum_{n=1}^{N} \mathrm{d}(\boldsymbol{R}_n, \boldsymbol{R})^2$, where $\mathrm{d}(\cdot,\cdot)$ represents a distance in $SO(3)$. Now the two distance functions (2.5) and (2.6) define the two different means.

Definition 3.1. *The mean rotation in the Euclidean sense, i.e., associated with the metric (2.5), of N given rotation matrices $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N$ is defined as*

$$\mathfrak{A}(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N) := \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \sum_{n=1}^{N} \|\boldsymbol{R}_n - \boldsymbol{R}\|_F^2. \tag{3.3}$$

Definition 3.2. *The mean rotation in the Riemannian sense, i.e., associated with the metric (2.6), of N given rotation matrices $\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N$ is defined as*

$$\mathfrak{G}(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N) := \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \sum_{n=1}^{N} \|\operatorname{Log}(\boldsymbol{R}_n^T \boldsymbol{R})\|_F^2. \tag{3.4}$$

The minimum here is understood to be the global minimum. We remark that in $\mathbb{R}^d$, or in the set of positive numbers, the objective functions to be minimized are convex over their domains, and therefore the means are well defined and unique. However, in $SO(3)$, as we shall see, the objective functions in (3.3) and (3.4) are not (geodesically) convex, and therefore the means may not be unique.

Before we proceed to study these two means, we note that both satisfy the following desirable properties that one would expect from a mean in $SO(3)$, and that are counterparts of properties of means of numbers, namely,

[1] We borrow this terminology from the hyperbolic geometry of the Poincaré upper half-plane. In fact, the hyperbolic length of the geodesic segment joining the points $P(a, y_1)$ and $Q(a, y_2)$, $y_1, y_2 > 0$ is $|\log \frac{y_1}{y_2}|$, (see [26]).

1. Invariance under permutation: For any permutation σ of the numbers 1 through N, we have $\mathfrak{M}(\boldsymbol{R}_{\sigma(1)}, \dots, \boldsymbol{R}_{\sigma(N)}) = \mathfrak{M}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N)$.

2. Bi-invariance: If $\boldsymbol{R}$ is the mean rotation of $\{\boldsymbol{R}_n\},\ n = 1, \dots, N$, then $\boldsymbol{PRQ}$ is the mean rotation of $\{\boldsymbol{P}\boldsymbol{R}_n\boldsymbol{Q}\},\ n = 1, \dots, N$, for every $\boldsymbol{P}$ and $\boldsymbol{Q}$ in $SO(3)$. This property follows immediately from the bi-invariance of the two metrics defined above.

3. Invariance under transposition: If $\boldsymbol{R}$ is the mean rotation of $\{\boldsymbol{R}_n\},\ n = 1, \dots, N$, then $\boldsymbol{R}^T$ is the mean rotation of $\{\boldsymbol{R}_n^T\},\ n = 1, \dots, N$.

We remark that the bi-invariance property is in some sense the counterpart of the homogeneity property of means of positive numbers (but here left and right multiplication are both needed because the rotation group is not commutative).

3.1. Characterization of the Euclidean mean. The following proposition gives a relation between the Euclidean mean and the usual arithmetic mean.

PROPOSITION 3.3. *The mean rotation $\mathfrak{A}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N)$ of $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N \in SO(3)$ is the orthogonal projection of $\overline{\boldsymbol{R}} = \sum_{n=1}^{N} \frac{\boldsymbol{R}_n}{N}$ onto the special orthogonal group $SO(3)$. In other words, the mean rotation in the Euclidean sense is the projection of the arithmetic mean $\overline{\boldsymbol{R}}$ of $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ in the linear space $\mathcal{M}(3)$ onto $SO(3)$.*

Proof. As $\boldsymbol{R}_n,\ n = 1, \dots, N$ and $\boldsymbol{R}$ are all orthogonal, it follows that

$$\mathfrak{A}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N) = \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \sum_{n=1}^{N} \|\boldsymbol{R}_n - \boldsymbol{R}\|_F^2 = \operatorname*{arg\,max}_{\boldsymbol{R}\in SO(3)} \operatorname{tr}(\overline{\boldsymbol{R}}^T \boldsymbol{R}).$$

On the other hand, the orthogonal projection of $\overline{\boldsymbol{R}}$ onto $SO(3)$ is given by

$$\begin{aligned} \Pi(\overline{\boldsymbol{R}}) &= \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \|\overline{\boldsymbol{R}} - \boldsymbol{R}\|_F = \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \|\overline{\boldsymbol{R}} - \boldsymbol{R}\|_F^2 \\ &= \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \left[\sum_{n=1}^{N} \sum_{m=1}^{N} \operatorname{tr}\Big(\frac{\boldsymbol{R}_n}{N} \frac{\boldsymbol{R}_m^T}{N}\Big) - 2 \operatorname{tr}\Big(\sum_{n=1}^{N} \frac{\boldsymbol{R}_n^T}{N} \boldsymbol{R}\Big) + \operatorname{tr} \boldsymbol{I} \right] \\ &= \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} -2 \operatorname{tr}\Big(\sum_{n=1}^{N} \frac{\boldsymbol{R}_n^T}{N} \boldsymbol{R}\Big) = \operatorname*{arg\,max}_{\boldsymbol{R}\in SO(3)} \operatorname{tr}(\overline{\boldsymbol{R}}^T \boldsymbol{R}). \qquad \square \end{aligned}$$

Because of Proposition 3.3, the mean in the Euclidean sense will be termed the *projected arithmetic mean* to reflect the fact that it is the orthogonal projection of the usual arithmetic mean in $\mathcal{M}(3)$ onto $SO(3)$.

REMARK 3.4. *The projected arithmetic mean can now be seen to be related to the classical orthogonal Procrustes problem [10], which seeks the orthogonal matrix that most closely transforms a given matrix into a second one.*

PROPOSITION 3.5. *If $\det \overline{\boldsymbol{R}}$ is positive, then the mean rotation in the Euclidean sense $\mathfrak{A}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N)$ of $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N \in SO(3)$ is given by the unique polar factor in the polar decomposition [10] of $\overline{\boldsymbol{R}}$.*

Proof. Critical points of the objective function

$$F(\boldsymbol{R}) = \sum_{n=1}^{N} \|\boldsymbol{R} - \boldsymbol{R}_n\|_F^2 \tag{3.5}$$

defined on $SO(3)$ and corresponding to the minimization problem (3.3) are those elements of $SO(3)$ for which the covariant derivative of (3.5) vanishes. Using (2.8) we get $\nabla F = \sum_{n=1}^{N} \boldsymbol{R}\left(\boldsymbol{R}_n^T\boldsymbol{R} - \boldsymbol{R}^T\boldsymbol{R}_n\right)$. Therefore, critical points of (3.5) are the rotation matrices $\boldsymbol{R}$ such that $\sum_{n=1}^{N} \boldsymbol{R}\left(\boldsymbol{R}_n^T\boldsymbol{R} - \boldsymbol{R}^T\boldsymbol{R}_n\right) = \boldsymbol{0}$, or, equivalently, for which the matrix $\boldsymbol{S}$ defined by

$$\boldsymbol{S} = \boldsymbol{R}^T\sum_{n=1}^{N}\boldsymbol{R}_n = N\boldsymbol{R}^T\overline{\boldsymbol{R}} \tag{3.6}$$

is symmetric.

Since $\boldsymbol{R}$ is orthogonal, and both $\boldsymbol{S}$ and $\boldsymbol{M} = \overline{\boldsymbol{R}}^T\overline{\boldsymbol{R}}$ are symmetric, it follows that $\boldsymbol{S}^2 = N^2\boldsymbol{M}$. Therefore, there exists an orthogonal matrix $\boldsymbol{U}$ such that $\boldsymbol{S}^2 = N^2\boldsymbol{U}^T\boldsymbol{D}\boldsymbol{U}$, where $\boldsymbol{D} = \operatorname{diag}(\Lambda_1, \Lambda_2, \Lambda_3)$ with $\Lambda_1 \geq \Lambda_2 \geq \Lambda_3 \geq 0$ being the eigenvalues of $\boldsymbol{M}$. The eight possible square roots of $\boldsymbol{M}$ are $\boldsymbol{U}^T\operatorname{diag}(\pm\sqrt{\Lambda_1}, \pm\sqrt{\Lambda_2}, \pm\sqrt{\Lambda_3})\boldsymbol{U}$. To determine the square root $\boldsymbol{S} = \boldsymbol{U}^T\operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)\boldsymbol{U}$ of $N^2\boldsymbol{M}$ that corresponds to the minimum of (3.5) we require that the Hessian of the objective function (3.5) at $\boldsymbol{R}$ given by (3.6) be positive for all tangent vectors $\boldsymbol{\Delta}$ at $\boldsymbol{R}$. From (2.9) we obtain $\operatorname{Hess} F(\boldsymbol{\Delta}, \boldsymbol{\Delta}) = 2N\operatorname{tr}\left(\overline{\boldsymbol{R}}^T\boldsymbol{R}\boldsymbol{\Delta}\boldsymbol{\Delta}^T\right)$, and therefore at $\boldsymbol{R}$ given by (3.6) we have

$$\operatorname{Hess} F(\boldsymbol{\Delta}, \boldsymbol{\Delta}) = 2[(\lambda_2+\lambda_3)a^2 + (\lambda_1+\lambda_3)b^2 + (\lambda_1+\lambda_2)c^2],$$

where a, b, c are such that $\boldsymbol{\Delta} = \boldsymbol{U}^T\boldsymbol{R}\boldsymbol{B}\boldsymbol{U}$ and $\boldsymbol{B} = \begin{bmatrix} 0 & -c & b \\ c & 0 & -a \\ -b & a & 0 \end{bmatrix}$.

As we are looking for a proper rotation matrix, i.e., an orthogonal matrix with determinant one, it follows from (3.6) that $\det\boldsymbol{S} = N\det\overline{\boldsymbol{R}}$. We therefore conclude that $\operatorname{Hess} F(\boldsymbol{\Delta}, \boldsymbol{\Delta})$ is positive for all tangent vectors $\boldsymbol{\Delta}$ at $\boldsymbol{R}$ if and only if $\lambda_1 = N\sqrt{\Lambda_1}$, $\lambda_2 = N\sqrt{\Lambda_2}$ and $\lambda_3 = sN\sqrt{\Lambda_3}$ where $s = 1$ if $\det\overline{\boldsymbol{R}}$ is positive and $s = -1$ otherwise. In fact, (3.5) has four critical points belonging to $SO(3)$ which consist of a minimum $[(\lambda_1, \lambda_2, \lambda_3) = N(\sqrt{\Lambda_1}, \sqrt{\Lambda 2}, s\sqrt{\Lambda_3})]$, a maximum $[(\lambda_1, \lambda_2, \lambda_3) = N(-\sqrt{\Lambda_1}, -\sqrt{\Lambda_2}, -s\sqrt{\Lambda_3})]$ and two saddle points $[(\lambda_1, \lambda_2, \lambda_3) = N(-\sqrt{\Lambda_1}, s\sqrt{\Lambda_2}, -\sqrt{\Lambda_3})$ and $(\lambda_1, \lambda_2, \lambda_3) = N(s\sqrt{\Lambda_1}, -\sqrt{\Lambda_2}, -\sqrt{\Lambda_3})]$.

Hence, the projected arithmetic mean is given by

$$\boldsymbol{R} = \overline{\boldsymbol{R}}\boldsymbol{U}\operatorname{diag}(\frac{1}{\sqrt{\Lambda_1}}, \frac{1}{\sqrt{\Lambda_2}}, \frac{s}{\sqrt{\Lambda_3}})\boldsymbol{U}^T, \tag{3.7}$$

which, when $\det\overline{\boldsymbol{R}} > 0$, coincides with the polar factor of the polar decomposition of $\overline{\boldsymbol{R}}$. Of course uniqueness fails when the smallest eigenvalue of $\boldsymbol{M}$ is not simple. ∎

REMARK 3.6. *The case where* $\det\overline{\boldsymbol{R}} = 0$ *is a degenerate case. However, if* $\overline{\boldsymbol{R}}$ *has rank 2, i.e., when* $\Lambda_1 \geq \Lambda_2 > \Lambda_3 = 0$, *one can still find a unique closest proper orthogonal matrix to* $\overline{\boldsymbol{R}}$ *(see [6] for details), and hence can define the mean rotation in the Euclidean sense.*

3.2. Characterization of the Riemannian mean. First, we compute the derivative of the real-valued function $H(\boldsymbol{P}(t)) = \frac{1}{2}\|\operatorname{Log}(\boldsymbol{Q}^T\boldsymbol{P}(t))\|_F^2$ with respect to t where $\boldsymbol{P}(t) = \boldsymbol{R}\exp(t\boldsymbol{A})$ is the geodesic emanating from $\boldsymbol{R}$ in the direction of $\boldsymbol{\Delta} = \dot{\boldsymbol{P}}(0) = \boldsymbol{R}\boldsymbol{A}$. As $\boldsymbol{\Delta}$ is in the tangent space at $\boldsymbol{R}$, we have $\boldsymbol{A} = \boldsymbol{R}^T\boldsymbol{\Delta} = -\boldsymbol{\Delta}^T\boldsymbol{R}$. Let $\theta(t) \in (-\pi, \pi)$ be the angle of rotation of $\boldsymbol{Q}^T\boldsymbol{P}(t)$, i.e., such that

$$\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{P}(t)) = 1 + 2\cos\theta(t). \tag{3.8}$$

Differentiate (3.8) to get $\frac{d}{dt}H(\boldsymbol{P}(t))\big|_{t=0} = -\frac{\phi}{\sin\phi}\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A})$, where $\phi = \theta(0)$ is the angle of rotation of $\boldsymbol{Q}^T\boldsymbol{R}$ and we have used the fact that $H(\boldsymbol{P}(t)) = \theta(t)^2$.

Recall that, since $\boldsymbol{A}$ is skew symmetric, $\operatorname{tr}(\boldsymbol{S}\boldsymbol{A}) = 0$ for any symmetric matrix $\boldsymbol{S}$. It follows that $\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A}) = \frac{1}{2}\operatorname{tr}([\boldsymbol{Q}^T\boldsymbol{R} - \boldsymbol{R}^T\boldsymbol{Q}]\boldsymbol{A})$. Hence

$$\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A}) = \frac{1}{2}\operatorname{tr}[(\boldsymbol{Q}^T\boldsymbol{R} - \boldsymbol{R}^T\boldsymbol{Q})\boldsymbol{R}^T\boldsymbol{\Delta}] = \frac{1}{2}\operatorname{tr}[\boldsymbol{\Delta}^T\boldsymbol{R}(\boldsymbol{R}^T\boldsymbol{Q} - \boldsymbol{Q}^T\boldsymbol{R})].$$

Then, with the help of (2.4) we obtain $\frac{d}{dt}H(\boldsymbol{P}(t))\big|_{t=0} = \operatorname{tr}[\boldsymbol{\Delta}^T\boldsymbol{R}\operatorname{Log}(\boldsymbol{Q}^T\boldsymbol{R})]$. Therefore, the covariant derivative of H is given by

$$\nabla H = \boldsymbol{R}\operatorname{Log}(\boldsymbol{Q}^T\boldsymbol{R}). \tag{3.9}$$

The second derivative of (3.8) gives

$$\frac{d^2}{dt^2}H(\boldsymbol{P}(t))\bigg|_{t=0} = \frac{\sin\phi - \phi\cos\phi}{4\sin^3\phi}[\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A})]^2 - \frac{\phi}{2\sin\phi}\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A}^2).$$

Let $\boldsymbol{U}$ be an orthogonal matrix and $\boldsymbol{B}$ the skew-symmetric matrix such that

$$\boldsymbol{Q}^T\boldsymbol{R} = \boldsymbol{U}^T\boldsymbol{V}\boldsymbol{U},\ \boldsymbol{B} = \boldsymbol{U}\boldsymbol{A}\boldsymbol{U}^T = \begin{bmatrix} 0 & -c & b \\ c & 0 & -a \\ -b & a & 0 \end{bmatrix} \text{ where } \boldsymbol{V} = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Then, as $\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A}) = \operatorname{tr}(\boldsymbol{V}\boldsymbol{B})$ and $\operatorname{tr}(\boldsymbol{Q}^T\boldsymbol{R}\boldsymbol{A}^2) = \operatorname{tr}(\boldsymbol{V}\boldsymbol{B}^2)$, it is easy to see that

$$\frac{d^2}{dt^2}H(\boldsymbol{P}(t))\bigg|_{t=0} = \frac{\phi\sin\phi}{1-\cos\phi}(a^2+b^2) + 2c^2. \tag{3.10}$$

The RHS of (3.10) is always positive for arbitrary a, b, c in $\mathbb{R}$ and $\phi \in (-\pi, \pi)$. It follows that $\operatorname{Hess} H(\boldsymbol{\Delta}, \boldsymbol{\Delta})$ is positive for all tangent vectors $\boldsymbol{\Delta}$.

Now, let G denote the objective function of the minimization problem (3.4), i.e.,

$$G(\boldsymbol{R}) = \sum_{n=1}^{N} \|\operatorname{Log}(\boldsymbol{R}_n^T\boldsymbol{R})\|_F^2. \tag{3.11}$$

Using the above, the covariant derivative of G is found to be $\nabla G = \boldsymbol{R}\sum_{n=1}^{N}\operatorname{Log}(\boldsymbol{R}_n^T\boldsymbol{R})$. Therefore, a necessary condition for regular extrema of (3.11) is

$$\sum_{n=1}^{N}\operatorname{Log}(\boldsymbol{R}_n^T\boldsymbol{R}) = \boldsymbol{0}. \tag{3.12}$$

By (3.10) we conclude that the Hessian $\operatorname{Hess} G(\boldsymbol{\Delta}, \boldsymbol{\Delta})$ of the objective function (3.11) is positive for all tangent vectors $\boldsymbol{\Delta}$. Therefore, equation (3.12) characterizes local minima of (3.11) only. As a matter of fact, local maxima are not regular points, i.e., they are points where (3.11) is not differentiable.

It is worth noting that, as $\boldsymbol{R}_n^T = \boldsymbol{R}_n^{-1}$, the characterization for the Riemannian mean given in (3.12) is similar to the characterization

$$\sum_{n=1}^{N}\ln(x_n^{-1}x) = 0 \tag{3.13}$$

of the geometric mean (3.2) of positive numbers. However, while in the scalar case the characterization (3.13) has the geometric mean as unique solution, the characterization (3.12) has multiple solutions, and hence is a necessary but not a sufficient condition to determine the Riemannian mean. The lack of uniqueness of solutions of (3.12) is akin to the fact that, due to the existence of a cut point for each element of $SO(3)$, the objective function (3.11) is not convex over its domain.

In general, closed-form solutions to (3.12) cannot be found. However, for some special cases solutions can be given explicitly. In the following subsections, we will present some of these special cases.

REMARK 3.7. *The Riemannian mean of* $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ *may also be called the Riemannian barycenter of* $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$*, which is a notion introduced by Grove, Karcher and Ruh [11]. In [17] it was proven that for manifolds with negative sectional curvature, the Riemannian barycenter is unique.*

3.2.1. Riemannian mean of two rotations. Intuitively, in the case $N = 2$, the mean rotation in the Riemannian sense should lie midway between $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ along the shortest geodesic curve connecting them, i.e., it should be the rotation $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$. Indeed, straightforward computation shows that $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$ does satisfy condition (3.12). Alternatively, equation (3.12) can be solved analytically as follows. First, we rewrite it as

$$\operatorname{Log}(\boldsymbol{R}_1^T\boldsymbol{R}) = -\operatorname{Log}(\boldsymbol{R}_2^T\boldsymbol{R}),$$

then we take the exponential of both sides to obtain $\boldsymbol{R}_1^T\boldsymbol{R} = \boldsymbol{R}^T\boldsymbol{R}_2$. After left multiplying both sides with $\boldsymbol{R}_1^T\boldsymbol{R}$ we get $(\boldsymbol{R}_1^T\boldsymbol{R})^2 = \boldsymbol{R}_1^T\boldsymbol{R}_2$. Such an equation has two solutions in $SO(3)$ that correspond to local minima of (3.11). However, the global minimum is the one that corresponds to taking the square root of the above equation that has eigenvalues with positive real part, i.e., $(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$. Therefore, for two non-antipodal rotation matrices $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, the mean in the Riemannian sense is given explicitly by

$$\mathfrak{G}(\boldsymbol{R}_1, \boldsymbol{R}_2) = \boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2} = \boldsymbol{R}_2(\boldsymbol{R}_2^T\boldsymbol{R}_1)^{1/2}. \tag{3.14}$$

The second equality can be easily verified by pre-multiplying $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$ by $\boldsymbol{R}_2\boldsymbol{R}_2^T$ which is equal to $\boldsymbol{I}$. This makes it clear that $\mathfrak{G}$ is symmetric with respect to $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, i.e., $\mathfrak{G}(\boldsymbol{R}_1, \boldsymbol{R}_2) = \mathfrak{G}(\boldsymbol{R}_2, \boldsymbol{R}_1)$.

3.2.2. Riemannian mean of rotations in a one-parameter subgroup. In the case where all matrices $\boldsymbol{R}_n,\ n = 1, \dots, N$ belong to a one-parameter subgroup of $SO(3)$, i.e., they represent rotations about a common axis, we expect that their mean is also in the same subgroup. Further, one can easily show that equation (3.12) reduces to saying that $\boldsymbol{R}$ is an Nth root of $\prod_{n=1}^{N}\boldsymbol{R}_n$. Therefore, the Riemannian mean is the Nth root that yields the minimum value of the objective function (3.11).

In this case, all rotations lie on a single geodesic curve. One can show that the geometric mean $\mathfrak{G}(\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3)$ of three rotations $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$ such that $\mathrm{d}_R(\boldsymbol{R}_i, \boldsymbol{R}_j) < \pi,\ i, j = 1, 2, 3$, is the rotation that is located at $\frac{2}{3}$ of the length of the shortest geodesic segment connecting $\boldsymbol{R}_1$ and $\mathfrak{G}(\boldsymbol{R}_2, \boldsymbol{R}_3)$, i.e., the rotation $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2(\boldsymbol{R}_2^T\boldsymbol{R}_3)^{1/2})^{2/3}$. By induction, when $\mathrm{d}_R(\boldsymbol{R}_i, \boldsymbol{R}_j) < \pi,\ i, j = 1, \dots, N$, we have

$$\mathfrak{G}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N) = \boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2(\boldsymbol{R}_2^T\boldsymbol{R}_3(\cdots\boldsymbol{R}_{N-1}(\boldsymbol{R}_{N-1}^T\boldsymbol{R}_N)^{\frac{1}{2}})^{\frac{2}{3}}\cdots)^{\frac{N-2}{N-1}})^{\frac{N-1}{N}}. \tag{3.15}$$

This explicit formula does not hold in the general case due to the inherent curvature of $SO(3)$, see the discussion at the end of Example 2 below.

When the rotations $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ belong to a geodesic segment of length less than π and centered at the identity, the above formula reduces to

$$\mathfrak{G}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N) = \boldsymbol{R}_1^{1/N} \cdots \boldsymbol{R}_N^{1/N}. \tag{3.16}$$

Once again we see the close similarity between the geometric mean of positive numbers and the Riemannian mean of rotations. This is to be expected since both the set of positive numbers and $SO(3)$ are multiplicative groups, and we have used their intrinsic metrics to define the mean. For this reason, we will call the mean in the Riemannian sense the *geometric mean*.

3.3. Equivalence of both notions of mean of two rotations. In the following, we show that for two rotations the projected arithmetic mean and the geometric mean coincide. First, we prove the following lemma.

LEMMA 3.8. *Let* $\boldsymbol{R}_1$ *and* $\boldsymbol{R}_2$ *be two elements of* $SO(3)$*, then* $\det(\boldsymbol{R}_1 + \boldsymbol{R}_2) \geq 0$.

Proof. Consider the real-valued function defined on $[0, 1]$ by $f(t) = \det(\boldsymbol{R}_1 + t\boldsymbol{R}_2)$. We see that this function is continuous with $f(0) = 1$ and $f(1) = \det(\boldsymbol{R}_1 + \boldsymbol{R}_2)$. Assume that $f(1) < 0$, i.e., $\det(\boldsymbol{R}_1 + \boldsymbol{R}_2) < 0$, then there exists τ in $[0, 1]$ such that $f(\tau) = \det(\boldsymbol{R}_1 + \tau\boldsymbol{R}_2) = 0$. Since $\det \boldsymbol{R}_2 = 1$, it follows that $\det(\boldsymbol{R}_2^T\boldsymbol{R}_1 + \tau\boldsymbol{I}) = 0$. Hence, τ must be in the spectrum of $\boldsymbol{R}_2^T\boldsymbol{R}_1$ which is a proper orthogonal matrix. But this cannot happen, which contradicts the assumption that $\det(\boldsymbol{R}_1 + \boldsymbol{R}_2) < 0$. ∎

In general, the result of the above lemma does not hold for more than two rotations matrices. We will see examples of three rotation matrices for which the determinant of their sum can be negative.

PROPOSITION 3.9. *The polar factor of the polar decomposition of* $\boldsymbol{R}_1 + \boldsymbol{R}_2$*, where* $\boldsymbol{R}_1$ *and* $\boldsymbol{R}_2$ *are two rotation matrices, is given by* $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$.

Proof. Let $\boldsymbol{Q}$ be the proper orthogonal matrix and $\boldsymbol{S}$ be the positive-definite matrix such that $\boldsymbol{QS}$ is the unique polar decomposition of $\boldsymbol{R}_1 + \boldsymbol{R}_2$. Then $\boldsymbol{S}^2 = (\boldsymbol{R}_1^T + \boldsymbol{R}_2^T)(\boldsymbol{R}_1 + \boldsymbol{R}_2) = 2\boldsymbol{I} + \boldsymbol{R}_1^T\boldsymbol{R}_2 + \boldsymbol{R}_2^T\boldsymbol{R}_1$. One can easily verify that $(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2} + (\boldsymbol{R}_1^T\boldsymbol{R}_2)^{-1/2}$ is the positive-definite square root of $2\boldsymbol{I} + \boldsymbol{R}_1^T\boldsymbol{R}_2 + \boldsymbol{R}_2^T\boldsymbol{R}_1$ and that the inverse of this square root is given by $\boldsymbol{S}^{-1} = (\boldsymbol{R}_1 + \boldsymbol{R}_2)^{-1}\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$. Hence, the polar factor is $\boldsymbol{Q} = (\boldsymbol{R}_1 + \boldsymbol{R}_2)\boldsymbol{S}^{-1} = \boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$. ∎

Since the polar decomposition is unique, the result of this proposition together with the previous lemma shows that both notions of mean agree for the case of two rotation matrices. For more than two rotations, however, both notions of mean coincide only in special cases that present certain symmetries. In Example 2 of § 4 below, we shall consider a two-parameter family of cases illustrating this coincidence.

4. Analytically solvable examples. In this section we present two cases in which we can solve for both the projected arithmetic mean and the geometric mean explicitly. These examples help us gain a deeper and concrete insight to both notions of mean. Furthermore, Example 2 confirms our intuitive idea that for "symmetric" cases, both notions of mean agree.

4.1. Example 1. We begin with a simple example where all rotation matrices for which we want to find the mean lie in a one-parameter subgroup of $SO(3)$. Using the bi-invariance property we can reduce the problem to that of finding the mean of

$$\boldsymbol{R}_n = \begin{bmatrix} \cos\theta_n & -\sin\theta_n & 0 \\ \sin\theta_n & \cos\theta_n & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad n = 1, \dots, N. \tag{4.1}$$

Projected arithmetic mean: The arithmetic sum of these matrices has a positive determinant $r^2 = (\sum_{n=1}^{N} \cos\theta_n)^2 + (\sum_{n=1}^{N} \sin\theta_n)^2$. Hence, the projected arithmetic mean of the given matrices is given by the polar factor of the polar decomposition of their sum. After performing such a decomposition we find that

$$\mathfrak{A}(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N) = \begin{bmatrix} \cos\Theta_a & -\sin\Theta_a & 0 \\ \sin\Theta_a & \cos\Theta_a & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{where} \quad \begin{cases} \cos\Theta_a = \dfrac{1}{r}\displaystyle\sum_{n=1}^{N} \cos\theta_n, \\ \sin\Theta_a = \dfrac{1}{r}\displaystyle\sum_{n=1}^{N} \sin\theta_n. \end{cases}$$

Such a mean is well defined as long as $r \neq 0$. This mean agrees with the notion of directional mean used in the statistics literature for circular and spherical data [20, 7, 9, 8]. The quantity $1 - r/N$, which is called the circular variance, is a measure of dispersion of the circular data $\theta_1, \ldots, \theta_N$. The direction defined by the angle Θ_a is called the mean direction of the directions defined by $\theta_1, \ldots, \theta_N$.

Geometric mean: Solutions of (3.12) are given by

$$\begin{bmatrix} \cos\Theta_l & -\sin\Theta_l & 0 \\ \sin\Theta_l & \cos\Theta_l & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \text{where} \quad \Theta_l = \frac{1}{N}(\sum_{n=1}^{N} \theta_n + 2\pi l), \ l = 0, \ldots, N-1.$$

The geometric mean of these rotation matrices is therefore the solution that yields the minimum value of the objective function (3.11). Of course, as we have seen in § 3, the geometric mean is given explicitly by (3.15).

Note that, even though elements of a one-parameter subgroup commute, the two rotations (3.15) and (3.16) are different. This is due to choice of the kth root of a rotation matrix to be the one with eigenvalues that have the largest positive real parts. To see this, consider the case $N = 2$, $\theta_1 = \frac{2\pi}{3}$ and $\theta_2 = -\frac{2\pi}{3}$. Then $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2} = \boldsymbol{P}$ where $\boldsymbol{P}$ is a rotation of an angle π about the z-axis while $\boldsymbol{R}_1^{1/2}\boldsymbol{R}_2^{1/2} = \boldsymbol{I}$.

If the rotation matrices $\boldsymbol{R}_n$ are such that $\alpha \leq \theta_n < \alpha + \pi$, $n = 1, \ldots, N$ for a certain number $\alpha \in \mathbb{R}$, then their geometric mean is a rotation about the z-axis of an angle $\Theta_g = \dfrac{1}{N}\displaystyle\sum_{n=1}^{N} \theta_n$.

The geometric mean rotation of the rotations given by (4.1) coincides with the concept of median direction of circular data [20, 7].

REMARK 4.1. *When $\theta_1 = \theta$, $\theta_2 = \theta + \pi$ and $N = 2$ in (4.1), neither the projected arithmetic mean nor the geometric mean is well defined. On the one hand $\boldsymbol{R}_1 + \boldsymbol{R}_2 = \boldsymbol{0}$, so the projected arithmetic mean is not defined, while on the other hand the objective function (3.11) for the geometric mean has two local minima with the same value, namely, $\boldsymbol{R}_1(\boldsymbol{R}_1^T\boldsymbol{R}_2)^{1/2}$ and its cut value $\boldsymbol{R}_1 \exp(\dfrac{\theta+\pi}{2\theta} \operatorname{Log}(\boldsymbol{R}_1^T\boldsymbol{R}_2))$, and therefore the global minimum is not unique.*

Let $\tilde{F}$ and $\tilde{G}$ be the functions defined on $[-\pi, \pi]$ such that $\tilde{F}(\theta) = F(\boldsymbol{R})$ and $\tilde{G}(\theta) = G(\boldsymbol{R})$ for any rotation $\boldsymbol{R}$ about the z-axis through an angle θ, i.e., $\tilde{F}$ and $\tilde{G}$ are the restrictions of the objective functions (3.5) and (3.11) to the subgroup considered in this example. In Fig. 4.1 we give the plots of $\tilde{F}$ and $\tilde{G}$ for the sets of data $N = 4$ and $\theta_1 = -\frac{\pi}{2}$, $\theta_2 = 0$, $\theta_3 = \frac{\pi}{2}$, $\theta_4 = \pi - \alpha$ where α takes several different values. It is clear that neither (3.5) nor (3.11) is convex. While the function (3.5)

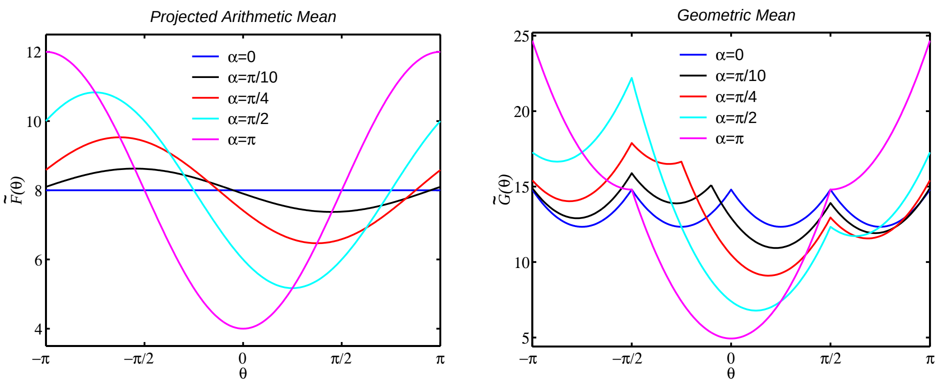

FIG. 4.1. *Plots of the objective functions $\tilde{F}(\theta)$ and $\tilde{G}(\theta)$ for different values of α. Note that when $\alpha = 0$, $\tilde{F}$ is constant and $\tilde{G}$ has four local minima with an equal value. Consequently, neither the projected arithmetic mean nor the geometric mean is well defined.*

is smooth the function (3.11) has cusp points but only at local maxima. However, if the given rotations are located in a geodesic ball of radius less than $\pi/2$, i.e., in this example have angles θ_i such that $|\theta_i - \theta_j| < \pi, 1 \leq i, j \leq N$, then the objective functions restricted to this geodesic ball are convex and hence the means are well defined. Such case is illustrated in Fig. 4.2 which shows plots of $\tilde{F}$ and $\tilde{G}$ for the following sets of data $N = 3$ and $\theta_1 = -\frac{\pi}{4}$, $\theta_2 = \frac{\pi}{4}$, $\theta_3 = \frac{3\pi}{4} - \alpha$ where α takes several different values.

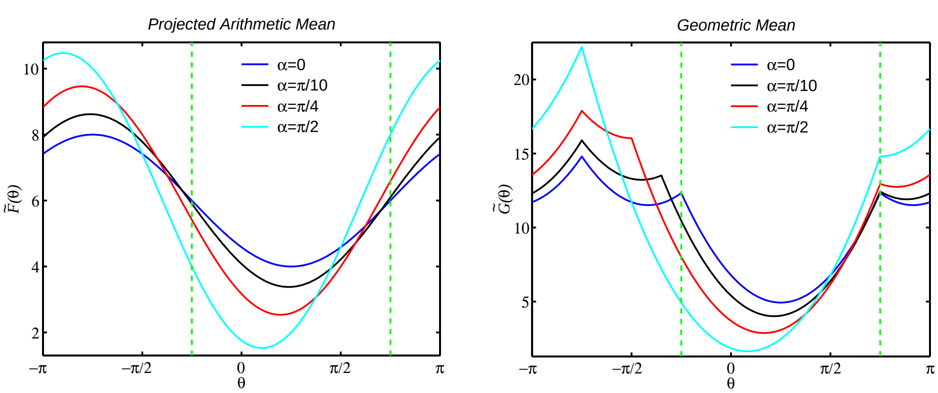

FIG. 4.2. *Plots of the objective functions $\tilde{F}(\theta)$ and $\tilde{G}(\theta)$ for different values of α. Restricted to $[-\pi/4, 3\pi/4]$, i.e., between the dashed lines, the objective functions are indeed convex.*

4.2. Example 2. In the second example we consider N elements of $SO(3)$ that represent rotations through an angle θ about the axes defined by the unit vectors $\boldsymbol{u}_n = [\sin\alpha\cos\beta_n, \sin\alpha\sin\beta_n, \cos\alpha]^T$, where $\beta_n = \frac{2(n-1)\pi}{N}$, $n = 1, \ldots, N$, and $\alpha \in [0, \frac{\pi}{2})$.

Projected arithmetic mean: Straightforward computations show that the projected arithmetic mean is given by

$$\mathfrak{A}(\boldsymbol{R}_1,\dots,\boldsymbol{R}_N)=\begin{bmatrix}\cos\Theta_a & -\sin\Theta_a & 0\\ \sin\Theta_a & \cos\Theta_a & 0\\ 0 & 0 & 1\end{bmatrix},\qquad \begin{cases}\cos\Theta_a=\dfrac{2\cos\theta-\sin^2\alpha(\cos\theta-1)}{2+\sin^2\alpha(\cos\theta-1)},\\ \sin\Theta_a=\dfrac{2\cos\alpha\sin\theta}{2+\sin^2\alpha(\cos\theta-1)}.\end{cases}$$

By using half-angle tangent formulas in the above we obtain the following simple relation between Θ_a and θ

$$\tan\frac{\Theta_a}{2}=\cos\alpha\tan\frac{\theta}{2}. \tag{4.2}$$

Geometric mean: Since the rotation axes are symmetric about the z-axis, and the rotations share the same angle, we expect that their geometric mean is a rotation about the z-axis through a certain angle Θ_g. Furthermore, because of this symmetry we also expect that the mean in the Euclidean sense agrees with the one in the Riemannian sense.

From the Campbell-Baker-Hausdorff formula for elements of $SO(3)$ [23] we have

$$\operatorname{Log}(\boldsymbol{R}_n^T\boldsymbol{R})=\phi\left(-a\operatorname{Log}\boldsymbol{R}_n+b\operatorname{Log}\boldsymbol{R}-c\left[\operatorname{Log}\boldsymbol{R}_n,\operatorname{Log}\boldsymbol{R}\right]\right),$$

where the coefficients a,b,c and ϕ are given by

$$a\theta\sin\frac{\phi}{2}=\sin\frac{\theta}{2}\cos\frac{\Theta_g}{2},\qquad b\Theta_g\sin\frac{\phi}{2}=\cos\frac{\theta}{2}\sin\frac{\Theta_g}{2},$$
$$c\theta\Theta_g\sin\frac{\phi}{2}=\sin\frac{\theta}{2}\sin\frac{\Theta_g}{2},\qquad \cos\frac{\phi}{2}=\cos\frac{\theta}{2}\cos\frac{\Theta_g}{2}-\cos\alpha\sin\frac{\theta}{2}\sin\frac{\Theta_g}{2}.$$

Therefore, the characterization (3.12) of the geometric mean reduces to

$$a\sum_{n=1}^{N}\operatorname{Log}\boldsymbol{R}_n-bN\operatorname{Log}\boldsymbol{R}+c\sum_{n=1}^{N}\left[\operatorname{Log}\boldsymbol{R}_n,\operatorname{Log}\boldsymbol{R}\right]=\boldsymbol{0}.$$

This is a matrix equation in $\mathfrak{so}(3)$, which is equivalent to a system of three nonlinear equations. Because the axes of rotation of $\boldsymbol{R}_n$ are symmetric about the z-axis we have $\sum_{n=1}^{N}\cos\beta_n=\sum_{n=1}^{N}\sin\beta_n=0$. It follows that $\sum_{n=1}^{N}[\operatorname{Log}\boldsymbol{R}_n,\operatorname{Log}\boldsymbol{R}]=\boldsymbol{0}$ and $\Theta_g\sum_{n=1}^{N}\operatorname{Log}\boldsymbol{R}_n=\theta\cos\alpha N\operatorname{Log}\boldsymbol{R}$. Therefore, this system reduces to the following single equation for the angle Θ_g

$$\tan\frac{\Theta_g}{2}=\cos\alpha\tan\frac{\theta}{2}, \tag{4.3}$$

which when compared with (4.2) indeed shows that $\Theta_a=\Theta_g$ and therefore the projected arithmetic mean and the geometric mean coincide.

This example provides a family of mean problems parameterized by θ and α where the projected arithmetic and geometric mean coincide. We now further examine the problem of finding the mean of three rotations about the three coordinate axes through the same angle θ, which, by the bi-invariance property of both means, can be considered as a special case of this two-parameter family with $N = 3$ and $\cos\alpha = \frac{1}{\sqrt{3}}$. Therefore the mean of these three rotations is a rotation through an angle Φ about the axis generated by the vector $[1, 1, 1]^T$ with $\tan\frac{\theta}{2} = \sqrt{3}\tan\frac{\Phi}{2}$. The rotations $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$ form a geodesic equilateral triangle in $SO(3)$. By symmetry arguments the geometric mean should be the intersection of the three geodesic medians, i.e., the geodesic segments joining the vertices of the geodesic triangle to the midpoints of the opposite sides. In flat geometry, this intersection is located at two-thirds from the vertices of the triangle. However, in the case of $SO(3)$, due to its intrinsic curvature, this is not true. The ratio γ of the length of the geodesic segment joining one rotation and the geometric mean, to the length of the geodesic median joining this rotation and the midpoint of the geodesic curve joining the two other rotations is plotted as a function of the angles θ in Fig. 4.3.

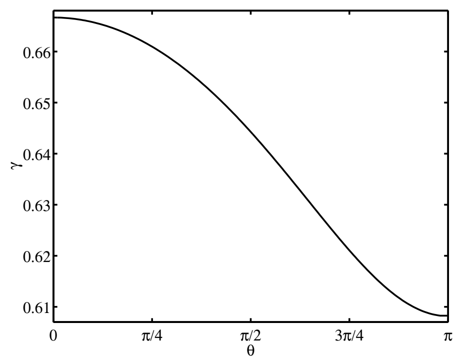

FIG. 4.3. *Plot of the ratio γ of the geodesic distance from one vertex to the barycenter over the geodesic distance from this vertex to the midpoint of the opposed edge in the geodesic equilateral triangle in $SO(3)$. The departure of γ from 2/3, which is due to the curvature of $SO(3)$, increases with the length, θ, of the sides of the triangle.*

5. Weighted means and power means. Our motivation of this work was to construct a filter that smooths the rotation data giving the relative orientations of successive base pairs in a DNA fragment, see [19] for details. Such a filter can be a generalization of moving window filters, which are based on weighted averages, used in linear spaces to smooth noisy data. The construction of such filters and the direct analogy we have found between the arithmetic and geometric means in the group of positive numbers, and the projected arithmetic and geometric means in the group of rotations, have led us to the introduction of weighted means and power means of rotations that we discuss next.

DEFINITION 5.1. *The weighted projected arithmetic mean of N given rotations $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ with weights $\boldsymbol{w} = (w_1, \dots, w_N)$ is defined as*

$$\mathfrak{A}_w(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N; \boldsymbol{w}) := \operatorname*{arg\,min}_{\boldsymbol{R}\in SO(3)} \sum_{n=1}^{N} w_n \|\boldsymbol{R} - \boldsymbol{R}_n\|_F^2. \tag{5.1}$$

This mean satisfies the bi-invariance property. Using similar arguments as for the projected arithmetic mean one can show that the weighted projected arithmetic mean is given by the polar factor of the polar decomposition of the matrix $\boldsymbol{A} = \sum_{n=1}^{N} w_n \boldsymbol{R}_n$

provided that $\det \boldsymbol{A}$ is positive.

DEFINITION 5.2. *The weighted geometric mean of N rotations $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ with weights $\boldsymbol{w} = (w_1, \dots, w_N)$ is defined as*

$$\mathfrak{G}_w(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N; \boldsymbol{w}) := \underset{\boldsymbol{R} \in SO(3)}{\arg\min} \sum_{n=1}^{N} w_n \| \operatorname{Log}(\boldsymbol{R}^T \boldsymbol{R}_n) \|_F^2. \tag{5.2}$$

This mean also satisfies the bi-invariance property. Using arguments similar to those used for the geometric mean, we can show that the weighted geometric mean is characterized by $\sum_{n=1}^{N} w_n \operatorname{Log}(\boldsymbol{R}_n^T \boldsymbol{R}) = \boldsymbol{0}$.

DEFINITION 5.3. *For a real number s such that $0 < |s| \leq 1$, we define the weighted s-th power mean rotation of N rotations $\boldsymbol{R}_1, \boldsymbol{R}_2, \dots, \boldsymbol{R}_N$ with weights $\boldsymbol{w} = (w_1, \dots, w_N)$ as*

$$\mathfrak{M}_w^{[s]}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N; \boldsymbol{w}) := \underset{\boldsymbol{R} \in SO(3)}{\arg\min} \sum_{n=1}^{N} w_n \| \boldsymbol{R}^s - \boldsymbol{R}_n^s \|_F^2. \tag{5.3}$$

We note that $\left[\mathfrak{M}_w^{[s]}(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N; \boldsymbol{w})\right]^s = \mathfrak{A}_w(\boldsymbol{R}_1^s, \dots, \boldsymbol{R}_N^s; \boldsymbol{w})$. Of course for $s = 1$ this is the weighted projected arithmetic mean. Because elements of $SO(3)$ are orthogonal, and the trace operation is invariant under transposition, the weighted s-th power mean is the same as the weighted $(-s)$-th power mean. Therefore, it is immediate that the *weighted projected harmonic mean*, defined by

$$\mathfrak{H}_w(\boldsymbol{R}_1, \dots, \boldsymbol{R}_N; \boldsymbol{w}) = \left[\mathfrak{M}_w(\boldsymbol{R}_1^{-1}, \dots, \boldsymbol{R}_N^{-1}; \boldsymbol{w})\right]^{-1}$$

coincides with the weighted projected arithmetic mean.

This is a natural generalization of the s-th power mean of positive numbers and it is in line with the fact that for positive numbers $(x_1, \dots, x_N)$ the s-th power mean is given by the s-th root of the arithmetic mean of $(x_1^s, \dots, x_N^s)$ [12, 2]. One has to note, however, that for s such that $0 < |s| < 1$ this mean is not invariant under the action of elements of $SO(3)$. This is not a surprise as the power mean of positive numbers also does not satisfy the homogeneity property.

For the set of positive numbers [12] and similarly for the set of Hermitian definite positive operators [25], there is a natural ordering of elements and the classical arithmetic-geometric-harmonic mean inequalities holds. Furthermore, it is well known [12, 25] that the s-th power mean converges to the geometric mean as s goes to 0. However, for the group of rotations such a natural ordering does not exists. Nonetheless, one can show that if all rotations $\boldsymbol{R}_1, \dots, \boldsymbol{R}_N$ belong to a geodesic ball of radius less than $\frac{\pi}{2}$ centered at the identity, then the projected power mean indeed converges to the geometric mean as s tends to 0.

Analysis of numerical algorithms for computing the geometric mean rotation and the use of the different notions of mean rotation for smoothing three-dimensional orientation data will be published elsewhere.

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