

MIXED MAPS FOR LEARNING A KOLMOGOROFF-NAGUMO-TYPE AVERAGE ELEMENT ON THE COMPACT STIEFEL MANIFOLD

S. Fiori

Dipartimento di Ingegneria dell'Informazione,
Università Politecnica delle Marche
s.fiori@univpm.it

T. Kaneko, and T. Tanaka

Dept. of Electrical and Electronic Eng.,
Tokyo Univ. of Agriculture and Technology
tanakat@cc.tuat.ac.jp

ABSTRACT

The present research work proposes a new fast fixed-point average-value learning algorithm on the compact Stiefel manifold based on a mixed retraction/lifting pair. Numerical comparisons between fixed-point algorithms based on the proposed non-associated retraction/lifting map pair and two associated retraction/lifting pairs confirm that the averaging algorithm based on a combination of mixed maps is remarkably less computationally demanding than the same averaging algorithm based on any of the constituent associated retraction/lifting pairs.

Index Terms— Fixed-point iteration, Compact Stiefel manifold, Empirical averaging, Kolmogoroff-Nagumo mean, Manifold retraction/lifting maps.

1. INTRODUCTION

The question about how to define the notion of *mean value* over a set of structured samples has no intrinsic answer. Even in the simple case of a data set made of two positive real-valued numbers, there exist a variety of methods to define their mean value, each of which possesses different properties and leads to a different numerical result. The most known averages of two numbers $x, y > 0$ are the arithmetic mean $\frac{1}{2}(x + y)$, the harmonic mean $\frac{2xy}{x+y}$ and the geometric mean $\sqrt{xy}$. A generalization of these is the Heinz mean $\frac{1}{2}(x^\alpha y^{1-\alpha} + y^\alpha x^{1-\alpha})$, with $0 \leq \alpha \leq \frac{1}{2}$, that interpolates between the arithmetic ($\alpha = 0$) and the geometric ($\alpha = \frac{1}{2}$) mean. Another averaging formula is given by the Heronian mean $\frac{1}{3}(x + \sqrt{xy} + y)$, that corresponds to a weighted sum of the arithmetic and the geometric means of the positive numbers x and y . Most averaging formulas lead to instances of the *Chisini mean* as defined in [6]. Also, see [20] for a detailed discussion on its properties. The Chisini mean provides a good illustration of the fact that it is possible to define a mean value of a set of numbers without any particular requirement about, e.g., convexity. A function f of N real-valued variables leads to a Chisini mean value μ if, for every tuple $(x_1, x_2, \dots, x_N)$, there exists a unique μ such that

$$f(x_1, x_2, \dots, x_N) = f(\mu, \mu, \dots, \mu). \quad (1)$$

The arithmetic mean $\mu_a \stackrel{\text{def}}{=} \frac{1}{N} \sum_{k=1}^N x_k$ of a tuple $(x_1, x_2, \dots, x_N)$ is a Chisini mean with $f(x_1, x_2, \dots, x_N) \stackrel{\text{def}}{=} x_1 + x_2 + \dots + x_N$. In fact, with this choice of the function f , (1) reads: $\sum_{k=1}^N x_k = \sum_{k=1}^N \mu = N\mu$. A rather general definition of mean value of a

set of real-valued numbers is the *Kolmogoroff-Nagumo* (or *quasi-arithmetic*) mean

$$\mu_{\text{KN}} \stackrel{\text{def}}{=} \varphi \left(\frac{1}{N} \sum_{k=1}^N \varphi^{-1}(x_k) \right) \quad (2)$$

for a continuous strictly monotonic function φ (for a review, see [20]). In the case of structured samples, such as structured matrices, the question about how to extend the definition of Kolmogoroff-Nagumo mean is rather involved. The Kolmogoroff-Nagumo mean turns out to be a special case of the Chisini mean. In fact, upon defining $f(x_1, x_2, \dots, x_N) \stackrel{\text{def}}{=} \varphi^{-1}(x_1) + \varphi^{-1}(x_2) + \dots + \varphi^{-1}(x_N)$, it is readily verified that the mean μ_{KN} is the unique solution to the Chisini equation (1)

$$\sum_{k=1}^N \varphi^{-1}(x_k) = \sum_{k=1}^N \varphi^{-1}(\mu) = N\varphi^{-1}(\mu). \quad (3)$$

Structured matrices appear in a variety of neural network applications and learning theories, such as medical imaging [4], statistical analysis on manifolds [5], adaptive filtering [9], computational ophthalmology [11] and radio polarimetry [14]. The empirical mean is perhaps the most often invoked statistical characterization of a set of structured matrices [3, 4, 9, 18, 21], along with the associated empirical variance, which measures the spread of a cloud of points around their empirical mean. A successful application of empirical mean on a structured-matrix space concerns the problem of computing the average character of a set of ‘geometric eyes’ in computational ophthalmology [10]. When the matrices to average obey internal constraints such as orthogonality, the result of simple summation and division by the number of summands, which would represent an arithmetic mean, does not obey the same constraints, in general. Therefore, in order to obtain an empirical arithmetic mean of orthogonal matrices, it is necessary to establish a learning method by considering the geometric structure of the matrix-space that the matrices to average belong to.

To solve such problem, Kaneko, Tanaka and Fiori [16] constructed an averaging algorithm on the compact Stiefel manifold which is a non-trivial extension of averaging algorithms on Lie-group-type manifolds introduced by Fiori and Tanaka in [12]. The underlying idea behind the algorithms developed in the contributions [16] is that the sample-points on the Stiefel manifold are mapped onto a tangent space, where the average is taken, and then the obtained average point on the tangent space is brought back to the Stiefel manifold, via appropriate maps which are referred to as a *retraction map* and a *lifting map*. A variety of algorithms on the compact Stiefel manifold utilizing such maps were explained in [17],

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whose convergence features and computational runtime were compared and which were applied to averaging real-world samples.

The key point is that, in order to construct an averaging algorithm on the compact Stiefel manifold, it is necessary to construct an appropriate retraction/lifting pair. The averaging algorithms proposed in [17] utilize QR-decomposition-based, Cayley-transform-based, polar-decomposition-based and orthographic-type retraction/lifting pairs. All these algorithms, however, suffer of a bloating of computational demand with the increase of the size of the processed matrices. For example, in the case of the polar-decomposition-based retraction/lifting pair, the retraction map may be expressed in closed form, while the computation of the associated lifting map requires solving a continuous-time algebraic Riccati equation.

In the present paper, in order to ease the computational demand of the previously-introduced class of averaging algorithms, a new Kolmogoroff-Nagumo-type averaging algorithm is proposed which exploits a combination of a closed form polar retraction map and a closed form orthographic lifting map. The implication of the proposed choice are evaluated analytically as well as numerically.

2. AVERAGING ALGORITHM BASED ON A COMBINATION OF RETRACTION/LIFTING PAIRS

The aim of the present section is to build-up an average-value learning algorithm on the compact Stiefel manifold based on the notion of *mixed manifold retraction/lifting pair*. The learning algorithm, stemming from a non-linear matrix-type equation, is implemented by a fast fixed-point iteration scheme.

The compact Stiefel manifold [7] is defined by:

$$\text{St}(p, n) \stackrel{\text{def}}{=} \{X \in \mathbb{R}^{p \times n} | X^T X = I_n\}$$

where symbol I_n denotes a $n \times n$ identity matrix and $n \leq p$, namely, $\text{St}(p, n)$ is the space of the ‘tall-skinny’ orthogonal matrices. Its tangent space at a point $X \in \text{St}(p, n)$ is expressed as:

$$T_X \text{St}(p, n) = \left\{ V \in \mathbb{R}^{p \times n} | X^T V + V^T X = 0 \right\}.$$

Each tangent space is a vector space under standard matrix addition and multiplication by a real scalar.

The following measure of discrepancy $\delta: \text{St}(p, n) \times \text{St}(p, n) \rightarrow \mathbb{R}_+^0$ between two Stiefel-manifold matrices is made use of:

$$\delta(X, Y) \stackrel{\text{def}}{=} \|I_n - X^T Y\|_F, \quad X, Y \in \text{St}(p, n), \quad (4)$$

where symbol $\|\cdot\|_F$ denotes the Frobenius norm.

A *retraction* at a point $X \in \text{St}(p, n)$ of a Stiefel manifold is defined as a map $P_X: T_X \text{St}(p, n) \rightarrow \text{St}(p, n)$, while a map $P_X^{-1}: \text{St}(p, n) \rightarrow T_X \text{St}(p, n)$ such that $P_X(P_X^{-1}(Q)) = Q$, for $Q \in \text{St}(p, n)$, is termed *lifting* map (for complete definitions see, e.g., [8, 17]). Both maps are defined only locally, therefore, hereafter it is assumed that X and Q lay sufficiently close to each other to evaluate $P_X^{-1}(Q)$ and that V is sufficiently close to 0 to evaluate $P_X(V)$.

Given a point $X \in \text{St}(p, n)$ and a vector $V \in T_X \text{St}(p, n)$, the *polar-decomposition retraction* on the Stiefel manifold may be written in closed form:

$$P_X(V) = (X + V)(I_n + V^T V)^{-\frac{1}{2}}. \quad (5)$$

The associated *polar-decomposition lifting* is denoted by P_X^{-1} .

The *orthographic lifting map* [1] may be defined as follows:

$$\hat{P}_X^{-1}(Q) = \pi_{T_X \text{St}(p, n)}(Q - X), \quad (6)$$

where $X, Q \in \text{St}(p, n)$ and $\pi_{T_X \text{St}(p, n)}: \mathbb{R}^{p \times n} \rightarrow T_X \text{St}(p, n)$ denotes a projection from the ambient space $\mathbb{R}^{p \times n}$ onto a tangent space $T_X \text{St}(p, n)$. One such a projector is:

$$\pi_{T_X \text{St}(p, n)}(A) = (I_p - X X^T)A - X \text{sk}(X^T A), \quad (7)$$

where $A \in \mathbb{R}^{p \times n}$ and $\text{sk}(A) \stackrel{\text{def}}{=} \frac{1}{2}(A^T - A)$. Plugging (7) into (6) gives:

$$\begin{aligned} \hat{P}_X^{-1}(Q) &= (I_p - X X^T)(Q - X) - X \text{sk}(X^T(Q - X)) \\ &= (I_p - X X^T)Q + \frac{1}{2}X(X^T Q - Q^T X). \end{aligned} \quad (8)$$

The associated *orthographic retraction map* is denoted by $\hat{P}_X$.

2.1. Averaging method based on a mixed retraction/lifting pair

The following steps lead to an equation characterizing the unknown empirical mean matrix $X \in \text{St}(p, n)$, which represents an empirical estimate of the actual center of mass $C \in \text{St}(p, n)$, on the basis of N available Stiefel samples $X_k \in \text{St}(p, n)$:

1. Map the points $X_k \in \text{St}(p, n)$ belonging to a neighborhood of the sought-for mean-matrix $X \in \text{St}(p, n)$ onto $T_X \text{St}(p, n)$ by applying the lifting map $\hat{P}_X^{-1}$. Denote such points as $V_k \stackrel{\text{def}}{=} \hat{P}_X^{-1}(X_k)$.
2. Compute the linear combination $\bar{V} = N^{-1} \sum_{k=1}^N V_k$.
3. Bring back the mean vector $\bar{V}$ to $\text{St}(p, n)$ by the retraction P_X and get an empirical mean matrix $X = P_X(\bar{V})$.

Summarizing the above procedure, a mean matrix $X \in \text{St}(p, n)$ is the solution of the non-linear, matrix-type equation:

$$X = P_X \left(\frac{1}{N} \sum_{k=1}^N \hat{P}_X^{-1}(X_k) \right) \quad (9)$$

in the variable X . The analogy between the quasi-arithmetic mean for real numbers (2) and the equation (9) is apparent, except that the equation (9) is an implicit function of the mean (as both sides of the equation depend on the unknown mean value X) instead of being an explicit function as in the case of Kolmogoroff-Nagumo mean.

The equation (9) is solved numerically by means of a fixed-point learning algorithm, that generates a sequence $X^{(i)} \in \text{St}(p, n)$ of estimates of the sought-for empirical mean matrix X , and that may be written as:

$$X^{(i+1)} = P_{X^{(i)}} \left(\frac{1}{N} \sum_{k=1}^N \hat{P}_{X^{(i)}}^{-1}(X_k) \right), \quad i \geq 0, \quad (10)$$

where matrix $X^{(0)} \in \text{St}(p, n)$ denotes an initial guess. In the previous contributions [16, 17], the algorithm (10) was based on associated retraction/lifting pairs, namely, either P_X/P_X^{-1} or $\hat{P}_X/\hat{P}_X^{-1}$, while, in the present paper, the mixed retraction/lifting pair $P_X/\hat{P}_X^{-1}$ is made use of with the aim to decrease the computational burden of the algorithm.

Although, by definition of retraction/lifting pair, it holds $P_X \circ P_X^{-1} = \hat{P}_X \circ \hat{P}_X^{-1} = \text{Id}_{\text{St}(p, n)}$, it is recognized that the composition $P_X \circ \hat{P}_X^{-1}$ does not equal the identity map in $\text{St}(p, n)$. In other terms, given matrices $X, Q \in \text{St}(p, n)$, the discrepancy

$$\Delta_X(Q) \stackrel{\text{def}}{=} \delta(P_X(\hat{P}_X^{-1}(Q)), Q)$$

differs from zero, in general, although numerical tests show that such discrepancy lays several logarithmic units below zero (see Section 3 for a statistical/quantitative analysis). Such a discrepancy may be evaluated as follows. First, note that:

$$\Delta_X(Q) = \|I_n - Q^T P_X(\hat{P}_X^{-1}(Q))\|_F, \quad (11)$$

define $M \stackrel{\text{def}}{=} Q^T X$ and set $V = (I_p - XX^T)Q + \frac{1}{2}X(X^T Q - Q^T X)$. It holds that:

$$V^T V = I_n + \frac{1}{4}(M^T M - M^{2T} - M^2 - 3MM^T), \quad (12)$$

$$Q^T(X + V) = I_n + M - \frac{1}{2}M(M + M^T), \quad (13)$$

hence, the discrepancy (11) takes on the expression:

$$\Delta = \left\| I_n - \left[I_n + M - \frac{1}{2}M(M + M^T) \right] \times \left[2I_n - \frac{1}{4}(M - M^T)^2 - MM^T \right]^{-\frac{1}{2}} \right\|_F. \quad (14)$$

Note that, when $Q = X$, it results $M = I_n$ and the above expression gives $\Delta = 0$.

2.2. Relationships with other contributions

The iteration rule (10) generalizes the averaging methods proposed independently in [13, 17]. The fixed-point solution X of the iteration (10) satisfies the equation:

$$\sum_{k=1}^N \hat{P}_X^{-1}(X_k) = 0, \quad (15)$$

namely, the fixed point X is a zero of the vector field

$$\mathcal{V}(X) \stackrel{\text{def}}{=} \sum_{k=1}^N \hat{P}_X^{-1}(X_k).$$

The Proposition 2.3 proved in [13] holds and ensures that, if the samples X_k are not too spread (see [13] for a precise definition), the zero of the vector field $\mathcal{V}(X)$ is unique, hence, the iteration rule (10) is locally well-defined and leads to a unique average.

The fixed-point-type iteration rule (10) also generalizes the averaging methods based on the minimization of a spread function based on the Riemannian distance. A complete study of the convergence properties of such methods, based on a gradient-descent-type optimization procedure, is available in [2]. An earlier study of an averaging method based on a Newton-type optimization procedure was proposed in [15].

The iteration rule (10) could be further generalized by introducing an unequal weighting scheme of the tangent-vectors $\hat{P}_{X^{(i)}}^{-1}(X_k)$ as suggested in the contribution [19] (see Algorithm 2). Such weighting scheme would lead to an iteration rule of the type:

$$X^{(i+1)} = P_{X^{(i)}} \left(\frac{1}{N} \sum_{k=1}^N w_k^{(i)} \hat{P}_{X^{(i)}}^{-1}(X_k) \right), \quad i \geq 0, \quad (16)$$

where weights $w_k^{(i)} > 0$ depend on the mutual distance between the samples X_k and the current value of the iteration $X^{(i)}$.

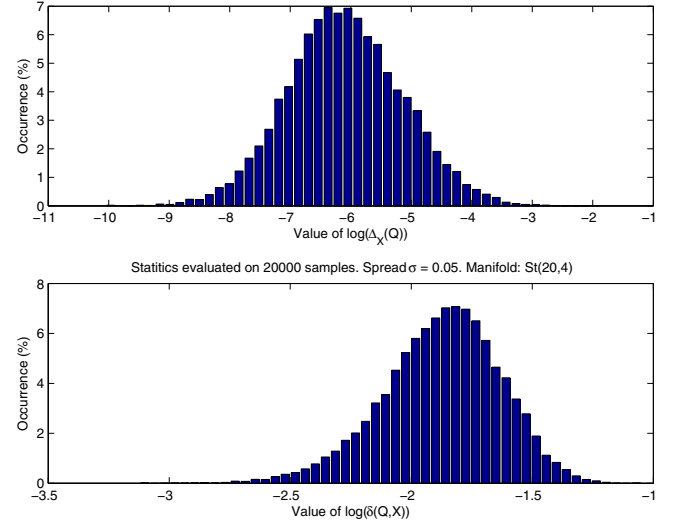


Fig. 1. Upper panel: Statistical distribution of the discrepancies $\Delta_X(Q)$ obtained by setting $X = C$ (center of the distribution) and $Q = X_k$ (random samples). Lower panel: Statistical distribution of the discrepancies $\delta(X, Q)$, again with $X = C$ and $Q = X_k$ (in logarithmic scales).

3. NUMERICAL EXPERIMENTS

In the present Section, the results of different experiments are illustrated to get an insight into the numerical behavior of the discussed retraction/lifting map pairs in the context of averaging over the compact Stiefel manifold. In the numerical experiments, the center $C \in \text{St}(p, n)$ of the distribution of the samples X_k is generated by computing the Q-factor of a thin-QR decomposition of a matrix randomly generated in $\mathbb{R}^{p \times n}$ with normally-distributed entries. The N samples to average are generated by the rule $X_k = \exp(\sigma \Omega_k)C$, with $\Omega_k \stackrel{\text{def}}{=} \text{sk}(A_k)$, where A_k is a matrix randomly generated in $\mathbb{R}^{p \times p}$ with normally-distributed entries, and $\sigma > 0$ controls the spread of the distribution [16, 17]. The initial guess $X^{(0)}$ in the fixed-point iteration algorithm (10) was chosen by slightly rotating the sample X_1 via a quasi-unit random rotation. The numerical tests were performed by running a MATLAB[®] 7 (64 bit) code on platform featuring an Intel[®] Xeon[®] (2.93 GHz) with 8 cores and 12GB RAM.

The first experiment aims at evaluating the numerical behavior of the compound map $P_X \circ \hat{P}_X^{-1}$. Figure 1 illustrates the statistical distribution of the discrepancy $\Delta_C(X_k)$ compared to the distribution of the discrepancies $\delta(C, X_k)$. $N = 20,000$ samples $X_k \in \text{St}(20, 4)$ were generated by a spread factor of $\sigma = 0.05$. The discrepancy values $\Delta_C(X_k)$ distribute approximately around 10^{-6} , confirming that the composition $P_X \circ \hat{P}_X^{-1}$, although not being an identity map, numerically behaves similarly to an identity map in the considered range. Figure 2 shows the scatter plot of the values of the discrepancies $\Delta_C(X_k)$ versus the values of the discrepancies $\delta(C, X_k)$. The relationship between them has a positive-correlation trend, showing that the more the arguments Q and X deviate from each other, the more the compound map $P_X \circ \hat{P}_X^{-1}$ deviates from the identity map.

The second experiment concerns the convergence properties of

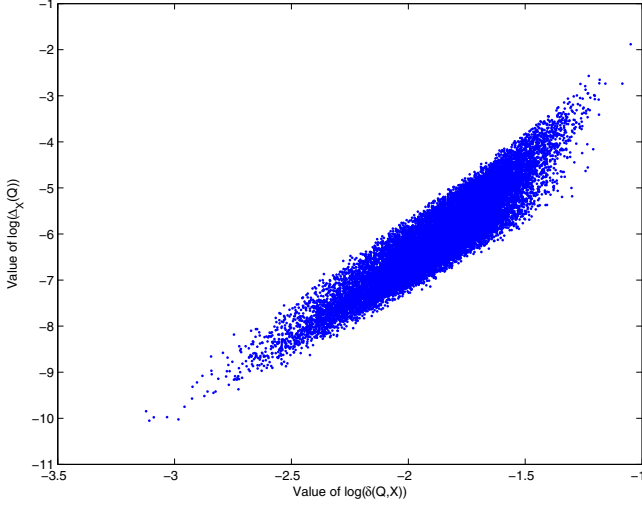


Fig. 2. Scatter plot of the values of the discrepancies $\Delta_X(Q)$ versus the values of the discrepancies $\delta(X, Q)$ obtained by setting $X = C$ and $Q = X_k$ (in logarithmic scales).

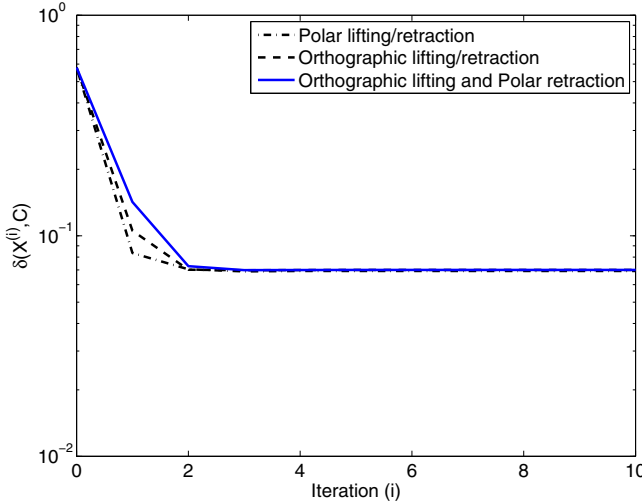


Fig. 3. Experiment about averaging on the manifold $\text{St}(20, 4)$. Index $\delta(X^{(i)}, C)$ during iteration.

the fixed-point iteration algorithm (10) based on the polar retraction and orthographic lifting (namely, the mixed retraction/lifting pair $P_X/\hat{P}_X^{-1}$), the orthographic retraction/lifting pair ($\hat{P}_X/\hat{P}_X^{-1}$) and the polar retraction/lifting pair (P_X/P_X^{-1}). For this experiment, a number $N = 30$ of samples were generated on the manifold $\text{St}(20, 4)$ with a spread parameter $\sigma = 0.2$. Figure 3 shows the values of the index $\delta(X^{(i)}, C)$. The three algorithms behave satisfactorily and converge to solution-matrices that locate at similar distances to the actual center of the distribution.

The third experiment aims at illustrating a comparison about the computational complexity of the algorithm (10) endowed again with the polar retraction and orthographic lifting, with the orthographic retraction/lifting pair, and with the polar retraction/lifting pair. A

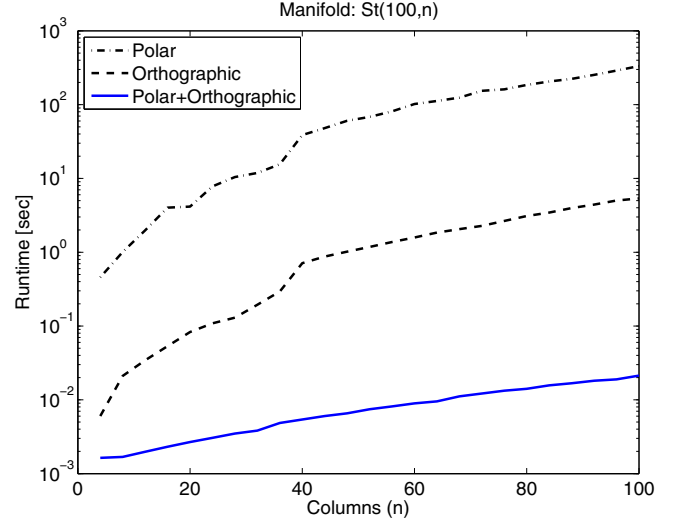


Fig. 4. Runtimes for the manifold $\text{St}(100, n)$ with the integer parameter n varying.

close inspection of the fixed-point algorithm (10) reveals that, for a general compact Stiefel manifold $\text{St}(p, n)$, the computational complexity is essentially a function of the number n . The Figure 4 shows the runtimes corresponding to the tested algorithms run on the manifold $\text{St}(100, n)$ with varying n . Such numerical simulation was performed with $N = 50$ samples generated with a spread-parameter value $\sigma = 0.01$. Each averaging experiment for each value of the index n was repeated 100 times to get rid of random fluctuations in the evaluation of runtimes. The obtained results indicate that the averaging algorithm based on a combination of the polar retraction map and the orthographic lifting map is much lighter than averaging methods based on associated retraction/lifting pairs in terms of computational burden.

4. CONCLUSION

The present research work proposed a new averaging method on the compact Stiefel manifold based on a combination of non-associated (mixed) retraction and lifting maps. The combined retraction/lifting pair was studied both analytically and numerically and the new averaging algorithm was tested numerically.

The obtained numerical results confirm that the composition $P_X \circ \hat{P}_X^{-1}$, although not being an identity map, numerically behaves like an identity map in the considered range and that the new algorithm behaves satisfactorily and converges to solution-matrices that deviate from the actual center of the distribution of a similar amount.

A comparison between three fixed-point algorithms based on the non-associated polar retraction and orthographic lifting, on the associated orthographic retraction/lifting pair and on the associated polar retraction/lifting pair reveals that the averaging algorithm based on a combination of the polar retraction map and the orthographic lifting map is remarkably superior to the averaging algorithms based on associated retraction/lifting pairs in terms of computational demand, resulting the lightest one.

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