Visualization of Manifold-Valued Elements by Multidimensional Scaling

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Abstract

The present contribution suggests the use of a multidimensional scaling (MDS) algorithm as a visualization tool for manifold-valued elements. A visualization tool of this kind is useful in signal processing and machine learning whenever learning/adaptation algorithms insist on high-dimensional parameter manifolds.

Keywords: Parameter manifold; Multidimensional scaling; Visualization tool.

1 Introduction

In machine learning, signal processing and intelligent data analysis, data to analyze and adaptive systems’ parameters are oftentimes organized as vectors or matrices whose entries satisfy non-linear constraints. Exemplary cases of interest and related applications are summarized below:

- Symmetric positive-definite matrices find a wide range of applications. For instance: Analysis of deformation [42, 44], image analysis [3], statistical analysis of diffusion tensor data in medicine [23], automatic and intelligent control [7], pattern recognition [40, 50], speech emotion classification [52] as well as design and analysis of wireless cognitive dynamic systems [28];
- Calculation of the center of mass of Lie-group-valued and manifold-valued data collections [20, 21, 24];
- Several applications deal with special orthogonal group connection patterns like, for instance: invariant visual perception [43], modeling of DNA chains [29, 36], automatic object pose estimation [30], distributed consensus optimization among agents [45], study of plate tectonics [41], blind source separation and independent component analysis [34], curve subdivision in nonlinear spaces [42, 53];
- There is a number of signal/data processing algorithms that learn parameter-vectors on the unit-hypersphere for applications such as blind channel deconvolution [17, 19, 40],
one-unit independent component analysis [30], robust constrained beamforming [16] and data classification by linear discrimination based on non-Gaussianity discovery [38];

- Stiefel-manifold-based algorithms have become increasingly popular in the scientific literature, with applications to optimal linear data compression, noise reduction and signal representation by principal/minor component analysis and principal/minor subspace decomposition [1, 15, 31, 37], smart sensor arrays [6, 39], direction of arrival estimation [1, 35], linear programming [5], electronic structures computation within local density approximation (e.g. for understanding the thermodynamics of bulk materials, the structure and dynamics of surfaces and the nature of point-defects in crystals) [13], factor analysis in psychometric [14];

- Non-compact manifolds play a role in signal/data processing and modeling. A prominent example is the real symplectic group, whose known applications range from quantum computing [4, 25] to control of beam systems in particle accelerators [11], from computational ophthalmology [26, 27] to vibration analysis [47] and control theory [10]. Recent studies have shown that non-compact manifolds are better framed as pseudo-Riemannian manifolds rather than Riemannian manifolds [22]. (The case of pseudo-Riemannian manifolds is not considered within the present manuscript, though.)

The above-mentioned cases may be framed as manifold-valued data analysis.

A problem of practical impact is the visualization of such high-dimensional data. Whenever the dimension of a manifold exceeds the number 3, direct visualization is impossible. In applications, the dimension of the manifolds that the data belong to is much higher than three.

A possible solution to the visualization problem is provided by multidimensional scaling (MDS). Multidimensional scaling is a numerical technique whose goal is to find out a low-dimensional representation of high-dimensional abstract objects suitable for graphical representation. The aim of multidimensional scaling is to reduce the dimensionality of data while retaining their proximity properties.

The aim of the present manuscript is to suggest the use of multidimensional scaling as a tool to visualize manifold-valued elements. Such a tool is intended as a support for testing and evaluating signal processing and machine learning algorithms insisting on manifolds.

As MDS computes a set of coordinate vectors (in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \), for visualization purpose) whose distribution reflects a pattern of proximity, a key point in visualization is the possibility to compute distances among objects on a manifold. For this reason, the present manuscript deals with Riemannian manifolds.

The Section 2 of the present manuscript briefly reviews metric notions of Riemannian manifolds and the basic theory of MDS (as well as details on its implementation). Section 3 shows numerical examples about high-dimensional manifold-valued data visualization.

## 2 Manifolds of interest and multidimensional scaling

The present section reviews some metric notions of smooth manifolds and recalls the way that multidimensional scaling works, its fundamental properties and implementation details.

### 2.1 Geodesic distance on Riemannian manifolds

Let the dataspace of interest be denoted as \( X \). It is supposed to be a Riemannian manifold. Its tangent space at point \( x \in X \) is denoted as \( T_xX \). On a Euclidean space \( \mathbb{E} \), the distance
Table 1: Summary of the features of a few manifolds of interest in applications. Symbol $e$ denotes identity matrix of appropriate size, operator $\text{tr}(\cdot)$ denotes matrix trace, symbol $^T$ denotes ordinary transpose while symbol $^H$ denotes Hermitian transpose.

| Symbol | Description                                      | Dimension | Inner product | Distance function |
|--------|--------------------------------------------------|-----------|---------------|-------------------|
| $SO(q)$ | Special orthogonal group: Manifold of continuous rotations | $\frac{1}{2}q(q-1)$ | $\langle v, w \rangle_x := \text{tr}(v^T w)$ | $d(x, y) = \sqrt{-\text{tr}(\log^2(x^T y))}$ |
| $S^+(q)$ | Manifold of symmetric positive-definite matrices | $\frac{1}{2}q(q+1)$ | $\langle v, w \rangle_x := \text{tr}(v^{-1}w^{-1} w^{-1} v^{-1})$ | $d(x, y) = \sqrt{\text{tr}(\log^2(x^{-1} y^{-1}))}$ |
| $SU(q)$ | Special unitary group                             | $q^2 - 1$ | $\langle v, w \rangle_x := \text{tr}(v^H w)$ | $d(x, y) = \sqrt{-\text{tr}(\log^2(x^H y))}$ |

between two points $x, y \in \mathbb{E}$ may be measured as $d(E)(x, y) \overset{\text{def}}{=} \|x - y\|$, where symbol $\| \cdot \|$ denotes the 2-norm. Such a distance is indeed the length of a straight line connecting endpoints $x$ and $y$. Such a notion of distance may be extended to a generic Riemannian manifold via the notion of geodesic arcs (which generalize straight lines) and arc length on manifolds.

A Riemannian manifold is equipped by a symmetric, positive-definite inner product. Given any pair of tangent vectors $v, w \in T_x X$, their inner product is denoted by:

$$\langle v, w \rangle_x \in \mathbb{R}. \quad (1)$$

Let $c_{x,v} : [0 1] \to X$ denote a smooth curve on the manifold $X$ such that $c_{x,v}(0) = x \in X$ and $\dot{c}_{x,v}(0) = v \in T_x X$. The length of the curve $c_{x,v}$ is given by:

$$\ell(c_{x,v}) \overset{\text{def}}{=} \int_0^1 \langle \dot{c}_{x,v}(t), \dot{c}_{x,v}(t) \rangle_{c_{x,v}(t)} dt. \quad (2)$$

Given arbitrary $x \in X$ and $v \in T_x X$, the curve $g_{x,v} : [0 1] \to X$ of shortest length is termed geodesic. Normal parametrization is assumed here, namely the quantity $\langle \dot{g}_{x,v}(t), \dot{g}_{x,v}(t) \rangle_{g_{x,v}(t)}$ keeps constant for every $t \in [0 1]$. Such minimal length, namely $\ell(g_{x,v})$, is termed geodesic distance between endpoints, namely between points $g_{x,v}(0) = x$ and $g_{x,v}(1)$. The Riemannian distance between endpoints is denoted by:

$$d(g_{x,v}(0), g_{x,v}(1)) \overset{\text{def}}{=} \ell(g_{x,v}). \quad (3)$$

Because of normal parametrization, it holds:

$$\ell(g_{x,v}) = \langle \dot{g}_{x,v}(0), \dot{g}_{x,v}(0) \rangle_{g_{x,v}(0)}^{\frac{1}{2}} = \langle v, v \rangle_x^{\frac{1}{2}}. \quad (4)$$

The above setting may be extended to include pseudo-Riemannian manifolds. Also, more general metric spaces may be taken into account, although this exceeds the scope of the present paper.

The table summarizes the features of a few manifolds of interest in applications. Except for the unit hyper-sphere, the dimension of the manifolds of interest grows quickly.

For a general reference on differential geometry, see [48].
2.2 Multidimensional Scaling (MDS)

One of the purposes of multidimensional scaling [8, 32, 33] is to provide a visual representation of the pattern of proximities among a set of high-dimensional objects. In this instance, MDS finds a set of vectors in the two-dimensional or three-dimensional Euclidean space such that the matrix of Euclidean distances among them corresponds – as closely as possible – to some function of the objects’ proximity matrix according to a criterion function termed stress.

Formally, let \( X \) be a high-dimensional Riemannian manifold with distance function \( d(\cdot, \cdot) \) and let \( \{x_k\}_k \) be a given collection of \( n \) elements of \( X \). The aim of MDS is to determine a collection of \( n \) Euclidean coordinate-vectors \( \{z_k\}_k (z_k \in \mathbb{R}^p, \text{ with } p = 2 \text{ or } p = 3) \) that replicates the pattern of proximities among the elements \( x_k \). This may be achieved by minimizing the Kruskal stress function that may be written – for a generic Riemannian manifold – as:

\[
\Phi(\{z_k\}_k) \overset{\text{def}}{=} \frac{1}{\sum_i \sum_{j<i} d(x_i, x_j)} \sum_i \sum_{j<i} \frac{(||z_i - z_j|| - d(x_i, x_j))^2}{d(x_i, x_j)},
\]

(5)

where symbol \( ||\cdot|| \) denotes Euclidean norm.

Alternatively, the Sammon stress function [51] may be used to measure the discrepancy between the proximity pattern of the original data and the proximity pattern of their low-dimensional versions. The Sammon stress function may be written – for a generic Riemannian manifold – as:

\[
\Phi(\{z_k\}_k) \overset{\text{def}}{=} \sum_i \sum_{j<i} w_{i,j} \frac{(||z_i - z_j|| - d(x_i, x_j))^2}{d(x_i, x_j)}.
\]

(6)

The Sammon stress function differs from the Kruskal stress function in that the former emphasizes the relevance of distances that were originally small.

Indeed, the Kruskal and the Sammon stress functions may be unified by the weighted stress function:

\[
\Phi(\{z_k\}_k) \overset{\text{def}}{=} M \sum_i \sum_{j<i} w_{i,j} (||z_i - z_j|| - d(x_i, x_j))^2,
\]

(7)

where the quantities \( w_{i,j} = w_{j,i} > 0 \) denote weights and \( M > 0 \) denotes a normalization constant. In summary:

- **Kruskal stress function**: \( M = 1, w_{i,j} = 1 \).
- **Sammon stress function**: \( M = \left( \sum_i \sum_{j<i} d(x_i, x_j) \right)^{-1}, w_{i,j} = d^{-1}(x_i, x_j) \).
- **Dwyer-Koren-Marriott stress function**: In [12], the weighting scheme \( w_{i,j} = d^{-2}(x_i, x_j) \) and \( M = 1 \) are proposed.

The correspondence \( x_k \leftrightarrow z_k \) induced by multidimensional scaling is not unique. In fact, if \( \{z_k\}_k \) is a minimizer set of the stress function, for a given dimensionality reduction problem, \( c \in \mathbb{R}^p \) is a constant displacement vector and \( R \in SO(p) \) is a \( p \)-dimensional rotation, also \( \{Rz_k + c\}_k \) is a minimizer set.

Multidimensional scaling may be used as a proximity/similarity visualization tool for high-dimensional data as it computes two-dimensional or three-dimensional vectors \( z_k \in \mathbb{R}^p \), corresponding to the original elements \( x_k \in X \), that captures the fundamental information about mutual distances.

The axes corresponding to the coordinates of the vectors \( z_k \) referred to as ‘fictitious coordinates’, do not possess any physical meaning, in general. All that matters in an MDS
map are the proximity properties. On a MDS-based visualization corresponding to a non-zero stress, the distances among objects are imperfect representations of the relationships among original data: The greater the stress, the greater the distortion.

A key observation in the implementation of multidimensional scaling is that, rather than optimizing the actual stress function \((7)\), it is more computationally convenient to optimize a quadratic majorization of it [9]. The following details on optimization of a majorizing function are drawn from [12]. Define the matrix \(A \in \mathbb{R}^{n \times n}\) as follows:

\[
A_{i,j} = \begin{cases} 
-w_{i,j} & \text{for } i \neq j, \\
\sum_{s \neq i} w_{i,s} & \text{for } i = j.
\end{cases}
\]  

(8)

Moreover, given a collection of \(n\) vectors \(\{u_k\}_k\) \((u_k \in \mathbb{R}^p)\), define the matrix \(C(\{u_k\}_k)\) as:

\[
C_{i,j}(\{u_k\}_k) = \begin{cases} 
-w_{i,j}d(x_i, x_j) & \text{for } i \neq j, \\
\sum_{s \neq i} C_{i,s}(\{u_k\}_k) & \text{for } i = j.
\end{cases}
\]  

(9)

To ease the notation, define matrix \(Z \in \mathbb{R}^{n \times p}\), whose rows coincide with the \(n\) coordinate-vectors \(z_T^k\) and matrix \(U \in \mathbb{R}^{n \times p}\), whose rows coincide with the \(n\) coordinate-vectors \(u_T^k\).

The stress function \((7)\) is bounded from above by the quadratic form \(\Psi(Z; U)\) defined as:

\[
\Psi(Z; U) \overset{\text{def}}{=} \sum_i \sum_{j<i} w_{i,j}d^2(x_i, x_j) + \sum_a (Z_a^T A Z_a - 2Z_a^T C(U) U_a),
\]  

(10)

where \(Z_a\) denotes the \(a^{th}\) column of the matrix \(Z\) and \(U_a\) denotes the \(a^{th}\) column of the matrix \(U\) \((a = 1, \ldots, p)\). It holds \(\Phi(Z) \leq \Psi(Z; U)\) with equality holding when \(Z = U\). In order to iteratively solve the optimization problem of minimizing the criterion \((7)\), one may use the following scheme:

0. Set initial guess \(U\),
1. \(U \leftarrow \arg \min_{V \in \mathbb{R}^{n \times p}} \Psi(V; U)\),
2. Repeat from 1 until done,
3. \(Z \leftarrow U\).

It is immediate to verify that the optimization problem of minimizing the criterion \((10)\) is equivalent to \(p\) independent optimization problems, one for each axis. Consequently, the optimization problem \((10)\) may be reduced to the solution of \(p\) quadratic problems of the kind:

\[
Z_a^T A Z_a - 2Z_a^T C(U) U_a.
\]  

(11)

As the matrix \(A\) is positive semi-definite, each of the above problem has only global minima. Moreover, note that the matrix \(A\) is constant across the \(p\) optimization problems. In order to iteratively solve the quadratic optimization problem:

\[
\min_{z \in \mathbb{R}^n} (z^T A z + z^T b), \quad A \geq 0, \quad b \in \mathbb{R}^n,
\]  

(12)
one may use the following gradient steepest descent algorithm with line search \cite{12}:

0. Set initial guess \( x \),
1. \( g \leftarrow 2Ax + b \),
2. \( s \leftarrow \frac{1}{2} g^T g \),
3. \( x \leftarrow x - sg \),
4. Repeat from 1 until done.

As the matrix \( A \) is semi-definite, it is rank-deficient. As a consequence, the optimization problem \cite{12} may not be solved in closed form and does not admit a unique solution.

2.3 Spherical MDS

As mentioned, multidimensional scaling is a method for embedding a general distance matrix into a low dimensional Euclidean space, used both as a pre-processing step as well as a visualization tool.

There are also applications where the target space, rather than being a Euclidean space, is a smooth manifold. In particular, Spherical MDS is the problem of embedding a matrix of distances onto a (low-dimensional) sphere. Spherical MDS has applications in texture mapping, image analysis as well as dimensionality reduction for finite dimensional distributions. A spherical dimensionality reduction method may have considerable impact in domains that represent data as histograms or distributions, such as in document processing and speech recognition \cite{2}.

An algorithmic framework for spherical multidimensional scaling has recently been described in \cite{2}.

3 Numerical Illustrative Examples

The present section aims at illustrating the behavior of the MDS-based manifold-valued elements visualization tool. In all the following examples, the stress function proposed in \cite{12} is made use of.

The first example aims at making the reader acquainted with the purpose of multidimensional scaling. It concerns the famous experiment with city-distances: The distance pattern among 9 cities inputs the MDS algorithm which computes the coordinates of 9 bi-dimensional points as shown in the Figure 1. The figure shows that the MDS optimization algorithm tends to minimize the stress which indeed is a measure of discrepancy between the pattern of proximity among cities (\( 9 \times 9 = 81 \) distances shown on the upper-right panel) and the pattern of proximity of the coordinate vectors (81 distances shown on the lower-right panel). As an example, Los Angeles and San Francisco are close to each other and far from New York and the computed set of coordinate-vectors reflect this fact.

The following two (toy) examples of MDS maps concern a distribution of random points in \( \mathbb{R}^2 \) visualized on \( \mathbb{R}^2 \). As the minimum distance problem \cite{7} does not possess an unique solution, it is not reasonable to expect that a MDS map \( \mathbb{R}^2 \rightarrow \mathbb{R}^2 \) is necessarily an identity.

Figure 2 shows a result obtained with initial guess just slightly randomly shifted with respect to the actual points. In this case, the computed coordinate-points and the actual points coincide. The same hold true for the \( 10 \times 10 \) matrices of actual and computed distances.

\footnote{Calculations show that the optimal stepsize \( s \) given in \cite{12} is incorrect of a factor 2.}
Figure 1: Example on city-distances. Upper-left panel: Locations of the computed coordinate-points (labeled for clarity). Lower-left panel: Stress function during iteration normalized to initial stress function (ratio expressed in decibels). Upper-right and lower-right panels: Pattern of distances among actual points and computed coordinate-points, respectively.

The same experiment was repeated with a random initial guess: Figure 3 shows that, although the set of coordinate-points replicate the distance pattern of the actual points, their locations are seemingly unrelated with those of the actual points. However, points that are actually close to each other (for example, points marked as 3 and 9) keep close to each other in the computed representation.

A further example concerns the bi-dimensional visualization of a distribution of points on a three-dimensional unit sphere. Figure 4 shows the actual points on a three-dimensional spherical surface, labeled for clarity. Figure 5 shows an obtained result. The points that are close to each other on the sphere (for example, points 4 and 13) are close to each other on the bi-dimensional plane too.

The MDS-based visualization tool may be profitably used to inspect the trajectory of the manifold-valued state of a signal processing algorithm. Figure 6 refers to the trajectory of a non-negative independent component analysis (NNICA) algorithm which learns on SO(9). Every time-step of the algorithm generates a $9 \times 9$ orthogonal matrix with +1-determinant that may be parameterized with no less than $9 \times 8/2 = 36$ angles, whose visualization ‘as is’ is impossible. The present visualization by multidimensional scaling is based on a map $SO(9) \rightarrow \mathbb{R}^3$. The NNICA algorithm run through 200 time-steps, downsampled to 20 for visual tidiness (initial point labeled as ‘1’, final point labeled as ‘20’).
succession of points clearly evidences a convergent adaptation trajectory.

4 Conclusion

The aim of the present contribution was to suggest the use of multidimensional scaling, a well-known dimensionality reduction technique, as a visualization tool for manifold-valued data.

Visualization tools are useful in signal processing and machine learning as they help inspecting the distribution of high-dimensional vectors and matrices. The MDS-based visualization tool suggested in the present paper captures the pattern of proximity among high-dimensional manifold-valued elements and computes a set of 2-dimensional or 3-dimensional vectors that retain the same pattern of proximity.
Figure 3: Toy experiment on finding a $\mathbb{R}^2 \rightarrow \mathbb{R}^2$ MDS map starting from a random initial guess. Upper-left panel: Locations of the actual points (diamond) and the computed coordinate-points (open circles). Note that the points are numbered for clarity. Lower-left panel: Stress function during iteration normalized to initial stress function (ratio expressed in decibels). Upper-right and lower-right panels: Pattern of distances among actual points and computed coordinate-points, respectively.

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