Riemannian optimization on the simplex of positive definite matrices

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Abstract

We discuss optimization-related ingredients for the Riemannian manifold defined by the constraint $X_1 + X_2 + \ldots + X_K = I$, where the matrix $X_i > 0$ is symmetric positive definite of size $n \times n$ for all $i = \{1, \ldots, K\}$. For the case $n = 1$, the constraint boils down to the popular standard simplex constraint.

1 Introduction

Column (or row) stochastic matrices are those where each column (or row) has non-negative entries that sum to 1. Such matrices are shown to be useful in many machine learning applications [LL04, ZCL05, IM07, RBCG08, SGH+15]. The constraint of interest for those matrices is $x_1 + x_2 + \ldots + x_K = 1$, where $x_i \geq 0$ for all $i = \{1, \ldots, K\}$, (1)

which is also called the standard simplex constraint. Sun et al. [SGH+15] proposed a Riemannian geometry for set obtained from the constraint (1) with strictly positive entries. The strict positivity ensures that the set obtained from the constraint (1) has a differentiable manifold structure. They develop optimization-related ingredients to enable first- and second-order optimization.

In this work, we propose to generalize the constraint (1) to constraints with matrices, i.e., the matrix simplex constraint $X_1 + X_2 + \ldots + X_K = I$, (2)

where $X_i \succeq 0$ is a symmetric positive semidefinite of size $n \times n$ for all $i = \{1, 2, \ldots, K\}$. Although the constraint (2) is a natural generalization of (1), its study is rather limited [REK05, LSC+08]. To that end, we discuss a novel Riemannian geometry for the set obtained from the constraint (2) with strict positive definiteness of the matrices. The main aim of the work is to focus on developing optimization-related ingredients that allow to propose optimization algorithms on this constraint set. The expressions of the ingredients extend to the case of Hermitian positive definite matrices. We provide manifold description files for easy integration with the manifold optimization toolbox Manopt [BMAS14].

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1Strict positive definiteness of matrices is needed to obtain a differentiable manifold structure. The proposed Riemannian structure allows to handle potentially semidefinite, i.e., rank deficient, matrices gracefully by scaling those elements to the boundary of the manifold.
2 The matrix simplex manifold

We define the matrix simplex manifold of interest as

$$\mathcal{M}_n^K := \{(X_1, X_2, \ldots, X_K) : X_1 + X_2 + \ldots + X_K = I, X_i \in \mathbb{R}^{n \times n}, \text{ and } X_i > 0 \text{ for all } i \in \{1, 2, \ldots, K\}\}. \tag{3}$$

It should be noted that the positive semidefiniteness constraint $X_i \succeq 0$ is replaced with the positive definiteness constraint $X_i > 0$ to ensure that the set $\mathcal{M}_n^K$ is differentiable. Below, we impose a Riemannian structure to the matrix simplex manifold \((3)\) and discuss ingredients that allow to develop optimization algorithms systematically [AMS08].

2.1 Riemannian metric and tangent space projector

An element $x$ of $\mathcal{M}_n^K$ is numerically represented as the structure $(X_1, X_2, \ldots, X_K)$ which is a collection of $K$ symmetric positive definite matrices of size $n \times n$.

The tangent space of $\mathcal{M}_n^K$ at an element $x$ is the linearization of the manifold, i.e., the constraint (2). Accordingly, the tangent space characterization of $\mathcal{M}_n^K$ at $x$ is

$$T_x \mathcal{M}_n^K = \{(\xi_1, \xi_2, \ldots, \xi_K) : \xi_1, \xi_2, \ldots, \xi_K \in \mathbb{R}^{n \times n}, \text{ and } \xi_i^T = \xi_i \text{ for all } i \in \{1, 2, \ldots, K\}\}. \tag{4}$$

It can be shown that $\mathcal{M}_n^K$ is an embedding submanifold of the $S_n^K := \text{SPD}_n \times \text{SPD}_n \times \cdots \times K \text{SPD}_n$, which is the Cartesian product of $K$ manifolds of symmetric positive definite matrices of size $n \times n$ [AMS08, Chapter 3.3]. Here $\text{SPD}_n$ denotes the manifold of $n \times n$ symmetric positive definite matrices that has a well-known Riemannian geometry [Bha09]. The dimension of the manifold $\mathcal{M}_n^K$ is $(K - 1)n(n + 1)/2$. We endow the manifold with a smooth metric $g_x : T_x \mathcal{M}_n^K \times T_x \mathcal{M}_n^K \to \mathbb{R}$ (inner product) at every $x \in \mathcal{M}_n^K$ [AMS08]. A natural choice of the metric is based on the well-known bi-invariant metric of $\text{SPD}_n$ [Bha09], i.e.,

$$g_x(\xi, \eta) := \sum_i \text{trace}(X_i^{-1} \xi \eta_i). \tag{5}$$

Once the manifold $\mathcal{M}_n^K$ is endowed with the metric (5), the manifold $\mathcal{M}_n^K$ turns into a Riemannian submanifold of $S_n^K$. Following [AMS08] Chapters 3 and 4), the Riemannian submanifold structure allows the computation of the Riemannian gradient and Hessian of a function (on the manifold) in a straightforward manner from the partial derivatives of the function.

A critical ingredient in those computations is the computation of the linear projection operator of a vector in the ambient space $\mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n} \times \cdots \times K \mathbb{R}^{n \times n}$ onto the tangent space (4) at an element of $\mathcal{M}_n^K$. In particular, given $z = (Z_1, Z_2, \ldots, Z_K) \in \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n} \times \cdots \times K \mathbb{R}^{n \times n}$ in the ambient space, we compute the projection operator $\Pi_x : \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times n} \times \cdots \times K \mathbb{R}^{n \times n} \to T_x \mathcal{M}_n^K$, orthogonal with respect to the metric (5), as [MS16]

$$\Pi_x(z) = \arg \min_{\xi \in T_x \mathcal{M}_n^K} -g_x(z, \xi) + \frac{1}{2} g_x(\xi, \xi),$$

2
which has the expression

$$\Pi_x(z) = (Z_1 + X_1 \Lambda X_1, Z_2 + X_2 \Lambda X_2, \ldots, Z_K + X_K \Lambda X_K), \quad (6)$$

where $\Lambda$ is the symmetric matrix that is the solution to the linear system

$$\sum_i X_i \Lambda X_i = -\sum_i Z_i. \quad (7)$$

It is easy to verify that

- $\Pi_x(z)$ belongs to the tangent space $T_x \mathcal{M}_n^K$ and
- $z - \Pi_x(z)$ and $\Pi_x(z)$ are complementary to each other with respect to the chosen metric (6) for all choices of $z$.

### 2.2 Retraction operator

Given a vector in the tangent space, the retraction operator maps it to an element of the manifold \[AMS08\] Chapter 4]. Overall, the notion of retraction operation allows to move on the manifold, which is required by any optimization algorithm.

A natural choice of the retraction operator on the manifold $\mathcal{M}_n^K$ is inspired from the well-known exponential mapping operation on $\text{SPD}_n$, the manifold of positive definite matrices \[Bha09\]. However, this only ensures positive definiteness of the output matrices. To maintain the summation equal to $\mathbf{I}$ constraint, we additionally normalize in a particular fashion. Overall, given a tangent vector $\xi_x \in T_x \mathcal{M}_n^K$, the expression for the retraction operator $R_x : T_x \mathcal{M}_n^K \to \mathcal{M}_n^K$ is

$$R_x(\xi_x) := (Y_{\text{sum}}^{-1/2}Y_1 Y_{\text{sum}}^{-1/2}, Y_{\text{sum}}^{-1/2}Y_2 Y_{\text{sum}}^{-1/2}, \ldots, Y_{\text{sum}}^{-1/2}Y_K Y_{\text{sum}}^{-1/2}), \quad (8)$$

where $\xi_x = (\xi_{x_1}, \xi_{x_2}, \ldots, \xi_{x_K})$, $Y_i = X_i(\expm(X_i^{-1} \xi_{x_i}))$, $Y_{\text{sum}} = \sum_i Y_i$, and $\expm(\cdot)$ is the matrix exponential operator.

To show that the operator (8) is a retraction operator, we need to verify certain conditions \[AMS08\] Chapter 4], which are

1. the centering condition: $R_x(0_x) = x$ and
2. the local rigidity condition: $DR_x(0_x) = \text{id}_{T_x \mathcal{M}_n^K}$, where $\text{id}_{T_x \mathcal{M}_n^K}$ denotes the identity mapping on $T_x \mathcal{M}_n^K$.

The centering condition for (8) is straightforward to verify by setting $\xi_x = 0$. To verify the local rigidity condition, we analyze the differential of the retraction operator locally, which is the composition of two steps: the first one is through the matrix exponential and the second is through the normalization by pre and post multiplying with $Y_{\text{sum}}^{-1/2}$. The matrix exponential is locally rigid due to the fact that it defines the well-known exponential mapping on the $\text{SPD}_n$ manifold \[AMS08, Bha09\]. The normalization step (with pre and post multiplying by $Y_{\text{sum}}^{-1/2}$) does not change local rigidity. Hence, the overall composition (8) satisfies both the centering and local rigidity conditions needed to be a retraction operation.
2.3 Riemannian gradient and Hessian computations

As mentioned earlier, a benefit of the Riemannian submanifold structure is that it allows to compute the Riemannian gradient and Hessian of a function in a systematic manner. To that end, we consider a smooth function \( f : M^K_n \rightarrow \mathbb{R} \) on the manifold. We also assume that it is well-defined on \( S^K_n \).

If \( \nabla_x f \) is the Euclidean gradient of \( f \) at \( x \in M^K_n \), then the Riemannian gradient \( \text{grad}_x f \) has the expression

\[
\text{grad}_x f = \Pi_x (\text{gradient on } S^K_n) = \Pi_x (X_1\text{symm}(\nabla X_1 f)X_1, X_2\text{symm}(\nabla X_2 f)X_2, \ldots, X_K\text{symm}(\nabla X_K f)X_K),
\]

where \( \nabla X_i f \) is the partial derivative of \( f \) at \( x \) with respect to \( X_i \) and \( \Pi_x \) is the tangent space projection operator defined in (6). Here, \( \text{symm}(\cdot) \) extracts the symmetric part of a matrix, i.e., \( \text{symm}(\Delta) = (\Delta + \Delta^\top)/2 \).

The computation of the Riemannian Hessian on the manifold \( M^K_n \) involves the notion of Riemannian connection [AMS08, Section 5.5]. The Riemannian connection, denoted as \( \nabla_{\xi_x} \eta_x \), at \( x \in M^K_n \) generalizes the covariant-derivative of the tangent vector \( \eta_x \in T_x M^K_n \) along the direction of the tangent vector \( \xi_x \in T_x M^K_n \) on the manifold \( M^K_n \). Since \( M^K_n \) is a Riemannian submanifold of the manifold \( S^K_n \), the computation of the Riemannian connection enjoys a simple expression in terms of the computations on the symmetric positive definite manifold \( \text{SPD}_n \) [Bha09]. In particular, the Riemannian connection expression for \( M^K_n \) is

\[
\nabla_{\xi_x} \eta_x = \Pi_x (\text{connection on } S^K_n) = \Pi_x (D\eta_x[\xi_x] - (\text{symm}(\xi X_1 X_1^{-1} \eta X_1), \ldots, \text{symm}(\xi X_K X_K^{-1} \eta X_K))), \tag{9}
\]

where \( D\eta_x[\xi_x] \) denotes the directional derivative of \( \eta_x \) along \( \xi_x \). Based on the expression (9), the Riemannian Hessian operation \( \text{Hess}_x f[\xi_x] \) along a tangent vector \( \xi_x \in T_x M^K_n \) has the expression

\[
\text{Hess}_x f[\xi_x] = \nabla_{\xi_x} \text{grad}_x f,
\]

which is easy to compute.

2.4 Computational cost

The expressions shown earlier involve matrix operations that cost \( O(n^3 K) \). The solution to the system (7) can be obtained iteratively using standard linear equation solvers. The overall cost for the computations is linear in \( K \).

2.5 The Hermitian case

The developments in Section 2 easily extend to Hermitian positive definite matrices satisfying the constraint (2). The matrix transpose operation is replaced with the conjugate transpose operation [SH15]. All other expressions are similarly developed.
3 Conclusion

We discussed the matrix simplex manifold, as a generalization of the standard simplex constraint to symmetric positive definite matrices, from a Riemannian optimization point of view. As a future research direction, it would be interesting to identify machine learning applications where the matrix simplex constraint arises naturally.

References

[AMS08] P.-A. Absil, R. Mahony, and R. Sepulchre, *Optimization algorithms on matrix manifolds*, Princeton University Press, 2008.

[Bha09] R. Bhatia, *Positive definite matrices*, Princeton university press, 2009.

[BMAS14] N. Boumal, B. Mishra, P.-A. Absil, and R. Sepulchre, *Manopt, a Matlab toolbox for optimization on manifolds*, Journal of Machine Learning Research 15 (2014), no. Apr, 1455–1459.

[IM07] Ryo Inokuchi and Sadaaki Miyamoto, *C-means clustering on the multinomial manifold*, International Conference on Modeling Decisions for Artificial Intelligence (MDAI), 2007.

[LL04] G. Lebanon and J. Lafferty, *Hyperplane margin classifiers on the multinomial manifold*, International conference on Machine learning (ICML), 2004.

[LSC+08] K. L. Lee, J. Shang, W. K. Chua, S. Y. Looi, and B.-G. Engelert, *Somim: An open-source program code for the numerical search for optimal measurements by an iterative method*, Tech. report, arXiv preprint arXiv:0805.2847, 2008.

[MS16] B. Mishra and R. Sepulchre, *Riemannian preconditioning*, SIAM Journal on Optimization 26 (2016), no. 1, 635–660.

[RBCG08] A. Rakotomamonjy, F. R. Bach, S. Canu, and Y. Grandvalet, *Simplemkl*, Journal of Machine Learning Research 9 (2008), no. Nov, 2491–2521.

[ŘEK05] J. Řeháček, B.-G. Englert, and D. Kaszlikowski, *Iterative procedure for computing accessible information in quantum communication*, Physical Review A 71 (2005), no. 5, 054303.

[SGH+15] Y. Sun, J. Gao, X. Hong, B. Mishra, and B. Yin, *Heterogeneous tensor decomposition for clustering via manifold optimization*, IEEE transactions on pattern analysis and machine intelligence 38 (2015), no. 3, 476–489.

[SH15] S. Sra and R. Hosseini, *Conic geometric optimization on the manifold of positive definite matrices*, SIAM Journal on Optimization 25 (2015), no. 1, 713–739.

[ZCL05] D. Zhang, X. Chen, and W. S. Lee, *Text classification with kernels on the multinomial manifold*, International ACM SIGIR conference on Research and development in information retrieval (SIGIR), 2005.