Information Geometry of Operator Scaling

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Abstract

Matrix scaling is a classical problem with a wide range of applications. It is known that the Sinkhorn algorithm for matrix scaling is interpreted as alternating e-projections from the viewpoint of classical information geometry. Recently, a generalization of matrix scaling to completely positive maps called operator scaling has been found to appear in various fields of mathematics and computer science, and the Sinkhorn algorithm has been extended to operator scaling. In this study, the operator Sinkhorn algorithm is studied from the viewpoint of quantum information geometry through the Choi representation of completely positive maps. The operator Sinkhorn algorithm is shown to coincide with alternating e-projections with respect to the symmetric logarithmic derivative metric, which is a Riemannian metric on the space of quantum states relevant to quantum estimation theory.

1 Introduction

Given a nonnegative matrix \( A \in \mathbb{R}_{+}^{m \times n} \), the matrix scaling problem is to find nonnegative diagonal matrices \( L \in \mathbb{R}_{+}^{m \times m} \) and \( R \in \mathbb{R}_{+}^{n \times n} \) such that

\[
(LAR)1_n = \frac{1}{m}1_m \quad \text{and} \quad (LAR)^\top 1_m = \frac{1}{n}1_n,
\]

where \( 1_n = (1, \ldots, 1)^\top \) is the \( n \)-dimensional all-one vector. This problem arises in various applications such as Markov chain estimation [30], data ranking [22], data assimilation [29], and optimal transport [28]. See [19] for many other applications. Sinkhorn [30] proposed an alternating algorithm for matrix scaling. Starting from \( A^{(0)} = A \), the Sinkhorn algorithm\(^1\) iterates row normalization

\[
A^{(2k+1)} = \frac{1}{m} \text{Diag}(A^{(2k)}1_n)^{-1} A^{(2k)},
\]

and column normalization

\[
A^{(2k+2)} = \frac{1}{n} A^{(2k+1)} \text{Diag}((A^{(2k+1)^\top}1_m)^{-1}.
\]

\(^1\)The Sinkhorn algorithm is also known as RAS method or iterative proportional fitting procedure (IPFP) [19].
Note that $A^{(2k+1)}1_n = m^{-1}1_m$ and $(A^{(2k+2)})^\top 1 = n^{-1}1_n$. There have been many approaches to prove the convergence of the Sinkhorn algorithm [19], such as potential optimization, convex duality, nonlinear Perron–Frobenius theory, and entropy optimization.

Csiszár [6] analyzed the Sinkhorn algorithm by focusing on the geometry of probability distributions. Specifically, let

$$
\Pi_1 = \left\{ A \in \mathbb{R}^{m \times n}_{++} \mid A1_n = m^{-1}1_m \right\},
\Pi_2 = \left\{ A \in \mathbb{R}^{m \times n}_{++} \mid A^\top 1_m = n^{-1}1_n \right\}
$$

be the spaces of row-normalized and column-normalized positive matrices, respectively. Then, Csiszár [6] proved that each iteration of the Sinkhorn algorithm coincides with the projection with respect to the Kullback–Leibler divergence $D_{KL}$:

$$
D_{KL}(A^{(2k+1)} \parallel A^{(2k)}) = \min_{B \in \Pi_1} D_{KL}(B \parallel A^{(2k)}),
D_{KL}(A^{(2k+2)} \parallel A^{(2k+1)}) = \min_{B \in \Pi_2} D_{KL}(B \parallel A^{(2k+1)}).
$$

This is one of the early results of information geometry [3, 2], an interdisciplinary field that provides geometric insights into statistics, information theory, and optimization. In information geometry, the space of probability distributions is viewed as a Riemannian manifold with the Riemannian metric given by the Fisher information matrix. Then, a pair of dual affine connections called e-connection and m-connection is introduced to this manifold. In this context, the Sinkhorn algorithm is interpreted as alternating e-projections onto $\Pi_1$ and $\Pi_2$.

Further details will be presented in Section 2.

Recently, a quantum (non-commutative) generalization of matrix scaling called operator scaling has been attracting much interests [14, 11, 12, 13]. Let $\Phi : \mathbb{C}^{n \times n} \to \mathbb{C}^{m \times m}$ be a completely positive linear map given by

$$
\Phi(X) = \sum_{i=1}^{k} A_i X A_i^\dagger,
$$

where $A_1, \ldots, A_k \in \mathbb{C}^{m \times n}$ and $\dagger$ denotes the Hermitian conjugate. Its dual map $\Phi^* : \mathbb{C}^{m \times m} \to \mathbb{C}^{n \times n}$ is defined as

$$
\Phi^*(X) = \sum_{i=1}^{k} A_i^\dagger X A_i.
$$

The operator scaling problem is to find non-singular Hermitian matrices $L \in \mathbb{C}^{m \times m}$ and $R \in \mathbb{C}^{n \times n}$ such that

$$
\Phi_{L,R}(I_n) = \frac{1}{m} I_m \quad \text{and} \quad \Phi^*_{L,R}(I_m) = \frac{1}{n} I_n,
$$

where $I_n$ is the $n$-dimensional identity matrix and

$$
\Phi_{L,R}(X) = L\Phi(R^\dagger X R)L^\dagger
$$

is the scaled operator. The operator scaling problem was originally introduced by Gurvits [13] to study a major open problem in computational complexity theory called the Edmonds problem, which is to determine whether a given matrix subspace contains a non-singular matrix or
not. Later, operator scaling has been found to appear in surprisingly many fields of mathematics and computer science, such as matrix rank in non-commutative variables [12, 20, 21], Brascamp–Lieb inequalities [11], quantum Schrödinger bridge [13], multivariate scatter estimation [9], and computational invariant theory [1].

Gurvits [14] extended the Sinkhorn algorithm to operator scaling. Specifically, starting from $\Phi^{(0)} = \Phi$, the operator Sinkhorn algorithm iterates left normalization

$$\Phi^{(2k+1)} = \Phi^{(2k)}_{L,I_n} \text{ where } L = \frac{1}{\sqrt{m}} \Phi^{(2k)}(I_n)^{-1/2},$$

and right normalization

$$\Phi^{(2k+2)} = \Phi^{(2k+1)}_{I_m,R} \text{ where } R = \frac{1}{\sqrt{n}} (\Phi^{(2k+1)})^*(I_m)^{-1/2}.$$  

Note that $\Phi^{(2k+1)}(I_n) = m^{-1} I_m$ and $(\Phi^{(2k+2)})^*(I_m) = n^{-1} I_n$. Gurvits [14] studied the convergence of the operator Sinkhorn algorithm for the case of $m = n$ by extending the capacity-based analysis of matrix scaling by [23]. Later, full convergence analysis of the operator Sinkhorn algorithm was given by [12]. The general case was analyzed recently by [11, 8]. However, it is still unclear whether the operator Sinkhorn algorithm can be viewed as alternating projections with respect to some divergence measure as in matrix scaling. In fact, this question was already posed in the original paper of Gurvits [14] and even mentioned as “a major open question” of operator scaling in the survey of Idel [19].

1.1 Our contribution

In this study, we investigate the operator Sinkhorn algorithm from the viewpoint of quantum information geometry [3] by using the Choi representation [5] of completely positive maps. Quantum information geometry was originally introduced to study the geometry of the space of quantum states, and it involves many non-trivial problems compared to classical information geometry such as the non-uniqueness of monotone Riemannian metrics and torsion of e-connections. Among possible Riemannian metrics, the symmetric logarithmic derivative (SLD) metric has been found to be relevant to quantum estimation theory such as the quantum Cramér–Rao inequality [15]. Our main finding is that the operator Sinkhorn algorithm is interpreted as alternating e-projections with respect to the SLD metric. Thus, our result is viewed as a generalization of the result by Csiszár [6] to operator scaling. We believe that our new geometric insight shed new light on operator scaling and may lead to deeper understanding and effective algorithms.

1.2 Organization

This paper is organized as follows. In Section 2, we briefly review classical information geometry and explain the geometric interpretation of the matrix Sinkhorn algorithm. In Section 3, we briefly introduce quantum information geometry and present our main finding on the operator Sinkhorn algorithm. In Section 4, we touch on another geometric approach to operator scaling in previous work and discuss divergence characterization of the operator Sinkhorn algorithm. Finally, we conclude the paper in Section 5.
2 Information geometry of matrix scaling

In this section, we review the result that the Sinkhorn algorithm for matrix scaling is interpreted as alternating e-projections from the viewpoint of classical information geometry, which was originally shown by Csiszár [6].

2.1 Classical information geometry

Classical information geometry provides geometric insights into statistics, information theory, and optimization by regarding the space of probability distributions as a Riemannian manifold with dual affine connections. Here, we briefly introduce concepts of classical information geometry. See [3, 2] for more details.

Let $S_{n-1} = \left\{ p = (p_1, \ldots, p_n) \mid p_k > 0, \sum_{k=1}^{n} p_k = 1 \right\} \subset \mathbb{R}^n$ be the $(n-1)$-dimensional probability simplex. Each point of $S_{n-1}$ corresponds to a multinomial distribution on $\{1, \ldots, n\}$. We explain the information geometric structure of $S_{n-1}$ following [10].

First, we define a Riemannian metric on $S_{n-1}$. From statistical perspective, the Riemannian metric $g$ on $S_{n-1}$ should be monotone under Markov embeddings. Chentsov’s theorem states that such a Riemannian metric $g$ is uniquely given by the Fisher information matrix (up to constant). Thus, we adopt the Fisher information matrix as the Riemannian metric tensor on $S_{n-1}$ and call it the Fisher metric. To do calculation with the Fisher metric, the e-representation and m-representation of tangent vectors are useful. Recall that each tangent vector of a manifold is identified with a directional derivative operator. By using this correspondence, the e-representation $X^{(e)} \in \mathbb{R}^n$ and m-representation $X^{(m)} \in \mathbb{R}^n$ of a tangent vector $X$ at $p \in S_{n-1}$ are defined as

$$
X^{(e)} = (X(\log p_1), \ldots, X(\log p_n)),
$$
$$
X^{(m)} = (Xp_1, \ldots, Xp_n),
$$

respectively. Then, the inner product of two tangent vectors $X$ and $Y$ at $p \in S_{n-1}$ with respect to the Fisher metric is calculated as the product-sum of their e-representation and m-representation:

$$
g(X, Y) = \sum_{k=1}^{n} X^{(e)}_k Y^{(m)}_k. \tag{1}
$$

Next, we introduce a pair of dual affine connections called the e-connection and m-connection on $S_{n-1}$. Note that these connections are different from the Levi–Civita connection, which is the unique torsion-free affine connection that preserves the Riemannian metric. The e-connection and m-connection on $S_{n-1}$ are defined such that their connection coefficients vanish under the coordinate systems $\theta = (\log p_1 - \log p_n, \ldots, \log p_{n-1} - \log p_n)$ and $\eta = (p_1, \ldots, p_{n-1})$, respectively. In other words, $\theta$ and $\eta$ are e-affine and m-affine coordinate systems, respectively. Due to the existence of affine coordinate systems, $S_{n-1}$ is both e-flat and m-flat. In this sense, $S_{n-1}$ is said to be a dually flat space. Since the m-connection on $S_{n-1}$ coincides with the affine connection induced by the natural embedding of $S_{n-1}$ into $\mathbb{R}^n$, the m-geodesic from $p^{(1)} \in S_{n-1}$
to \( p(2) \in S_{n-1} \) is given by \( \eta(t) = (1-t)\eta(1) + t\eta(2) \), which means that \( p_k(t) = (1-t)p_k^{(1)} + tp_k^{(2)} \) for \( k = 1, \ldots, n \). Similarly, the e-geodesic from \( p^{(1)} \in S_{n-1} \) to \( p^{(2)} \in S_{n-1} \) is given by \( \theta(t) = (1-t)\theta^{(1)} + t\theta^{(2)} \), which means that \( \log p_k(t) = (1-t)\log p_k^{(1)} + t\log p_k^{(2)} + C(t) \) for \( k = 1, \ldots, n \), where \( C(t) \) is the normalization constant.

Finally, we explain the generalized Pythagorean theorem and e-projection on \( S_{n-1} \). Let

\[
D_{KL}(p \parallel q) = \sum_{k=1}^{n} p_k \log \frac{p_k}{q_k}
\]

be the Kullback–Leibler divergence between \( p \in S_{n-1} \) and \( q \in S_{n-1} \), which satisfies \( D_{KL}(p \parallel q) \geq 0 \) and \( D_{KL}(p \parallel q) = 0 \) if and only if \( p = q \). The Pythagorean theorem is generalized to the Kullback–Leibler divergence as follows.

**Lemma 2.1.** For points \( p, q, r \in S_{n-1} \), let \( \gamma_1 \) be the e-geodesic from \( p \) to \( q \) and \( \gamma_2 \) be the \( m \)-geodesic from \( q \) to \( r \). If \( \gamma_1 \) and \( \gamma_2 \) are orthogonal with respect to the Fisher metric at \( q \), then

\[
D_{KL}(r \parallel p) = D_{KL}(r \parallel q) + D_{KL}(q \parallel p).
\]

By using this, we obtain the following.

**Lemma 2.2.** Let \( M \) be an \( m \)-autoparallel connected submanifold of \( S_{n-1} \) and \( p \in S_{n-1} \). Then, a point \( q \in M \) satisfies \( D_{KL}(q \parallel p) = \min_{r \in M} D_{KL}(r \parallel p) \) if and only if the e-geodesic from \( p \) to \( q \) is orthogonal to \( M \) at \( q \) with respect to the Fisher metric.

The unique point \( q \in M \) in Lemma 2.2 is called the e-projection of \( p \) onto \( M \).

### 2.2 Sinkhorn as alternating e-projections

Now, we show that the Sinkhorn algorithm coincides with alternating e-projections. Note that this result was originally derived by Csiszár \[6\]. Here, we present a proof based on e-geodesics for later reference.

Recall that, given a nonnegative matrix \( A \in \mathbb{R}^{n \times n}_+ \), the matrix scaling problem is to find nonnegative diagonal matrices \( L \in \mathbb{R}^{m \times m}_+ \) and \( R \in \mathbb{R}^{n \times n}_+ \) such that \((LAR)1_m = m^{-1}1_m\) and \((LAR)\top 1_m = n^{-1}1_n\). Starting from \( A^{(0)} = A \), each iteration of the Sinkhorn algorithm is defined as

\[
A^{(2k+1)} = \frac{1}{m} \text{Diag}(A^{(2k)}) \text{Diag}(1_m)^{-1} A^{(2k)},
\]

\[
A^{(2k+2)} = \frac{1}{n} A^{(2k+1)} \text{Diag}(A^{(2k+1)}\top 1_m)^{-1}.
\]

Let

\[
\Pi = \{ A \in \mathbb{R}^{m \times n}_+ \mid 1_m \top A 1_n = 1 \},
\]

\[
\Pi_1 = \{ A \in \mathbb{R}^{m \times n}_+ \mid A 1_n = m^{-1}1_m \} \subset \Pi,
\]

\[
\Pi_2 = \{ A \in \mathbb{R}^{m \times n}_+ \mid A\top 1_m = n^{-1}1_n \} \subset \Pi.
\]

We identify \( \Pi \) with \( S_{mn-1} \) through vectorization and introduce the corresponding information geometric structure. Since \( \Pi_1 \) and \( \Pi_2 \) are affine subspaces of \( \Pi \) under the \( \eta \)-coordinate, they are \( m \)-autoparallel connected submanifolds of \( \Pi \). From the definition of the Sinkhorn algorithm, it is clear that \( A^{(2k+1)} \in \Pi_1 \) and \( A^{(2k+2)} \in \Pi_2 \) for every \( k \) if \( A^{(0)} = A \) is a positive matrix. Then, the Sinkhorn algorithm is interpreted as alternating e-projections onto \( \Pi_1 \) and \( \Pi_2 \) as follows.

\[2\]Csizsár used the term “l-projection” instead of e-projection.
Proposition 2.3. Assume that $A^{(0)} = A$ is a positive matrix. Then, each iteration of the Sinkhorn algorithm coincides with the e-projection onto $\Pi_1$ or $\Pi_2$. Namely, the e-geodesic from $A^{(2k)}$ to $A^{(2k+1)}$ (resp. from $A^{(2k+1)}$ to $A^{(2k+2)}$) is orthogonal to $\Pi_1$ (resp. $\Pi_2$) with respect to the Fisher metric for every $k$.

Proof. The e-geodesic from $A^{(2k)}$ to $A^{(2k+1)}$ is given by
\[
\log A(t) = (1-t) \log A^{(2k)} + t \log A^{(2k+1)} + C(t)1_m1_n^\top,
\]
where log is applied element-wise and $C(t)$ is the normalization constant. Therefore, the e-representation of the tangent vector $X$ of this e-geodesic at $A^{(2k+1)}$ is
\[
X^{(e)} = \left. \frac{d}{dt} \log A(t) \right|_{t=1} = \log A^{(2k+1)} - \log A^{(2k)} + C'(1)1_m1_n^\top.
\]
From the definition of the Sinkhorn algorithm,
\[
\log A^{(2k+1)}_{ij} - \log A^{(2k)}_{ij} = -\log \left( \sum_{j'} A^{(2k)}_{ij'} \right),
\]
which depends only on $i$. Hence, each row of $X^{(e)}$ is parallel to $1_n$. On the other hand, from the definition of $\Pi_1$, each row of the m-representation $Y^{(m)}$ of a tangent vector $Y$ of $\Pi_1$ is orthogonal to $1_n$. Therefore, from $\Pi_1$, $X$ and $Y$ are orthogonal to each other with respect to the Fisher metric. Hence, the e-geodesic from $A^{(2k)}$ to $A^{(2k+1)}$ is orthogonal to $\Pi_1$ with respect to the Fisher metric. The proof for the e-geodesic from $A^{(2k+1)}$ to $A^{(2k+2)}$ is similar.

For $A, B \in \Pi$, let
\[
D_{KL}(A \parallel B) = \sum_{i,j} A_{ij} \log \frac{A_{ij}}{B_{ij}}
\]
be the Kullback–Leibler divergence. From Proposition 2.3 and Lemma 2.2, we obtain the following.

Corollary 2.4. Assume that $A^{(0)} = A$ is a positive matrix. Then, each iteration of the Sinkhorn algorithm provides the unique minimizer of the Kullback–Leibler divergence:
\[
D_{KL}(A^{(2k+1)} \parallel A^{(2k)}) = \min_{B \in \Pi_1} D_{KL}(B \parallel A^{(2k)}),
\]
\[
D_{KL}(A^{(2k+2)} \parallel A^{(2k+1)}) = \min_{B \in \Pi_2} D_{KL}(B \parallel A^{(2k+1)}).
\]

3 Information geometry of operator scaling

In this section, we present our main result on a quantum information geometric interpretation of the operator Sinkhorn algorithm.

\[^{3}\text{Thus, it is different from the matrix logarithm.}\]
3.1 Prerequisites from matrix analysis

Here, we introduce necessary concepts of matrix analysis. See [17, 4] for more details.

For two matrices $A = (a_{ij}) \in \mathbb{C}^{p \times q}$ and $B = (b_{kl}) \in \mathbb{C}^{r \times s}$, their Kronecker product $A \otimes B \in \mathbb{C}^{pr \times qs}$ is the partitioned matrix given by

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1q}B \\ \vdots & \ddots & \vdots \\ a_{p1}B & \cdots & a_{pq}B \end{bmatrix}.$$

For a partitioned matrix

$$\begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}$$

with $A_{ij} \in \mathbb{C}^{m \times m}$ for every $(i, j)$, its partial traces are defined as

$$\text{tr}_1 \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix} = \sum_{i=1}^{n} A_{ii} \in \mathbb{C}^{m \times m},$$

$$\text{tr}_2 \begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix} = \begin{bmatrix} \text{tr} A_{11} & \cdots & \text{tr} A_{1n} \\ \vdots & \ddots & \vdots \\ \text{tr} A_{n1} & \cdots & \text{tr} A_{nn} \end{bmatrix} \in \mathbb{C}^{n \times n}.$$

A linear map $\Phi : \mathbb{C}^{n \times n} \to \mathbb{C}^{m \times m}$ is said to be completely positive if it has the Kraus representation:

$$\Phi(X) = \sum_{i=1}^{k} A_i X A_i^\dagger,$$

where $A_1, \ldots, A_k \in \mathbb{C}^{m \times n}$ and $\dagger$ denotes the Hermitian conjugate. Then, its dual map $\Phi^* : \mathbb{C}^{m \times m} \to \mathbb{C}^{n \times n}$ is also completely positive with the Kraus representation

$$\Phi^*(X) = \sum_{i=1}^{k} A_i^\dagger X A_i.$$

In quantum information theory, it is known that any quantum operation is described by a trace-preserving completely positive (TPCP) map [13, 27].

For a linear map $\Phi : \mathbb{C}^{n \times n} \to \mathbb{C}^{m \times m}$, its Choi representation $\text{CH}(\Phi) \in \mathbb{C}^{mn \times mn}$ is defined as

$$\text{CH}(\Phi) = \sum_{i,j=1}^{n} E_{ij} \otimes \Phi(E_{ij}) = \begin{bmatrix} \Phi(E_{11}) & \cdots & \Phi(E_{1n}) \\ \vdots & \ddots & \vdots \\ \Phi(E_{n1}) & \cdots & \Phi(E_{nn}) \end{bmatrix},$$

where $E_{ij}$ is the matrix unit with 1 in the $(i, j)$-th entry and 0s elsewhere. From definition, $\text{tr}_1 \text{CH}(\Phi) = \Phi(I_n)$ and $\text{tr}_2 \text{CH}(\Phi) = \Phi^*(I_m)$. In addition, Choi [5] showed the following important property.
Lemma 3.1 (Choi [5]). $\Phi$ is completely positive if and only if $\text{CH}(\Phi)$ is positive semidefinite.

For an Hermitian matrix $A \in \mathbb{C}^{n \times n}$ (i.e., $A = A^\dagger$), let

$$A = P \Lambda P^\dagger, \quad \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$$

be its spectral decomposition. Assume that the eigenvalues $\lambda_1, \ldots, \lambda_n$ of $A$ are contained in the interval $[a, b]$. Then, for a function $f : [a, b] \to \mathbb{R}$, we define the Hermitian matrix $f(A) \in \mathbb{C}^{n \times n}$ by

$$f(A) = Pf(\Lambda)P^\dagger, \quad f(\Lambda) = \text{diag}(f(\lambda_1), \ldots, f(\lambda_n)).$$

In particular, for a positive semidefinite matrix $A$ and the square root function $f(x) = x^{1/2}$, we denote $f(A)$ by $A^{1/2}$. A function $f$ is said to be operator monotone if $f(A) \succeq f(B)$ holds for every $A$ and $B$ satisfying $A \succeq B$.

Given $A \in \mathbb{C}^{n \times n}$ and $Q \in \mathbb{C}^{n \times n}$, the (continuous) Lyapunov equation $A^\dagger X + XA = Q$ has a unique solution of $X$ if $A$ is positively stable (i.e., all the eigenvalues of $A$ are contained in the open right half-plane of $\mathbb{C}$). Furthermore, if both $A$ and $Q$ are Hermitian, then the solution $X$ is also Hermitian.

For positive definite matrices $A \in \mathbb{C}^{n \times n}$ and $B \in \mathbb{C}^{n \times n}$, their geometric mean $A\#B \in \mathbb{C}^{n \times n}$ is defined as

$$A\#B = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}.$$

It is known that $A\#B$ is positive definite and $A\#B = B\#A$. Furthermore, $A\#B$ is the unique positive definite solution of the Riccati equation $XA^{-1}X = B$.

3.2 Quantum information geometry

The theory of classical information geometry has been extended to quantum systems. Here, we briefly introduce several concepts of quantum information geometry. See [3] for more details.

In quantum information theory [15, 27], each quantum system is associated with a complex Hilbert space. For example, a qubit system is associated with $\mathbb{C}^2$. A state of a quantum system associated with $\mathbb{C}^n$ is described by a density matrix $\rho \in \mathbb{C}^{n \times n}$, which is a positive semidefinite Hermitian matrix of trace one. Let

$$S(\mathbb{C}^n) = \{ \rho \in \mathbb{C}^{n \times n} \mid \rho > 0, \text{tr} \rho = 1 \}$$

be the set of positive definite density matrices on $\mathbb{C}^n$. In quantum information geometry, the set $S(\mathbb{C}^n)$ is regarded as a $(n^2 - 1)$-dimensional Riemannian manifold. We explain the information geometric structure of $S(\mathbb{C}^n)$ following [10].

First, we define a Riemannian metric on $S(\mathbb{C}^n)$. Whereas the Riemannian metric is uniquely specified as the Fisher metric by Chentsov’s theorem in classical information geometry, such uniqueness does not hold in quantum information geometry. Specifically, Petz [26] investigated Riemannian metrics on $S(\mathbb{C}^n)$ that are monotone under TPCP maps and showed that there is a one-to-one correspondence between monotone Riemannian metrics and operator monotone functions. Among them, here we focus on the symmetric logarithmic derivative (SLD) metric, which corresponds to the function $t \mapsto (t + 1)/2$. For a tangent vector $X$ at $\rho \in S(\mathbb{C}^n)$, its
e-representation $X^{(e)} \in \mathbb{C}^{n \times n}$ is defined by the unique Hermitian solution of the Lyapunov equation

$$X^{(e)} \rho + \rho X^{(e)} = 2X \rho. \quad (2)$$

On the other hand, the $m$-representation $X^{(m)} \in \mathbb{C}^{n \times n}$ of a tangent vector $X$ at $\rho \in S(\mathbb{C}^n)$ is defined by $X \rho$. Then, the inner product of two tangent vectors $X$ and $Y$ at $\rho \in S(\mathbb{C}^n)$ with respect to the SLD metric is given by $g^S(X, Y) = \text{tr}(X^{(e)} Y^{(m)})$. The SLD metric has been found to play a central role in extending the Cramér–Rao inequality to quantum estimation [21].

Next, we introduce dual affine connections on $S(\mathbb{C}^n)$. Similarly to the classical case, the $m$-connection on $S(\mathbb{C}^n)$ is defined as the torsion-free affine connection induced by the natural embedding of $S(\mathbb{C}^n)$ into $\mathbb{R}^n$:

$$\rho \mapsto (\rho_{11}, \ldots, \rho_{nn}, \text{Re} \rho_{12}, \text{Im} \rho_{12}, \ldots, \text{Re} \rho_{n-1,n}, \text{Im} \rho_{n-1,n}).$$

Thus, the $m$-geodesic from $\rho_1$ to $\rho_2$ is simply given by $\rho(t) = (1-t)\rho_1 + t\rho_2$ and the space $S(\mathbb{C}^n)$ is $m$-flat. On the other hand, the $e$-connection on $S(\mathbb{C}^n)$ is not unique and depends on which Riemannian metric is introduced to $S(\mathbb{C}^n)$. Namely, for each Riemannian metric $g$ on $S(\mathbb{C}^n)$, the $e$-connection on $S(\mathbb{C}^n)$ is defined to be the dual of the $m$-connection with respect to $g$. Let us adopt the SLD metric now. Then, the $e$-geodesic from $\rho_1$ to $\rho_2$ is explicitly given by

$$\rho(t) = C(t) K^t \rho_1 K^t, \quad (3)$$

where $K = \rho_1^{-1/2}\rho_2$ is the matrix geometric mean of $\rho_1^{-1}$ and $\rho_2$ and $C(t)$ is the normalization constant for $\text{tr} \, \rho(t) = 1$. However, this $e$-connection is not torsion-free. Thus, the space $S(\mathbb{C}^n)$ is not dually flat under the SLD metric and it is not clear whether there exists some canonical divergence and analogue of the generalized Pythagorean theorem in this case.

### 3.3 Main result

Now, we present our main result on the operator Sinkhorn algorithm. Recall that, given a completely positive linear map $\Phi : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times m}$, the operator scaling problem is to find nonsingular Hermitian matrices $L \in \mathbb{C}^{m \times m}$ and $R \in \mathbb{C}^{n \times n}$ such that $\Phi_{L,R}(I_n) = m^{-1}I_m$ and $\Phi^*_{L,R}(I_m) = n^{-1}I_n$, where $\Phi_{L,R}(X) = L\Phi(R\dagger XR)L\dagger$. Starting from $\Phi(0) = \Phi$, each iteration of the operator Sinkhorn algorithm is defined as

$$\Phi^{(2k+1)} = \Phi^{(2k)}_{L,I_n} \quad \text{where} \quad L = \frac{1}{\sqrt{m}} \Phi^{(2k)}(I_n)^{-1/2},$$

$$\Phi^{(2k+2)} = \Phi^{(2k+1)}_{I_m,R} \quad \text{where} \quad R = \frac{1}{\sqrt{n}} (\Phi^{(2k+1)*}(I_m)^{-1/2}.\quad (4)$$

For quantum information geometric consideration, we identify a completely positive map with its Choi representation. Then, we obtain the following formula.

**Lemma 3.2.** The Choi representation of $\Phi_{L,R}$ is given by

$$\text{CH}(\Phi_{L,R}) = (R\dagger \otimes L) \text{CH}(\Phi)(R \otimes L\dagger).$$

---

4The $e$-connection on $S(\mathbb{C}^n)$ is torsion-free if and only if the Bogoliubov–Kubo–Mori metric [21] is adopted [2][19].
Proof. Since $\Phi_{L,I_n}(X) = L\Phi(X)L^\dagger$, 
\begin{align*}
\text{CH}(\Phi_{L,I_n}) = \sum_{i,j} E_{ij} \otimes L\Phi(E_{ij})L^\dagger = (I_n \otimes L) \text{CH}(\Phi)(I_n \otimes L^\dagger),
\end{align*}
where we used the formula $(A \otimes B)(C \otimes D) = AC \otimes BD$ in the second equality.

On the other hand, since $\Phi_{I,R}(X) = \Phi(R^\dagger XR)$, 
\begin{align*}
\text{CH}(\Phi_{I,m,R}) = \sum_{i,j} E_{ij} \otimes \Phi(R^\dagger E_{ij}R) = (R^\dagger \otimes I_m) \text{CH}(\Phi)(R \otimes I_m),
\end{align*}
where we used
\begin{align*}
\Phi(R^\dagger E_{ij}R) = \Phi\left(\sum_{k,l} \bar{R}_{ik}R_{jl}E_{kl}\right) = \sum_{k,l} \bar{R}_{ik}R_{jl} \Phi(E_{kl}) = \sum_{k,l} \bar{R}_{ki}R_{lj} \text{CH}(\Phi)_{kl}.
\end{align*}
Therefore, from $\Phi_{L,R} = (\Phi_{L,I_n})_{I,m,R}$,
\begin{align*}
\text{CH}(\Phi_{L,R}) &= (R^\dagger \otimes I_m) \text{CH}(\Phi_{L,I_n})(R \otimes I_m) \\
&= (R^\dagger \otimes I_m)(I_n \otimes L) \text{CH}(\Phi)(I_n \otimes L^\dagger)(R \otimes I_m) \\
&= (R^\dagger \otimes L) \text{CH}(\Phi)(R \otimes L^\dagger).
\end{align*}
\hfill \Box

Let $\rho_k = \text{CH}(\Phi^{(k)}) \in \mathbb{C}^{mn \times mn}$ be the Choi representation of $\Phi^{(k)}$. Note that $\rho_k \succeq 0$ from Lemma 3.1. By using Lemma 3.2, the operator Sinkhorn algorithm is rewritten as follows.

\begin{lemma}
Each iteration of the operator Sinkhorn algorithm is given by
\begin{align*}
\rho_{2k+1} &= (I_n \otimes L)\rho_{2k}(I_n \otimes L), \quad L = \frac{1}{\sqrt{m}}(\text{tr}_1 \rho_{2k})^{-1/2}, \\
\rho_{2k+2} &= (R \otimes I_m)\rho_{2k+1}(R \otimes I_m), \quad R = \frac{1}{\sqrt{n}}(\text{tr}_2 \rho_{2k+1})^{-1/2}.
\end{align*}
\end{lemma}

Let
\begin{align*}
\Pi &= \{\rho \in \mathbb{C}^{mn \times mn} \mid \rho \succ O, \text{ tr } \rho = 1\}, \\
\Pi_1 &= \{\rho \in \mathbb{C}^{mn \times mn} \mid \rho \succ O, \text{ tr}_1 \rho = m^{-1}I_m\} \subset \Pi, \\
\Pi_2 &= \{\rho \in \mathbb{C}^{mn \times mn} \mid \rho \succ O, \text{ tr}_2 \rho = n^{-1}I_n\} \subset \Pi.
\end{align*}
We identify $\Pi$ with $S(\mathbb{C}^{mn})$ and introduce the corresponding information geometric structure with the SLD metric. From the definition of $\Pi_1$ and $\Pi_2$, they are $m$-autoparallel connected submanifolds of $\Pi$.

Since the partial trace of a positive definite matrix is also positive definite, we have the following.

\begin{lemma}
If $\rho_0 \succ O$, then $\rho_{2k+1} \in \Pi_1$ and $\rho_{2k+2} \in \Pi_2$ for every $k$.
\end{lemma}

Then, the operator Sinkhorn algorithm is interpreted as alternating e-projections as follows.
Theorem 3.5. Assume that $\rho_k \succ O$. Then, each iteration of the operator Sinkhorn algorithm coincides with the $e$-projection onto $\Pi_1$ or $\Pi_2$ with respect to the SLD metric. Namely, $\rho_{2k+1}$ (resp. $\rho_{2k+2}$) is the unique point in $\Pi_1$ (resp. $\Pi_2$) such that the $e$-geodesic from $\rho_k$ to $\rho_{2k+1}$ (resp. from $\rho_{2k+1}$ to $\rho_{2k+2}$) is orthogonal to $\Pi_1$ (resp. $\Pi_2$) with respect to the SLD metric for every $k$.

Proof. From Lemma 3.4 we have $\rho_k \succ O$ for every $k$. In the following, we prove the statement for $\rho_{2k+1}$. The proof for $\rho_{2k+2}$ is similar.

Let $K = \rho_{2k}^{-1} \# \rho_{2k+1}$. Since $\rho_{2k+1} = (I_n \otimes L)\rho_{2k}(I_n \otimes L)$ with $L = (\text{tr}_1 \rho_{2k})^{-1/2}/\sqrt{m} > O$ from Lemma 3.3,

$$K = \rho_{2k}^{-1/2} \cdot (\rho_{2k}^1 \rho_{2k+1} \rho_{2k}^1)'^{-1/2} \rho_{2k}^{-1/2} \rho_{2k}^{-1/2} \cdot (\rho_{2k}^1 (I_n \otimes L) \rho_{2k}(I_n \otimes L) \rho_{2k}^1)' \rho_{2k}^{-1/2} \rho_{2k}^{-1/2} = I_n \otimes L.$$

Then, the $e$-geodesic from $\rho_{2k}$ to $\rho_{2k+1}$ with respect to the SLD metric is given by

$$\rho(t) = C(t)K^t \rho_{2k}K^t.$$

Thus,

$$\left. \frac{\text{d}}{\text{d}t} \rho(t) \right|_{t=1} = C'(1)\rho_{2k+1} + C(1)(\log K)\rho_{2k+1} + C(1)\rho_{2k+1}(\log K).$$

Therefore, the $e$-representation $X^{(e)}$ of the tangent vector $X$ of this $e$-geodesic at $\rho_{2k+1}$ is the solution of the Lyapunov equation

$$X^{(e)} \rho_{2k+1} + \rho_{2k+1}X^{(e)} = 2 \left( C'(1)\rho_{2k+1} + C(1)(\log K)\rho_{2k+1} + C(1)\rho_{2k+1}(\log K) \right),$$

which has a unique solution since $\rho_{2k+1} \succ O$. Namely, we must have

$$X^{(e)} = C'(1)I_{nn} + 2C(1)\log K = I_n \otimes (C'(1)I_m + 2C(1)\log L).$$

On the other hand, from the definition of $\Pi_1$, the $m$-representation $Y^{(m)}$ of a tangent vector $Y$ of $\Pi_1$ satisfies $\text{tr}_1 Y^{(m)} = O$. Therefore,

$$g^S(X, Y) = \text{tr}(X^{(e)}Y^{(m)}) = \text{tr}[(C'(1)I_m + 2C(1)\log L)(\text{tr}_1 Y^{(m)})] = 0.$$

Hence, the $e$-geodesic from $\rho_{2k}$ to $\rho_{2k+1}$ is orthogonal to $\Pi_1$ with respect to the SLD metric.

Conversely, suppose that the $e$-geodesic from $\rho_{2k}$ to $\rho \in \Pi_1$ is orthogonal to $\Pi_1$ with respect to the SLD metric. Then, by following the above argument reversely, we must have $\rho_{2k}^{-1} \# \rho = I_n \otimes M$ with some $M$ and thus $\rho = (I_n \otimes M)\rho_{2k}(I_n \otimes M)$. Since $\rho_{2k}$ is the Choi representation of $\Phi^{(2k)}$,

$$\rho = (I_n \otimes M) \left( \sum_{i,j} E_{ij} \otimes \Phi^{(2k)}(E_{ij}) \right) (I_n \otimes M) = \sum_{i,j} E_{ij} \otimes (M \Phi^{(2k)}(E_{ij}) M).$$
Therefore,

\[
\text{tr}_1 \rho = \sum_{i,j} \text{tr}(E_{ij}) \cdot M \Phi^{(2k)}(E_{ij}) M \\
= \sum_i M \Phi^{(2k)}(E_{ii}) M \\
= M \left( \sum_i \Phi^{(2k)}(E_{ii}) \right) M \\
= M \Phi^{(2k)}(I_n) M \\
= M (\text{tr}_1 \rho)^2 M.
\]

By the linearity of \(\Phi^{(2k)}\)

Since \(\rho \in \Pi_1\), we must have \(\text{tr}_1 \rho = m^{-1}I_m\). Hence, from the uniqueness of the solution of the Riccati equation, we must have \(M = (\text{tr}_1 \rho)^{-1/2}/\sqrt{m} = L\) and thus \(\rho = \rho_{2k+1}\).

\[\Box\]

4 Discussion

In this section, we briefly introduce another Riemannian approach to operator scaling in previous study and discuss on divergence characterization of the operator Sinkhorn algorithm. For the sake of simplicity, we assume that \(m = n\) in the following.

4.1 Another Riemannian approach for operator scaling

In [1], the authors devised an efficient algorithm for operator scaling based on a Riemannian structure of the positive definite cone. They focused on the capacity \([14]\) of a completely positive map \(\Phi\) defined as

\[
cap(\Phi) = \inf_{X \succ O} \frac{\det(\Phi(X))}{\det X}.
\]

It is an extension of the capacity of a nonnegative matrix \(A\) in matrix scaling \([23]\):

\[
cap(A) = \inf_{X > 0} \prod_{i=1}^{n} (Ax_i) / \prod_{i=1}^{n} x_i.
\]

It is known that if one finds \(X \succ O\) achieving the (approximate) infimum of \([1]\), then one can recover the (approximate) solution of operator scaling \([12]\). Unfortunately, the problem \([1]\) is nonconvex. The main idea of \([1]\) is to consider an equivalent problem

\[
\inf_{X \succ O} \log \det \Phi(X) - \log \det X,
\]

and show that this problem is geodesically convex. Specifically, they regarded the positive definite cone \(\{X \succ O\}\) as a Riemannian manifold by taking the Hessian of \(\Psi(X) = -\log \det(X)\) as the Riemannian metric tensor and introducing the corresponding Levi–Civita connection. It is known \([17]\) that the geodesic from \(X_1\) to \(X_2\) on this Riemannian manifold is given by

\[
X(t) = X_1^{1/2} (X_1^{-1/2} X_2 X_1^{-1/2})^t X_1^{1/2},
\]
which is different from the e-geodesic \([\mathbf{3}]\) with respect to the SLD metric. Then, in the problem \([\mathbf{4}]\), the objective function is convex along with geodesic \([\mathbf{4}]\) and this property leads to an efficient algorithm \([\mathbf{1}]\). It may be interesting to investigate the relation of this approach with our quantum information geometric results and we leave it for future work. Information geometry of the positive definite cone \([\mathbf{25}]\) might be also relevant.

### 4.2 Divergence characterization of operator Sinkhorn algorithm

The Sinkhorn algorithm for matrix scaling is equivalent to alternating minimization of the Kullback–Leibler divergence (see Corollary \([\mathbf{2.4}]\)). Thus, it is natural to ask if some quantum analogue of the Kullback–Leibler divergence yields the same characterization of the operator Sinkhorn algorithm. This problem was already mentioned by Gurvits \([\mathbf{14}, \text{Remark 4.8}]\) and even said to be “a major open question” of operator scaling in the survey by Idel \([\mathbf{19}]\). Here, we discuss this problem from the viewpoint of quantum information geometry.

Although quantum generalization of the Kullback–Leibler divergence is not unique, the most important one may be the Umegaki quantum relative entropy \([\mathbf{31}]\):

\[
D(\rho \| \sigma) = \text{tr}[\rho \log(\rho) - \rho \log(\sigma)],
\]

which has been found to play a central role in quantum information theory \([\mathbf{18}, \mathbf{27}]\). Unfortunately, the trajectory of alternating minimization of the Umegaki quantum relative entropy does not coincide with that of the operator Sinkhorn algorithm. For the sake of completeness, we check this numerically with \(m = n = 2\). We generated a \(4 \times 4\) density matrix \(\rho_0\) by \(\rho_0 = P^T P / \text{tr}(P^T P)\), where \(P\) is a \(4 \times 4\) matrix of standard Gaussian random variables. Then, we applied the operator Sinkhorn algorithm and alternating minimization of the Umegaki quantum relative entropy, both starting from \(\rho_0\). In the minimization of the Umegaki quantum relative entropy, we used the MATLAB package CVXQUAD \([\mathbf{7}]\). Figure \([\mathbf{1}]\) plots the squared Frobenius norm \(\|\rho_t - \rho_*\|^2_F\) with respect to the iteration count \(t\), where \(\rho_*\) is the convergence point of the operator Sinkhorn algorithm and \(\rho_t\) is the \(t\)-th iterate of either operator Sinkhorn algorithm or alternating Umegaki relative entropy minimization. It is clear that the two procedures converge to distinct points.

In matrix scaling, it is known that the capacity can be characterized as the minimum of the Kullback–Leibler divergence:

\[
-\log \text{cap}(A) = \inf_{B: \text{doubly stochastic}} D_{\text{KL}}(B \| A).
\]

Hence, one may still hope that a similar characterization holds between the capacity \([\mathbf{3}]\) and the Umegaki quantum relative entropy in operator scaling. However, again we can numerically check that this is not the case. Figure \([\mathbf{2}]\) plots the Umegaki quantum relative entropy \(D(\rho_* \| \rho_0)\) and the negative logarithm of capacity \(-\log \text{cap}(\rho_0)\) over 30 random initial \(\rho_0\). It is clearly shown that they consistently disagree.

In quantum information geometry, the Umegaki quantum relative entropy appears as the canonical divergence between quantum states when we introduce the Bogoliubov–Kubo–Mori metric

\[
g^B(X, Y) = \text{tr}[X(\rho) \log(Y(\rho))],
\]

which is the unique monotone Riemannian metric that induces a dually flat structure on the space of quantum states \([\mathbf{3}]\). On the other hand, the SLD metric does not induce a
Figure 1: Convergence history of operator Sinkhorn algorithm and alternating Umegaki relative entropy minimization.

Figure 2: Comparison of Umegaki quantum relative entropy $D(\rho_0 \mid\!\mid \rho_0)$ and negative logarithm of capacity $-\log \text{cap}(\rho_0)$. 
dually flat structure, because the e-connection does not become torsion-free. Traditionally, the theory of information geometry has been mostly developed in the dually flat setting [3, 2] and the theory for statistical manifolds admitting torsion [24, 16] is still largely unexplored [10]. Therefore, although we found that the operator Sinkhorn algorithm coincides with alternating e-projections with respect to the SLD metric, it is still unclear whether it can be viewed as alternating minimization of some divergence.

5 Conclusion

In this study, we investigated the operator Sinkhorn algorithm [14] from the viewpoint of quantum information geometry [3]. Our main finding is that the operator Sinkhorn algorithm coincides with alternating e-projections with respect to the symmetric logarithmic derivative (SLD) metric, which is a Riemannian metric on the quantum state space and plays an important role in quantum estimation theory [15]. This result is viewed as a generalization of the result by Csiszár [6] to operator scaling.

Whereas the matrix Sinkhorn algorithm is viewed as alternating minimization of the Kullback–Leibler divergence, such divergence characterization is still unclear for the operator Sinkhorn algorithm. The main obstacle is that the e-connection induced by the SLD metric is not torsion-free and thus existing tools for dually flat spaces such as the generalized Pythagorean theorem are not directly applicable. It is an interesting future work to develop theories of statistical manifolds admitting torsion [24, 16] and obtain divergence characterization of the operator Sinkhorn algorithm.

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