

ORIGINAL RESEARCH

Interpolation of positive matrices by quantum-inspired optimal control

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Abstract

Interpolation of probability distributions can be formulated as an optimal transport problem. Positive matrix, which can be viewed as the generalization of probability distribution to higher dimension, is used in quantum theory to describe the state of a quantum system. Here, a quantum-inspired method for the interpolation of positive matrices is proposed. Particularly, this method employs the quantum state purification of the positive matrices in an extended space. Since pure state controllability can be easily achieved using open-loop coherent control, the continuous interpolation of positive matrices is given as a completely positive map induced by simulating the optimal control for pure state transfer. The quantum-inspired interpolation is shape-preserving with applications to tensor field processing.

1 | INTRODUCTION

Classical optimal transport problem seeks for the optimal plan that minimizes the cost of transforming one probability distribution of mass to another [1]. The optimal transport map defines a displacement interpolation of probability distributions and induces a transport-based distance function, which is considered to be more efficient and robust in comparing distributions than the Kullback–Leibler divergence. For example, the stability of training of generative adversarial networks can be improved using an optimal transport cost [2]. The optimal transport between positive matrices considers the transformation in a higher dimension. Positive matrices offer compact representations of visual and time-series data [3–6], which has led researchers to consider the distance function and interpolation method for positive matrices. In particular, the interpolation of positive matrices has become a useful tool in graphics and geometry processing, as the diffusion tensors of the images are characterized by 2×2 and 3×3 positive matrices [3, 4, 7, 8]. For example, Diffusion Tensor Imaging (DTI) [9, 10] has been

widely used in medical imaging, in which the diffusion of water molecules is characterized by a 3×3 positive matrix. In control theory, the interpolation method is proposed to reduce the computational complexity in solving the Lyapunov equations for linear parameter varying systems [11, 12], where the stabilizing Lyapunov matrices are computed for a few values of the parameters and the Lyapunov matrices for other values are obtained by interpolation.

Matricial analogues of mass transport for positive-definite matrices have been studied in [13–15]. By developing a suitable notion of control cost, the solution to the matrix optimal transport problem is the minimal amount of work needed for the dynamical deformation that connects positive matrices. The rotation and alignment of eigenvectors have to be considered for the transportation of matrices in addition to the scaling of mass [13, 15], as the principle directions of the diffusion tensors have to transform continuously and independently in order to eliminate the artifacts in the interpolation images. For example, in the context of DTI, the changes in orthogonal diffusion orientation must be decoupled to achieve a shape-preserving

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interpolation, which is critical in white matter fiber tracking [3, 16].

Since positive matrices can be related to quantum probability distributions as quantum density matrices [17], quantum dynamical path provides an alternative route for the transformation of positive matrices. It has been argued in [13–15] that quantum-inspired interpolation can remove the push-pop artifacts commonly generated by the linear interpolation between matrix-valued power spectra of multivariate time series. Moreover, in contrast to classical transport where each unit of mass is moved from the initial position to the target position in different paths, the quantum operation acts on the eigenvectors and changes the corresponding eigenvalues of the matrix simultaneously. On one hand, intensive efforts have been made to find an analog of the Wasserstein metric on the space of density matrices. The critical concept in these studies is finding a quantum operator which mimics the gradient operator of the classical continuity equation for the mass-preserving flow of probability distribution [14, 18], or trying to generalize certain invariance property to the quantum regime [19]. However, as quantum density matrix is intrinsically different from classical probability distribution, the optimal transport theory can only be adapted to accommodate a restricted set of quantum dynamics, which may render such generalization impossible [20]. On the other hand, inspired by the quantum Lindblad evolution [15, 21] formulates the interpolation problem of positive-definite matrices as the minimization of control cost subjected to a dynamical equation. Although the devised dynamical equation consists of two terms which are responsible for the rotation of eigenvectors and scaling of eigenvalues, respectively, the equation itself cannot be related to genuine quantum control process and does not allow controllability analysis.

Here, we consider the interpolation of positive matrices as an optimal control for quantum state transfer. The main results are as follows:

- We prove that the classical optimal transport always generates linear interpolation if the positive matrix is taken as a classical ensemble of quantum pure states. In particular, by taking the classical ensemble as a vector-valued probability distribution, its displacement interpolation can be solved exactly. The resulting linear interpolation is unable to decouple the rotation of orthogonal eigenvectors, which means the generated matrices are not shape-preserving and not suitable for applications such as DTI.
- We propose a quantum-inspired method to solve the interpolation problem via a completely positive map, which is the most general form of quantum evolution. The main idea is to purify the matrix to a quantum pure state in a higher-dimensional Hilbert space using the standard state purification protocol. The unitary operation taking one quantum pure state to the other induces a completely positive map for the transformation of density matrices in the subspace. Then the existence of a quantum path between any two density matrices is guaranteed by the pure state controllability in the larger space, as illustrated in Figure 1. In fact,

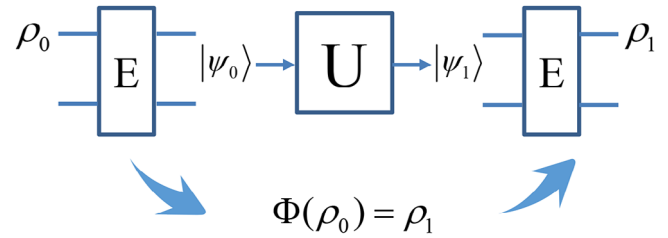


FIGURE 1 Positive matrices ρ_0 and ρ_1 are entangled with ancillary systems to create quantum pure states. A quantum dynamical path that connects ρ_0 and ρ_1 is derived by controlling the unitary transformation between the pure states, which can be simulated efficiently on classical computers with quantum optimal control algorithms.

the one-to-one correspondence between completely positive map and unitary evolution in an extended space is a key concept in the development of open quantum system theory [22, 23]. Quantum pure state controllability has been well studied in literature [24–28]. In particular, the conditions for pure state controllability can be easily satisfied by simulating open-loop coherent control. The optimal interpolation, or transport of density matrices is achieved when the control cost is minimized. As a result, we can solve the problem using any efficient optimal control algorithm such as Gradient Ascent Pulse Engineering (GRAPE) [29]. The resulting interpolation rotates the orthogonal eigenvectors and scales the corresponding eigenvalues simultaneously and independently, which ensures that the transformation of the tensor fields is smooth and natural.

The rest of the paper is organized as follows. A brief introduction to quantum state, quantum operation and classical optimal transport theory is presented in Section 2. Section 3 proves that the classical displacement interpolation for positive matrices is equivalent to linear interpolation. In Section 4, it is shown that an interpolation framework can be established based on the simulation of quantum optimal control. Two illustrative examples are given in Section 5. Section 6 concludes this paper.

Notation. Quantum pure states are denoted using Dirac notation. A *ket* represents a state vector, written as $|\psi\rangle$ (equivalent to a complex-valued column vector). The conjugate transpose \dagger of a state vector $|\psi\rangle$ is denoted as $\langle\psi|$. The commutator of two operators (matrices) X and Y on \mathcal{H} is defined as $[X, Y] \triangleq XY - YX$. Id is the identity map. \mathbb{R} denotes the set of real numbers. $\#$ is the notation for the push-forward operation in probability theory.

2 | PRELIMINARIES

2.1 | Quantum state representation

Here, quantum states are defined on the Hilbert space \mathcal{H} . A quantum state is pure if it can be represented as a

complex-valued unit vector in \mathcal{H} . A pure state vector can be expanded on the basis of \mathcal{H} as

$$|\psi\rangle = \sum_n c_n |n\rangle, \quad \sum_n |c_n|^2 = 1, \quad (1)$$

which is a probabilistic superposition of the basis states $\{|n\rangle\}$. Here c_n is a complex number and $|c_n|^2$ is the probability amplitude. In contrast, a classical ensemble of pure states is described by

$$\mathcal{E} = \{(\lambda_1, |\psi_1\rangle), \dots, (\lambda_M, |\psi_M\rangle)\}, \quad \sum_i \lambda_i = 1, \quad \lambda_i \geq 0. \quad (2)$$

The ensemble represents a classical mixture of these pure states $\{|\psi_i\rangle\}$, with λ_i being the ratio of a state $|\psi_i\rangle$. In order to unify the representation of quantum pure state and semi-classical mixed state, the density matrix formulation has been introduced [17]. The density matrix ρ of a quantum state has the following properties

$$\rho \geq 0, \quad \rho^\dagger = \rho, \quad \text{tr}(\rho) = 1. \quad (3)$$

The density matrix of a pure state $|\psi\rangle$ is given by $\rho = |\psi\rangle\langle\psi|$, while the density matrix of the ensemble \mathcal{E} is written as $\rho = \sum \lambda_i |\psi_i\rangle\langle\psi_i|$. We have $\text{tr}(\rho^2) = 1$ for a pure state and $\text{tr}(\rho^2) < 1$ for a mixed state.

2.2 | Quantum operation

Quantum operation is a physical process that generates the dynamical transformation between quantum states. For example, a unitary operation U maps a pure state to another pure state as

$$|\chi\rangle = U|\psi\rangle = \sum_n c_n U|n\rangle. \quad (4)$$

However, unitary operation usually is realized with a closed quantum system. A generalized quantum operation will take its environment into consideration, and such an operation can be characterized by a completely positive map as

$$\Phi(\rho) = \sum_k M_k \rho M_k^\dagger, \quad \sum_k M_k^\dagger M_k \leq I, \quad (5)$$

where $\{M_k\}$ are called Kraus operators [17]. The generalized quantum operation can be used to induce the transformation between pure states and mixed states. As can be seen from (4) and (5), quantum operations act on the entire set of orthogonal vectors $\{|n\rangle\}$ (pure state), or $\{|\psi_i\rangle\}$ (mixed state) in parallel, which constitutes the major difference between the semi-classical optimal transport and quantum dynamical optimal transport studied here. In particular, since the transformation of the orthogonal vectors is simultaneous and decoupled under quantum control, the diffusion with respect to the tensor

fields is guaranteed to be shape-preserving in the interpolated images.

2.3 | Classical optimal transport and displacement interpolation

Given measurable spaces (X_1, Σ_1) and (X_2, Σ_2) , a measurable mapping $T : X_1 \rightarrow X_2$ and a measure $\mu : \Sigma_1 \rightarrow [0, +\infty]$, the pushforward of μ is the measure expressed as

$$(T\#\mu)(B) = \mu(T^{-1}(B)), \quad B \in \Sigma_2, \quad (6)$$

and we have

$$\int_{X_2} f d(T\#\mu) = \int_{X_1} f \circ T d\mu, \quad (7)$$

for an arbitrary function f . The classical optimal transport cost is define by

$$\mathcal{T}(\mu, \nu) = \inf_{T\#\mu=\nu} \int_{\mathbb{R}^n} d(x, T(x)) d\mu(x), \quad (8)$$

where d is a distance function. According to (8), the optimal transport cost for discrete probability distributions $\mu = (\mu_i)$ and $\nu = (\nu_j)$ can be written as

$$\begin{aligned} \mathcal{T}(\mu, \nu) &= \min_{\{\gamma_{ij}\}} \sum_{i,j} \gamma_{ij} d(\mu_i, \nu_j), \\ \sum_j \gamma_{ij} &= \mu_i, \quad \sum_i \gamma_{ij} = \nu_j, \quad \gamma_{ij} \geq 0. \end{aligned} \quad (9)$$

Here γ_{ij} is the amount of mass moved from μ_i to ν_j . It is known that \mathcal{T} is a distance function (Equation (12), [1]) on the space of probability distributions.

Displacement interpolation (McCann's interpolation) is defined by

$$\rho_t = [(1-t)\text{Id} + tT]\#\mu, \quad t \in [0, 1], \quad (10)$$

with T being the optimal transport map. The family of probability measures $(\rho_t)_{0 \leq t \leq 1}$ interpolates between μ and ν , and it is the **natural** linear interpolation regarding the geometry of optimal transport. Consider the quadratic cost $d(x, y) = |x - y|^2$ in \mathbb{R}^n as an example, we have

$$\begin{aligned} \mathcal{T}_2(\mu, \rho_t) &= \int_{\mathbb{R}^n} |x - [(1-t)x + tT(x)]|^2 d\mu(x) \\ &= t^2 \int_{\mathbb{R}^n} |x - T(x)|^2 d\mu(x) = t^2 \mathcal{T}_2(\mu, \nu). \end{aligned} \quad (11)$$

In terms of the quadratic Wasserstein distance $\mathcal{W}_2 = \sqrt{\mathcal{T}_2}$ [1], Equation (11) can be rewritten as

$$\mathcal{W}_2(\mu, \rho_t) = t \mathcal{W}_2(\mu, \nu). \quad (12)$$

2.4 | Quantum state controllability

Pure state controllability for closed quantum systems is considered as a finite-level system driven by a time-dependent Hamiltonian

$$H(t) = H_0 + \sum_k u_k(t) H_k, \quad (13)$$

where H_0 and $\{H_k\}$ are the open-loop control fields. H_k is constant, with a time-dependent amplitude $u_k(t)$. The notions of controllability can be related to the dynamical Lie algebra \mathcal{L} of the control system, which is generated from $\{iH_k\}$ by taking all linear combinations and iterated commutators. For example, the system is pure-state controllable if and only if \mathcal{L} is isomorphic to either $U(N)$ or $SU(N)$.

Although characterizing the degree of controllability with the dynamical Lie algebra is useful for control design, it has been found that degeneracies reduce the number of degrees of freedom available to manipulate a system [30]. Therefore, steering between quantum states with non-degenerate energy levels are well studied and can be easily achieved, whereas controlling degenerate quantum states requires much more effort [31, 32].

Quantum density matrix controllability [25] is more complicated and beyond the scope of this paper.

3 | OPTIMAL TRANSPORT ON ENSEMBLES

The interpolation of a positive matrix can be studied by normalizing its trace to 1, which turns the positive matrix into a quantum state with density matrix representation. A quantum state with density matrix representation can be decomposed as the classical mixture of pure states by the following lemma.

Lemma 1. *Any quantum density matrix ρ admits a decomposition as*

$$\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|, \quad \sum_i \lambda_i = 1, \quad \lambda_i > 0. \quad (14)$$

If the positive eigenvalues $\{\lambda_i\}$ of ρ are distinct, then each λ_i is uniquely associated with its corresponding eigenvector $|\psi_i\rangle$. The density matrix ρ with distinct positive eigenvalues can be uniquely mapped to the pure-state-valued probability distribution $\{\lambda_i, |\psi_i\rangle\}$.

Proof. Note that (14) is just the spectral decomposition of the Hermitian matrix ρ without the possible eigensubspace associated with the eigenvalue 0. According to the Spectral Theorem [17], the decomposition is unique on the eigensubspaces whose eigenvalues are distinct, and the eigensubspaces corresponding to distinct eigenvalues are orthogonal. Therefore, a unique ensemble of $\{\lambda_i, |\psi_i\rangle\}$ can be determined by ρ as a trivial application of the Spectral Theorem [17] if $\{\lambda_i > 0\}$ are distinct. The injectivity of this mapping is clear from (14). Thus we have

established a one-to-one mapping between ρ and the ensemble $\{\lambda_i, |\psi_i\rangle\}$ if $\{\lambda_i\}$ are distinct. \square

Assumption 1. In the rest of this section we assume the positive eigenvalues of the matrices are non-degenerate, that is, $\lambda_i \neq \lambda_j$ for $i \neq j$, and the eigenvectors $\{|\psi_i\rangle\}$ are normalized pure state vectors located on the unit sphere.

When a distance function d is given for these pure states, a standard discrete optimal transport problem can be formulated based on the ensemble representation. To be more precise, suppose the ensemble representation of two density matrices ρ_0 and ρ_1 are denoted by $\{\lambda_{0,i}, |\psi_{0,i}\rangle\}$ and $\{\lambda_{1,j}, |\psi_{1,j}\rangle\}$, respectively. The optimal transport distance can be defined as

$$\begin{aligned} \mathcal{T}(\rho_0, \rho_1) &= \min_{\{\gamma_{ij}\}} \sum_{i,j} \gamma_{ij} d(|\psi_{0,i}\rangle, |\psi_{1,j}\rangle), \\ \sum_j \gamma_{ij} &= \lambda_{0,i}, \quad \sum_i \gamma_{ij} = \lambda_{1,j}, \quad \gamma_{ij} \geq 0. \end{aligned} \quad (15)$$

Theorem 1. \mathcal{T} is a distance function on the space of density matrices.

Proof. According to the classical optimal transport theory, $\min_{\{\gamma_{ij}\}} \sum_{i,j} \gamma_{ij} d(|\psi_{0,i}\rangle, |\psi_{1,j}\rangle)$ is a distance function between the ensembles if d is a distance function. Therefore, $\mathcal{T}(\rho_0, \rho_1) = \mathcal{T}(\rho_1, \rho_0)$, $\mathcal{T}(\rho_0, \rho_1) + \mathcal{T}(\rho_1, \rho_2) \geq \mathcal{T}(\rho_0, \rho_2)$ and $\mathcal{T} \geq 0$ are automatically satisfied. According to Lemma 1, the mapping from the density matrix to its ensemble representation is injective, which implies that $\rho_0 = \rho_1$ if $\mathcal{T}(\rho_0, \rho_1) = 0$. Thus \mathcal{T} satisfies all three axioms on the space of density matrices. \square

Theorem 2. *The displacement interpolation is linear with respect to the density matrices for any distance function d .*

Proof. As explained above, the density matrices ρ_0 and ρ_1 are uniquely mapped to two classical discrete distributions, with $\{\lambda_{0,i}\}, \{\lambda_{1,j}\}$ being the probabilities and the corresponding pure states $\{|\psi_{0,i}\rangle\}, \{|\psi_{1,j}\rangle\}$ representing the locations of the distributed mass. By substituting the classical distributions into (10), we can write the interpolated state as $\rho_t = \sum_{i,j} \rho_{ij}(t)$, where each $\rho_{ij}(t)$ is written as

$$\rho_{ij}(t) = \gamma_{ij}^* [(1-t)|\psi_{0,i}\rangle\langle\psi_{0,i}| + t|\psi_{1,j}\rangle\langle\psi_{1,j}|]. \quad (16)$$

Here $\{\gamma_{ij}^*\}$ is the optimal transport plan, which means that the mass of γ_{ij}^* will be moved from the state $|\psi_{0,i}\rangle$ to $|\psi_{1,j}\rangle$ in the optimal plan. Note that we have used $T(|\psi_{0,i}\rangle) = |\psi_{1,j}\rangle$ for this particular path, which is always true irrespective of the concrete expression of T . Intuitively, $\rho_{ij}(t)$ is the mass being transported between the pure states $|\psi_{0,i}\rangle\langle\psi_{0,i}|$ and $|\psi_{1,j}\rangle\langle\psi_{1,j}|$ at time t . Since we always have

$$\sum_{i,j} \gamma_{ij}^* = \sum_i \lambda_{0,i} = 1, \quad (17)$$

according to the second line of (15), the interpolated states constitute a discrete probability measure on $i \times j$ points.

If the discrete probability measure is taken as an ensemble and mapped back to a mixed state ρ_t , we have

$$\begin{aligned}\rho_t &= \sum_{i,j} \rho_{ij}(t) \\ &= \sum_{i,j} \gamma_{ij}^* [(1-t)|\psi_{0,i}\rangle\langle\psi_{0,i}| + t|\psi_{1,j}\rangle\langle\psi_{1,j}|] \\ &= \sum_i (1-t)\lambda_{0,i}|\psi_{0,i}\rangle\langle\psi_{0,i}| + \sum_j t\lambda_{1,j}|\psi_{1,j}\rangle\langle\psi_{1,j}| \\ &= (1-t)\rho_0 + t\rho_1.\end{aligned}\quad (18)$$

That is, the displacement interpolation with respect to the density matrices is equivalent to linear interpolation. Note that the equality (18) holds for any distance function d . Moreover, it can be seen that (18) holds even if we replace the optimal transport map with any transport map in the definition of displacement interpolation. \square

Consider a quadratic cost between the pure states as

$$d(|\psi_{0,i}\rangle\langle\psi_{0,i}|, |\psi_{1,j}\rangle\langle\psi_{1,j}|) = |\hat{x}_{0,i} - \hat{x}_{1,j}|^2,$$

where \hat{x} is the real-valued generalized Bloch vector defined by [33]

$$\rho = \frac{1}{n} \left(I + \sqrt{\frac{n(n-1)}{2}} \hat{x} \cdot \hat{\sigma} \right), \quad (19)$$

with $\hat{\sigma}$ denoting the generalized Pauli matrices which constitute the basis of n -dimensional quantum systems. $\hat{x} \in \mathbb{R}^{n^2-1}$ is the coordinate of the density matrix. Pure states are located on the unit sphere and we have $|\hat{x}|^2 = 1$. By definition, the quadratic cost is the Euclidean distance between the coordinate vectors. According to (11), for each transportation path the following property holds

$$\begin{aligned}\mathcal{T}(\rho_{ij}(0), \rho_{ij}(t)) &= t^2 \gamma_{ij}^* |\hat{x}_{0,i} - \hat{x}_{1,j}|^2 \\ &= t^2 \mathcal{T}(\rho_{ij}(0), \rho_{ij}(1)).\end{aligned}\quad (20)$$

After summation we have

$$\mathcal{T}(\rho_0, \rho_t) = \sum_{i,j} t^2 \gamma_{ij}^* |\hat{x}_{0,i} - \hat{x}_{1,j}|^2 = t^2 \mathcal{T}(\rho_0, \rho_1), \quad (21)$$

which is consistent with the classical case. It is clear that in general

$$\mathcal{T}(\rho_0, \rho_t) \neq t^2 \mathcal{T}(\rho_0, \rho_1), \quad (22)$$

if we use other distance functions such as quantum fidelity.

According to Theorem 2, the resulting interpolation is linear irrespective of the definition of the distance function, while the underlying transport costs may be significantly different.

Moreover, linear interpolation could create artifacts which are undesirable in many applications [3, 9, 14–16].

4 | QUANTUM-INSPIRED INTERPOLATION VIA OPTIMAL CONTROL

For an individual system or a particle which is not an ensemble, the quantum operations act on the eigenvectors of the state at the same time, which means the transportation between the pure eigenstates cannot be individually addressed. In this case, the optimal transport is equivalent to finding an optimal map that continuously transforms the matrices. However, the feasibility of quantum dynamical map is constrained by admissible controls. To be more specific, the transformation between mixed states and pure states are difficult to realize via controls that are allowed by quantum mechanics. Open-loop coherent control, even with the aid of dissipative dynamics, cannot always guarantee the density matrix controllability. Pure state controllability is much more easier to realize in comparison. We have the following result for controlling a pure state.

Lemma 2. *The transformation between any pure states can be realized via a unitary operation.*

Proof. This lemma is a straightforward consequence of the elementary fact that two unit vectors are unitarily equivalent in the Hilbert space. Here we give a constructive proof. Since the pure state is a unit vector in the Hilbert space, it is always possible to construct an orthonormal basis with the pure state being its first basis vector. The rotation matrix U inducing the change of basis of a linear space is always unitary, and this U can transform the pure states as desired. \square

According to Lemma 2 and noting that unitary operation can be easily realized by open-loop coherent control, we propose a unified framework for solving the interpolation problem based on the purification of quantum states. Let \mathcal{H}_S be the Hilbert space on which the density matrix ρ is defined, and \mathcal{H}_E be a copy of \mathcal{H}_S . Fix an orthonormal basis of \mathcal{H}_E as $\{|e_i\rangle\}$. Using the decomposition (14), the purification of ρ on $\mathcal{H}_S \otimes \mathcal{H}_E$ is given by

$$|\psi_\rho\rangle = \sum_i \sqrt{\lambda_i} |\psi_i\rangle \otimes |e_i\rangle, \quad \lambda_i > 0, \quad (23)$$

where we sort the eigenvectors $\{|\psi_i\rangle\}$ in descending order such that $\lambda_i > \lambda_{i-1}$. This kind of sorting is used to ensure the uniqueness of the state purification, and additionally, any other kind of sorting would have the same effect. We have the following theorem for the interpolation of density matrices based on their purifications.

Theorem 3. *The map from ρ to $|\psi_\rho\rangle$ is injective. There always exists a unitary transformation U that transports $|\psi_{\rho_0}\rangle$ to $|\psi_{\rho_1}\rangle$ for arbitrary*

ρ_0 and ρ_1 , and the reduced quantum dynamics on the density matrix space is given by the following completely positive map

$$\rho_1 = \sum_{k,i} \lambda_i M_{ki} |\psi_i\rangle\langle\psi_i| M_{ki}^\dagger, \quad (24)$$

with

$$M_{ki} = \langle e_k | U | e_i \rangle. \quad (25)$$

The summation of $\{k\}$ is carried out on the entire basis.

Proof. Since ρ is the reduced state of $|\psi_\rho\rangle$, it is clear that $\rho_0 \neq \rho_1$ implies $|\psi_{\rho_0}\rangle \neq |\psi_{\rho_1}\rangle$. The existence of the unitary transformation U is guaranteed by Lemma 2. We have

$$\begin{aligned} \rho_1 &= \text{tr}_E(U|\psi_{\rho_0}\rangle\langle\psi_{\rho_0}|U^\dagger) \\ &= \sum_k \left\langle e_k \left| U \left(\sum_i \lambda_i |\psi_i\rangle\langle\psi_i| \otimes |e_i\rangle\langle e_i| \right) U^\dagger \right| e_k \right\rangle, \end{aligned} \quad (26)$$

which proves (24). \square

The Kraus operator M_{ki} induces the transformation of the eigenvector $|\psi_i\rangle$, which includes both the rotation and scaling of the vector. Thus we have established a one-to-one map between the unitary evolution in the extended space and the completely positive dynamics in the density matrix space. To make it more explicit, according to (24), the transformation

$$\Phi_i(\lambda_i |\psi_i\rangle\langle\psi_i|) = \sum_k M_{ki}(\lambda_i |\psi_i\rangle\langle\psi_i|) M_{ki}^\dagger, \quad (27)$$

on the i -th eigenvector of ρ_0 is induced by the unitary control U on the extended space. Since the transformation of all the eigenvectors are induced by the same U simultaneously, the changes in the orthogonal vectors are well decoupled. Optimal control can then be derived in the extended space, which corresponds to the optimal transport process in the density matrix space. The gradient ascent pulse engineering (GRAPE) algorithm [29] is a simple yet efficient algorithm for optimizing the control field in quantum state engineering problems. The control amplitudes $\{u_k(j)\}$, consisting of N steps of duration $1/N$ discretized over $[0,1]$, are iteratively optimized. The first-order gradients are calculated to indicate how each amplitude $u_k(j)$ should be modified in the next iteration to improve the cost function. Denote the corresponding unitary evolutions as $\{U_1, \dots, U_N\}$, and the unitary evolutions are generated by open-loop coherent control in the following form

$$H_j = \sum_k u_k(j) H_k, \quad j = 1, \dots, N, \quad u_k(j) \in \mathbb{R}. \quad (28)$$

The fidelity between the controlled state and the target state at $t = 1$ is measured by

$$\begin{aligned} \mathcal{F}(|\psi_{\rho_1}\rangle) &= |\langle\psi_{\rho_1}|\psi(1)\rangle|^2 = |\langle\psi_{\rho_1}|U_N \dots U_1|\psi_{\rho_0}\rangle|^2 \\ &= |\langle\psi_{\rho_1}|\exp(-i\Delta t H_N) \dots \exp(-i\Delta t H_1)|\psi_{\rho_0}\rangle|^2, \end{aligned} \quad (29)$$

where $\Delta t = 1/N$. In the basic GRAPE, the cost function is \mathcal{F} and the first-order gradients are simply calculated by $\partial \mathcal{F}(|\psi_{\rho_1}\rangle)/\partial u_k(j)$. Alternatively, the cost function for the optimal control of this paper is defined by

$$J = \mathcal{F}(|\psi_{\rho_1}\rangle) - \beta \sum_{j,k} u_k(j)^2, \quad (30)$$

which aims to minimize the amount of work needed for the transformation of the positive matrices via a quantum dynamical path. β is a penalization parameter. In analog to the basic GRAPE algorithm, the gradient of $\mathcal{F}(|\psi_{\rho_1}\rangle)$ to first order in Δt is given by

$$\frac{\partial \mathcal{F}(|\psi_{\rho_1}\rangle)}{\partial u_k(j)} = - \left\langle U_j^N | i\Delta t \left[H_k, U_j^1 \right] \right\rangle, \quad (31)$$

with

$$\begin{aligned} U_j^N &= U_{j+1}^\dagger \dots U_N^\dagger |\psi_{\rho_1}\rangle\langle\psi_{\rho_1}| U_N \dots U_{j+1}, \\ U_j^1 &= U_j \dots U_1 |\psi_{\rho_0}\rangle\langle\psi_{\rho_0}| U_1^\dagger \dots U_j^\dagger. \end{aligned} \quad (32)$$

The gradient update of the control $u_k(j)$ with respect to the cost function J is thus given by

$$\begin{aligned} u_{k+1}(j) &= u_k(j) - \epsilon \frac{\partial J}{\partial u_k(j)} \\ &= u_k(j) - \epsilon \left(\left\langle U_j^N | i\Delta t \left[H_k, U_j^1 \right] \right\rangle + 2\beta u_k(j) \right), \end{aligned} \quad (33)$$

where ϵ is the step size.

Therefore, if a suitable set of $\{H_k\}$ has been chosen to guarantee the controllability of the pure states on $\mathcal{H}_S \otimes \mathcal{H}_E$, the interpolation could be solved using the penalized GRAPE algorithm by simulating the controlled quantum dynamics on classical computers.

5 | EXAMPLES

In this section, we provide examples of quantum-inspired interpolations for the most useful cases of 2×2 and 3×3 positive matrices [3].

Example 1. Consider the optimal interpolation between the density matrices $\rho_0 = |0\rangle\langle 0|$ and $\rho_1 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$ of a two-level quantum system (qubit). Note that the optimal cost for transforming between the quantum states could be considered as a distance function with operational meaning. Since ρ_0 is a pure state and ρ_1 is a mixed state, the transformation between ρ_0 and ρ_1 cannot be directly realized via unitary control on the qubit. Instead, we consider the optimal coherent control between the purifications of ρ_0 and ρ_1 , which are given by

$$\begin{aligned} |\psi_{\rho_0}\rangle &= |0\rangle \otimes |0\rangle, \\ |\psi_{\rho_1}\rangle &= \frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |1\rangle, \end{aligned} \quad (34)$$

whose density matrices can be written as

$$\begin{aligned} |\psi_{\rho_0}\rangle\langle\psi_{\rho_0}| &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \\ |\psi_{\rho_1}\rangle\langle\psi_{\rho_1}| &= \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix}. \end{aligned} \quad (35)$$

To ensure the pure state controllability of the extended two-qubit system, the control Hamiltonian are chosen as $H_1 := \sigma_{\tilde{x}} \otimes \sigma_{\tilde{x}}$, $H_2 := \sigma_x \otimes I_0$, $H_3 := I_0 \otimes \sigma_x$, $H_4 := \sigma_x \otimes \sigma_x$, $H_5 := \sigma_y \otimes I_0$, $H_6 := I_0 \otimes \sigma_y$, $H_7 := \sigma_y \otimes \sigma_y$, $H_8 := \sigma_{\tilde{x}} \otimes I_0$, $H_9 := I_0 \otimes \sigma_{\tilde{x}}$, where σ_x, σ_y and $\sigma_{\tilde{x}}$ are Pauli matrices [17, 34]. We let $\Delta t = 0.001$ and $\epsilon = 0.05$. The fidelities for different values of penalization parameter β are shown in Figure 2, in which the fidelities are calculated by (29). It is clear that the evolution of fidelity becomes more unstable when the control cost is not optimized ($\beta = 0$). The effects of optimizing control cost for interpolation are visualized in Figures 3 and 4, where the evolution of the reduced state is characterized using its Bloch vector representations. As shown in Figure 3b, the interpolation path is far from smooth when approaching the target state if no constraint on the control cost is imposed, which is consistent with the unstable evolution of fidelity observed in Figure 2. The interpolation becomes smoother with $\beta > 0$, for example, see Figure 4. If we continue to increase β , the interpolation path would look like a straight line that connects the initial state and the target state, which however, is at the cost of control precision.

Example 2. The diffusion tensors are given by 3×3 positive matrices in the analysis of diffusion tensor magnetic resonance images [9], in which the interpolation of tensors is vital for fiber tracking, registration and spatial normalization of the diffusion tensor images. Here we consider an example from [3], for

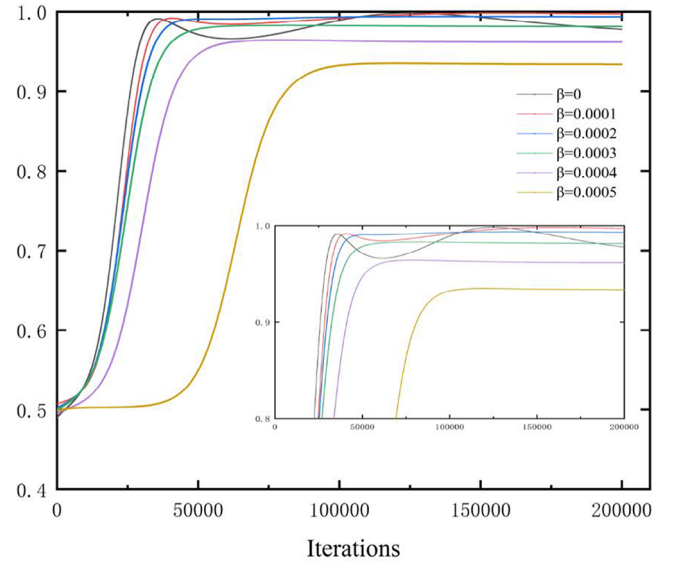


FIGURE 2 The evolution of fidelities between ρ_0 and ρ_1 under the coherent control.

which we can apply the quantum-inspired interpolation method to compute the Scaling-Rotation curves that transform the diffusion tensor matrix $X := \text{diag}(15, 2, 1)$ to a tensor matrix Y with different principal axes. First, the matrices have to be normalized to density matrices, and the normalized X and Y are written as

$$\begin{aligned} \rho_0 &= \begin{bmatrix} \frac{15}{18} & 0 & 0 \\ 0 & \frac{2}{18} & 0 \\ 0 & 0 & \frac{1}{18} \end{bmatrix}, \\ \rho_1 &= \begin{bmatrix} 0.1764 & -0.2220 & 0.2775 \\ -0.2220 & 0.3333 & -0.3924 \\ 0.2775 & -0.3924 & 0.4903 \end{bmatrix}. \end{aligned}$$

It is easy to verify that ρ_0 and ρ_1 both are mixed states. The purification of ρ_0 and ρ_1 are given by 9×9 matrices. Since the generalized Pauli matrices for 3×3 case are

$$\begin{aligned} \sigma_1 &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \sigma_2 &= \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\ \sigma_3 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \sigma_4 &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \\ \sigma_5 &= \begin{bmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, & \sigma_6 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \end{aligned}$$

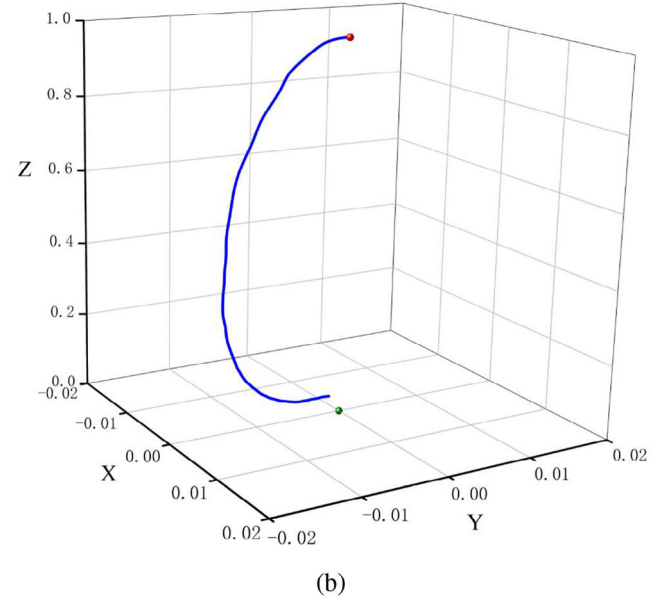
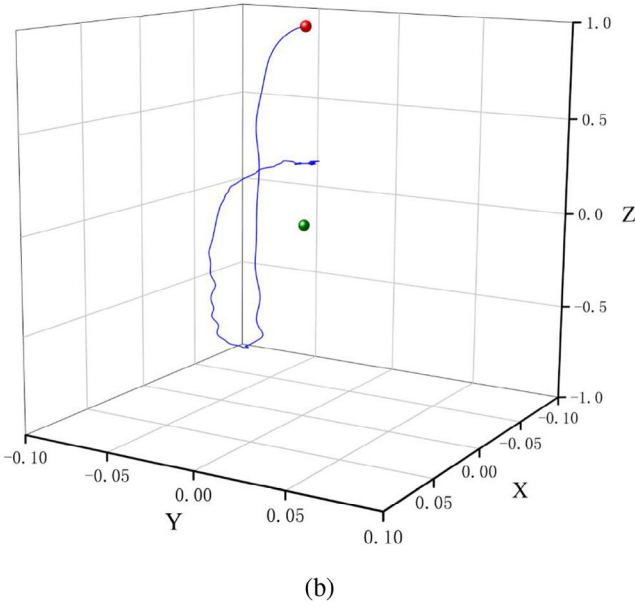
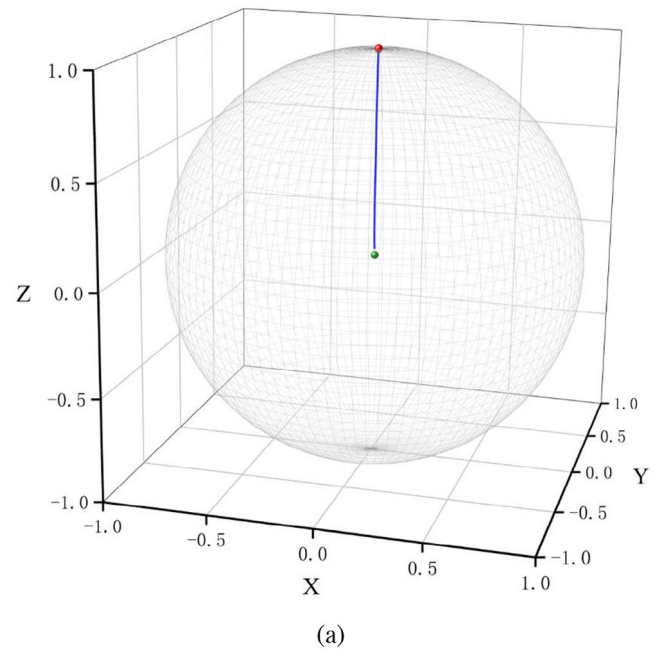
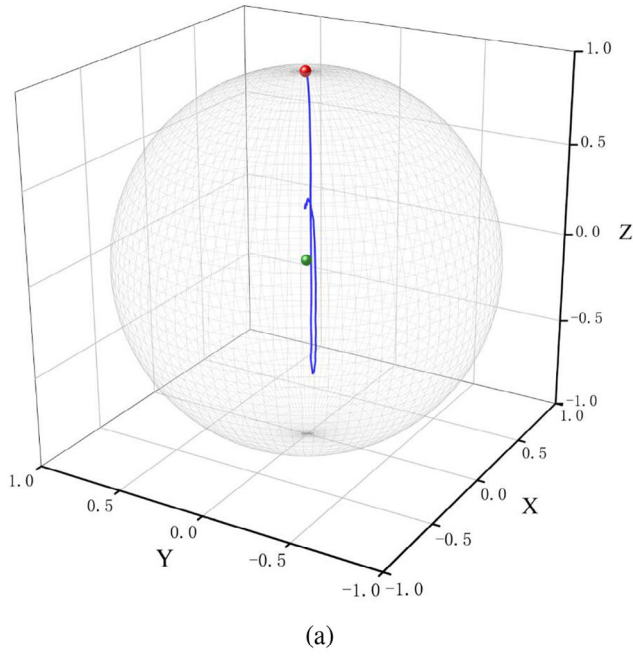


FIGURE 3 Interpolation between ρ_0 and ρ_1 with $\beta = 0$. (a) depicts the evolution of the state on the Bloch Sphere, and (b) is the locally enlarged view of the same trajectory. The red point is the Bloch vector representation of the initial state ρ_0 , and the green point is the Bloch vector representation of the target state ρ_1 . The blue line passes through the interpolating states.

$$\sigma_7 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad \sigma_8 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix},$$

the control Hamiltonians for the optimal interpolation in the extended space are chosen as $H_1 := \sigma_1 \otimes I_0$, $H_2 := I_0 \otimes \sigma_1$, $H_3 := \sigma_2 \otimes I_0$, $H_4 := I_0 \otimes \sigma_2$, $H_5 := \sigma_3 \otimes I_0$, $H_6 := I_0 \otimes \sigma_3$, $H_7 := \sigma_4 \otimes I_0$, $H_8 := I_0 \otimes \sigma_4$, $H_9 := \sigma_5 \otimes I_0$,

FIGURE 4 Interpolation between ρ_0 and ρ_1 with $\beta = 0.0002$. (a) depicts the evolution of the state on the Bloch Sphere, and (b) is the locally enlarged view of the same trajectory.

$H_{10} := I_0 \otimes \sigma_5$, $H_{11} := \sigma_6 \otimes I_0$, $H_{12} := I_0 \otimes \sigma_6$, $H_{13} := \sigma_7 \otimes I_0$, $H_{14} := I_0 \otimes \sigma_7$, $H_{15} := \sigma_8 \otimes I_0$, $H_{16} := I_0 \otimes \sigma_8$ and $H_{17} := I_0 \otimes I_0$. The optimization problem is solved by the penalized GRAPE algorithm. The optimal unitary path that connects the purified states in the extended space induces the simultaneous rotation and scaling of the orthogonal eigenvectors of the 3×3 matrix in the reduced subspace, which essentially decouples the changes in the orthogonal diffusion orientations to achieve a shape-preserving interpolation. Figure 5 shows the continuous rotation of the three initial eigenvectors in the subspace with $\beta = 0.0001$.

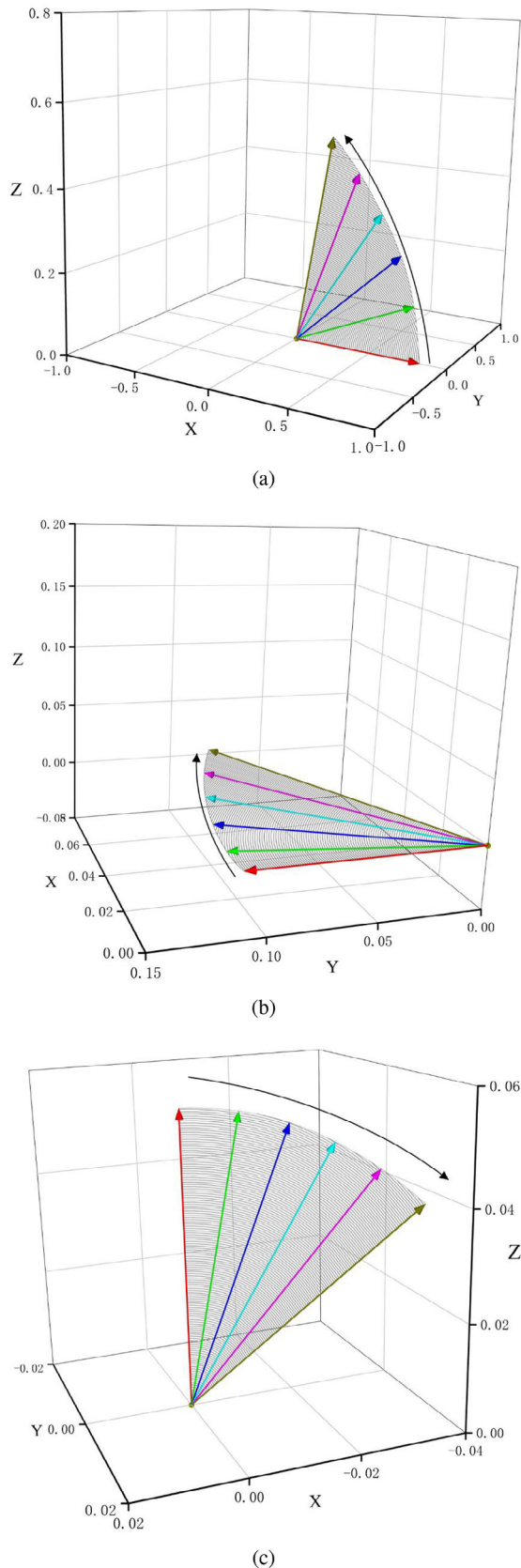


FIGURE 5 The rotation of three eigenvectors for the 3×3 positive matrix in the process of optimal interpolation with $\beta = 0.0001$. (a)–(c) depicts the evolution of the individual eigenvectors from $t = 0$ to $t = 1$ with a fixed time interval. The eigenvectors are normalized to have the same length.

6 | CONCLUSION

Here, we have proposed a quantum-inspired interpolation method for positive matrices. The positive matrices are normalized and purified to quantum states on an extended space, whose controllability can be easily guaranteed using unitary control. As a result, it is always possible to find an optimal control that induces the state transfer. In other words, the interpolation always exists under this framework. The optimal unitary control rotates the eigenvectors of the pure states in the extended space at the same time. Meanwhile, the trajectory is projected onto the subspace of positive matrices, generating a continuous completely positive map for interpolation. Since the rotation of the eigenvectors in the extended space is simultaneous and decoupled, the underlying transformation of the eigenvectors of the positive matrix in the subspace is also decoupled. The resulting interpolation is shape-preserving which could be used to reduce artifacts in many important applications of tensor field processing such as fiber tracking in medical imaging. Future work will focus on employing fast and robust quantum optimal control algorithms to further improve the performance of the interpolation problem.

AUTHOR CONTRIBUTIONS

Chen Jiang: Formal analysis; investigation; validation; visualization; writing—original draft; writing—review and editing. **Yu Pan:** Conceptualization; formal analysis; funding acquisition; investigation; methodology; project administration; resources; supervision; writing—original draft; writing—review and editing. **Yi Yang:** Investigation; methodology. **Daoyi Dong:** Funding acquisition; supervision; writing—review and editing.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflicts of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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