

Regularization and Interpolation of Positive Matrices

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Abstract—We construct certain matricial analogues of mass transport for positive-definite matrices of equal trace. The framework aims to devise ways of interpolating positive-definite matrices that tradeoff between “aligning up their eigenstructure” and “scaling the corresponding eigenvalues.” Motivation for the work is provided by power spectral analysis of multivariate time series where linear interpolation between matrix-valued power spectra generates push-pop unrealistic and undesirable artifacts.

Index Terms—Multivariate interpolation, optimal transport, signal processing, time series analysis.

I. INTRODUCTION

This paper is an attempt to develop a suitable matricial analogue of optimal mass transport (OMT). The basic problem of OMT refers to seeking a transportation plan that carries a given probability distribution to another so that a suitably defined transportation cost is minimized [1]–[3]. The original formulation of the problem by Monge in 1871 was motivated by civil engineering considerations, namely to transport dirt so as to level the ground. The mathematical problem achieved significant fame and notoriety due to inherent technical difficulties, which persisted until the 1940s when Kantorovich presented a relaxation of OMT in the form of a linear program. The relevance of this circle of ideas in the broader setting of resource allocation was already widely recognized and the impact secured a Nobel prize in economics for Kantorovich in 1975. A new transformative phase of development in OMT began in the 1990s [4]–[7] motivated by multitude

of applications in physics, probability theory, image analysis, optimal control, etc. In these, OMT was seen as an optimal control problem and stochastic formulations ensued (see [8]–[10] and the references therein). The work presented herein is motivated by Ning *et al.* [11] where a matrix-valued formulation of OMT was introduced to address certain issues in spectral analysis of multivariable time series and system identification. More specifically, recall that the spectral content of scalar (slowly time varying) time series is often displayed in the form of a spectrogram (time–frequency power distribution). The spectrogram illuminates any time drift of the spectral content, but suffers from the perennial tradeoff between variability and resolution (also known as the uncertainty principle of Fourier methods). Traditionally, windowing, kernel methods, and several other techniques have been used to enhance spectrograms. An alternative approach, highlighted in [12], is to interpolate spectral estimates in a suitable metric so as to track changes in the underlying spectral content in a natural manner. Further, in [13], the authors have argued that OMT induces the appropriate topology (Wasserstein metric) where small perturbations correspond to small changes in estimated moments and vice versa. However, there has been no matrix-valued analogue of the Wasserstein metric. The work in [11] was perhaps the first attempt and had its basis in Kantorovich’s idea of seeking a joint density (matrix valued in our case) in a suitable product space, necessitating a prohibitively high computational burden. In this paper, we explore alternative ideas that are rooted in control. More specifically, we seek a dynamical evolution that allows rotation of eigenvectors as well as scales the corresponding eigenvalues so as to generate a path between end-point matrices. Accordingly, the choice of parameters (affecting cost) in an optimization problem promotes rotation or scaling.

Being inspired by the close connection between the heat equation, the Schrödinger equation and the scalar version of OMT, [2], [3], we formulate our problem based on some concepts in quantum mechanics. More specifically, probability density functions are exchanged for *density matrices* ρ , i.e., positive-semidefinite Hermitian matrices with unit trace. Transport is then seen as a flow in the space of such matrices that minimizes a suitable cost functional.

The insight and techniques gained are aimed toward interpolating or regularizing sample covariances as well as matrix-valued power spectral densities of multivariate time series—they both reflect on how power varies with direction. More specifically, when dynamics that impact a vectorial process are slowly varying, it is of interest to track changes by interpolating input–output short-window spectral estimates in a nonparametric manner, e.g., tracking frequencies of resonances in the spectral content along with a corresponding direction that couples specific entries. The ability to do so in a natural manner is even more enabling in array processing, where changes in spectral content of a matrix-valued spectrogram may be directly attributed to a moving scatterer. In particular, OMT-based interpolation prevents push-pop artifacts as compared to linear interpolation (e.g., see [13] for scalar processes).

In this paper, we focus on interpolation of matrices. We see this as the first step toward the development of more general transport be-

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tween matrix-valued distributions (i.e., allowing for a spatial/frequency component). More specifically, at present, we focus on interpolating positive-definite matrices in ways that allow controlling the correspondence between their eigenstructures. To this end, we decompose the tangent space of the cones of positive-definite matrices into two subspaces, one that corresponds to rotating the eigenstructure and another that corresponds to scaling eigenvalues. In this way, by controlling these two complementing directions, we construct interpolating flows that have desired properties. Insights into setting up the problem are drawn from quantum mechanics where the principle object of study is the time evolution of noncommutative operators (i.e., of matrices, when restricted to finite dimensions). Thus, in order to make the paper self-contained, we include a brief exposition of certain basic facts from quantum mechanics upon which we draw insights for the needed analysis.

This paper is structured as follows. In Section II, we present certain basic ideas of quantum mechanics that relate to material used in this paper. In Section III, we consider the tangent space of the cone of positive-definite matrices. This leads to the material in Section IV on suitable cost functionals that promote a judicious balance between rotating the eigenstructure and scaling the eigenvalues. In Sections V and VI, numerical examples are discussed and in Section VII concluding remarks are provided.

Notation: We denote by $\mathbb{H}$ the set of $n \times n$ Hermitian matrices, $\mathbb{S}$ the set of $n \times n$ skew-Hermitian matrices, and $\mathbb{H}_+$ the cones of positive-semidefinite matrices. Since matrices are $n \times n$ throughout this paper, we will not explicitly note dependence on n . The commutator of two square matrices A and B is denoted by $[A, B] := AB - BA$.

II. QUANTUM INSIGHTS

The development draws on concepts from quantum mechanics and, therefore, we begin with a brief account of basics (see standard references, e.g., [15], for more).

A. Schrödinger Equation

The evolution of closed quantum systems, i.e., one having no interaction with other quantum systems or a heat bath, is given by the following *time-dependent Schrödinger equation* [15]:

$$\frac{\partial \psi}{\partial t} = X\psi \quad (1)$$

where $\psi \in \mathbb{C}^n$ and X is a skew-Hermitian matrix.¹ Equation (1) describes a unitary evolution for the wave function, in our case, vector ψ ; the quantum system is in a “pure state” in that the density matrix $\rho = \psi\psi^*$ has rank 1. A system is in a mixed state when the density matrix

$$\rho = \sum_k \lambda_k \psi_k \psi_k^*$$

with $\sum_k \lambda_k = 1$, has rank higher than 1. Either way, the density matrix evolves according to

$$\frac{\partial \rho}{\partial t} = X\rho - \rho X =: [X, \rho] \quad (2)$$

where the derivative is thought of entry-wise. It is evident that if the system is in a pure state, it remains so, as the rank of

$$\rho(t) = e^{Xt} \psi(0) \psi(0)^* e^{-Xt}$$

¹More generally, ψ belongs to a Hilbert space and accordingly X is a skew-Hermitian operator on that same Hilbert space. Typically X is expressed as $-\frac{i}{\hbar}H$ where H is a Hamiltonian (Hermitian) operator and $\hbar$ is the reduced Planck constant.

remains invariant. Likewise, if the system is in a mixed state

$$\begin{aligned} \rho(t) &= \sum_k \lambda_k(t) \psi_k(t) \psi_k^*(t) \\ &= e^{Xt} \left(\sum_k \lambda_k(t) \psi_k(0) \psi_k(0)^* \right) e^{-Xt} \end{aligned}$$

the eigenvalues $\lambda_k(t)$ of the density matrix remain invariant over time t , i.e., $\lambda_k(t) = \lambda_k(0)$ for all t . Thus, the evolution governed by (2) rotates in the same way the complete set of eigenvectors of the density matrix without changing the corresponding eigenvalues.

B. Evolution of Density Matrices

Decoherence and changes in the spectrum of ρ are typically modeled through coupling with an *ancilla*, which is another quantum system. The state of the original system is then obtained by *tracing out* the ancillary component of the joint density operator. *Lindblad's equation*, [16], [17], describes precisely such an evolution for the component of the original system. The Lindblad equation has the form

$$\frac{\partial \rho}{\partial t} = [X, \rho] - \sum_k \left(\frac{1}{2} (Y_k \rho + \rho Y_k^*) - Z_k \rho Z_k^* \right)$$

where $Y_k = Z_k^* Z_k$. The presence of $-Z \rho Z^*$ ensures that $\text{trace}(\rho)$ remains constant, whereas both the eigenvalues and the eigenstructure may change over time. Alternatively, one may consider more generally

$$\frac{\partial \rho}{\partial t} = [X, \rho] + u \quad (3)$$

where $\text{trace}(u) = 0$ so as to preserve the trace of ρ . In fact, additionally, we will do exactly that and consider flows in directions corresponding to traceless component u . Positivity of the flow will be ensured as an added (convex) condition and will not be intrinsically encoded in u (as in the Lindblad equation where the right-hand side is linear in ρ).

III. TRACE-PRESERVING LINEAR FLOW ON POSITIVE MATRICES

Consider the set of positive-semidefinite matrices that are normalized to have trace one

$$\mathcal{D} := \{\rho \in \mathbb{H}_+ \mid \text{trace}(\rho) = 1\}.$$

As we noted earlier, we seek flows on $\mathcal{D}$ that preserve trace. The tangent space of $\mathcal{D}$ at any $\rho \in \mathcal{D}$ is

$$T_\rho = \{u \mid u \in \mathbb{H}, \text{trace}(u) = 0\}.$$

In this, the subspace of traceless Hermitian components²

$$R_\rho := \{[X, \rho] \mid X \in \mathbb{S}\}$$

is responsible for rotating the eigensubspaces of ρ as we have noted in the previous section.

We now seek to identify the orthogonal complement of R_ρ so as to isolate the two directions that are responsible for rotation of eigenvectors and scaling of eigenvalues.³ To this end, consider $u \in \mathbb{H}$ such that

$$\text{trace}(u[X, \rho]) = 0 \quad \forall X \in \mathbb{S}. \quad (4)$$

Since the trace is invariant under cyclic permutations,

$$\text{trace}([u, \rho]X) = 0 \quad \forall X \in \mathbb{S}. \quad (5)$$

²If $X \in \mathbb{S}$ and $\rho \in \mathbb{H}$, both $[X, \rho]^* = [X, \rho] \in \mathbb{H}$ and $\text{trace}([X, \rho]) = 0$.

³The inner product of two matrices is $\langle u, v \rangle = \text{trace}(u^*v)$

But $[u, \rho]$ is already in $\mathbb{S}$, hence it is zero, and therefore u must commute with ρ . Thus, from (4) we have that u is in the orthogonal complement of R_ρ . We summarize our conclusion as follows.

Proposition 1: The tangent space T_ρ of $\mathcal{D} := \{\rho \in \mathbb{H}_+ \mid \text{trace}(\rho) = 1\}$ at $\rho \in \mathcal{D}$ can be decomposed as the direct sum

$$T_\rho = R_\rho \oplus C_\rho$$

of orthogonal components

$$R_\rho = \{[X, \rho] \mid X \in \mathbb{S}\} \text{ and}$$

$$C_\rho = \{u \mid u \in \mathbb{H}, [u, \rho] = 0, \text{ and } \text{trace}(u) = 0\}.$$

If $X(t) \in \mathbb{S}$ and $u(t) \in C_{\rho(t)}$ for all t , then $\text{trace}(\rho(t))$ remains constant with t .

IV. INTERPOLATING FLOWS BETWEEN ρ_0 AND ρ_1

Following on the previous rationale, we may seek paths between density matrices ρ_0 and ρ_1 , that minimize a suitable cost functional that allows trading off between the eigenstructure rotation specified by $X(t) \in \mathbb{S}$ and the eigenvalue scaling affected by $u(t) \in \mathbb{H}$. Assuming a constant rate of rotation and a constant “drift” of the spectrum, we formulate the following problem:

Problem 1: Minimize $\|X\|_2 + \epsilon\|Z\|_2$ subject to

$$\dot{\rho}(t) = [X, \rho(t)] + \underbrace{e^{Xt} Z e^{-Xt}}_{u(t)} \quad (6)$$

for $\rho(0) = \rho_0, \rho(1) = \rho_1$, along with $X \in \mathbb{S}, Z \in \mathbb{H}, [\rho_0, Z] = 0$, and $\text{trace}(Z) = 0$.

In the above-mentioned equation, the parameter $\epsilon \in [0, \infty)$ represents a weight that helps trading off the two alternative mechanisms for shifting eigenvalues and eigensubspaces to match the two end-point matrices. In general, “rotation” and “scaling” may vary over time, whereas in the case of (6) where the drift is constant, the solution has the explicit form $\rho(t) = e^{Xt}(\rho_0 + Zt)e^{-Xt}$.

In the setting of Problem 1, we readily verify that $u(t)$ commutes with $\rho(t)$ as long as Z commutes with ρ_0 . Thence, it can be seen that in fact, Problem 1 is equivalent to

$$\text{minimize } \|X\|_2 + \epsilon\|e^{-X} \rho_1 e^X - \rho_0\|_2 \quad (7a)$$

$$\text{subject to } X + X^* = 0 \text{ and } [\rho_0, e^{-X} \rho_1 e^X - \rho_0] = 0. \quad (7b)$$

This is a constrained nonconvex optimization problem that we approach, numerically, using `fmincon` in MATLAB. This utilizes an interior point method with computational complexity of order $O(n^3)$ at each iteration.

V. EXAMPLE: INTERPOLATION OF DENSITY MATRICES

In this section, we highlight how interpolation is effected, via solving Problem 1, as a proof of concept. Starting from two end-point density matrices, the framework allows constructing alternative paths connecting the two where one may tradeoff the two possible ways that the transition from one to the other may take place, i.e., allowing for the eigenvalues to adjust by “scaling” and the eigenvectors to “rotate,” respectively.⁴

⁴The examples we present involve matrices of sizes 2×2 and 3×3 . This is solely because we cannot display in a suggestive manner results in higher dimensions. The computational burden in higher dimensions scales reasonably well (interpolating 20×20 matrices requires of the order of 200 s using general purpose solvers on a laptop with Intel Core i7).

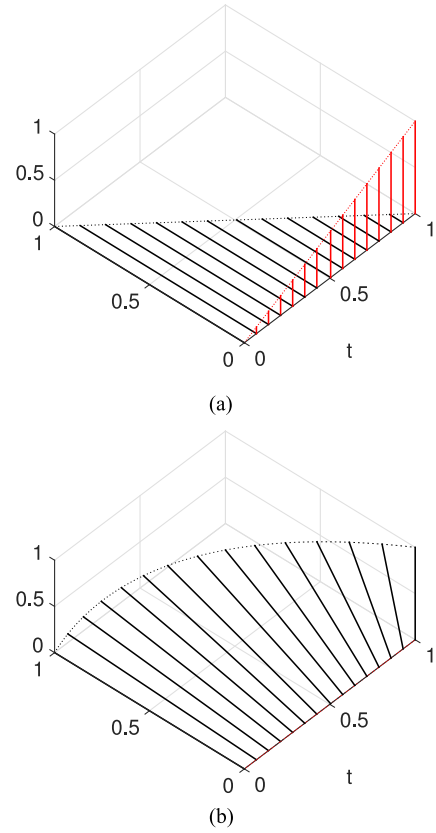


Fig. 1. Solutions are obtained by solving Problem 1: for illustration, eigenvectors, shown as line segments that vary with t , are scaled in proportion to corresponding eigenvalues. (a) shows a push-pop effect where eigenvalues are rescaled (hence two eigenvectors are shown, one increasing and the other decreasing in length as a function of t), whereas (b) indicates a correspondence through rotation of the eigenstructure along a path of rank-1 matrices (hence only one eigenvector is shown, and this rotates with t).

Example 1: Consider the two density matrices

$$\rho_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \text{ and } \rho_1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

On one end, a choice of ϵ (vanishingly small) in Problem 1 leads to a path that displays a fade-in/fade-out effect of scaling the eigenvalues, so as to connect the two end points [see Fig. 1 (a)]. No rotation of eigenvectors takes place. On the other end, for large ϵ (e.g., $\epsilon = 10$), we obtain a path where “rotation” of the eigenvectors is less costly [see Fig. 1(b)]; it is worth noting that in this case, since both matrices have rank 1, the path remains rank 1.

Motivation for our framework stems from multivariable time series analysis where power is often associated (e.g., in sensor arrays or radar) with the position of dominant scatterers. Fade-in–fade-out effects when interpolating or smoothing multivariable spectra are obviously undesirable as they create artifacts. Such fade-in–fade-out effects may be erroneously interpreted as due to the presence of additional scatterers beyond those that are present. The above-mentioned rudimentary example may correspond to the case of two sensors reading a constant frequency echo from a scatterer that changes its relative position with respect to the two. When recorded signals are correlated, the matrix-valued power spectrum at the corresponding frequency has (approximately) rank 1. Likewise, movement of the scatterer that corresponds to a path between the two matrices, ought to have rank 1 [as in Fig. 1(b)].

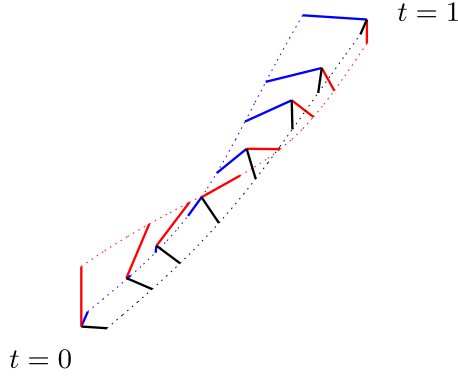


Fig. 2. Solutions are obtained by solving Problem 1: for illustration, eigenvectors (shown as colored line segments) are scaled in proportion to corresponding eigenvalues. It is seen how eigenstructure rotates while eigenvalues scale.

This exemplifies the need for paths that avoid push-pop for the corresponding eigenvalues (as linear interpolation would—one eigenvalue reducing while another increasing at the same time).

Example 2: In this example, we highlight a situation with matrices of higher dimension (three in this case). Fig. 2 shows a path between two matrices as follows:

$$\rho_0 = \begin{bmatrix} 0.2 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0.5 \end{bmatrix} \text{ and } \rho_1 = \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 0.3 & 0 \\ 0 & 0 & 0.2 \end{bmatrix}.$$

The solution to (7) with $\epsilon = 10$ is $\rho(t) = e^{Xt}(\rho_0 + Zt)e^{-Xt}$ with

$$X = \begin{bmatrix} 0 & 0 & 2.2 \\ 0 & 0 & 2.2 \\ -2.2 & -2.2 & 0 \end{bmatrix} \text{ and } Z = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 0.2 & 0 \\ 0 & 0 & -0.3 \end{bmatrix}.$$

In this case, we see that both rotation and scaling take place simultaneously.

VI. EXAMPLE: REGULARIZATION OF NOISY PATHS

Besides interpolation problems, i.e., finding a path for $\rho(t)$ connecting two density matrices ρ_0 and ρ_1 , the approach allows solving regularization problems where a smooth path is constructed to smooth out noisy measurements. More specifically, given a noisy data set

$$\{\tilde{\rho}(t_i) \mid 0 \leq t_1 \leq \dots \leq t_N \leq 1, \}$$

we seek a smooth path $\rho(t)$ that approximately fits the data in a suitable sense. The key is to parameterize the path in a way consistent with the two “orthogonal” actions of rotating eigenvectors and scaling eigenvalues (as both may be needed), and penalize one more (typically, scaling). To this end, we propose the following:

Problem 2: Minimize, over choice of ρ_0 , X , and Z

$$\sum_{i=1}^N \|e^{Xt_i}(\rho_0 + Zt_i)e^{-Xt_i} - \tilde{\rho}(t_i)\|_2$$

subject to $X \in \mathbb{S}$, $Z \in \mathbb{H}$, $\rho(\cdot) \geq 0$, $[\rho_0, Z] = 0$, and $\text{trace}(Z) = 0$.

The outcome is shown in Fig. 3. For illustration purposes, the data set $\tilde{\rho}(t_i)$ is generated by adding a symmetric matrix-valued (uniform) noise $w(t)$ to a nominal flow $e^{Xt}\rho_0e^{-Xt}$ for $t_i \in \{0.05, 0.1, 0.15, \dots, 1\}$

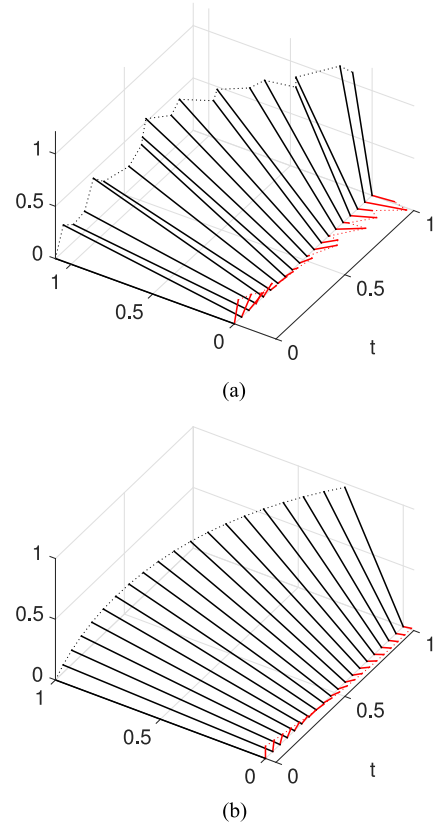


Fig. 3. Regularization of noisy matrixial data with eigenvectors scaled according to corresponding eigenvalues. (a) Data: noisy matrices $\tilde{\rho}(t_i)$. (b) Regularized path $\rho(t_i)$.

where

$$\rho_0 = \begin{bmatrix} 1.0 & 0 \\ 0 & 0.1 \end{bmatrix} \text{ and } X = \begin{bmatrix} 0 & -1.6 \\ 1.6 & 0 \end{bmatrix}.$$

VII. CONCLUDING REMARKS

We propose an approach to constructing flows on density matrices. This is intended for interpolation and regularization of sample covariances and power spectra of multivariable time series. The general approach is control theoretic in that we select the flow (tangent direction) that minimizes a suitable cost functional. The choice of functional allows trading off the two basic mechanisms (rotating eigenvectors versus scaling eigenvalues). Judicious balance between aligning up the eigenstructure and scaling the eigenvalues is necessitated by the fact that one of the two mechanisms alone may not suffice in generic situations. The choice of the parameter ϵ that dictates the respective tradeoff must be based on the application and priors on the problem. In closing, we refer the interested reader to [14] for a parallel alternative formulation of matrixial OMT, which also draws on the connection with quantum mechanics, but along a different angle altogether.

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