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Optimal steering to invariant distributions for networks flows

Yongxin Chen, Member, IEEE, Tryphon T. Georgiou, Fellow, IEEE, and Michele Pavon

Abstract—We derive novel results on the ergodic theory of irreducible, aperiodic Markov chains. We show how to optimally steer the network flow to a stationary distribution over a finite or infinite time horizon. Optimality is with respect to an entropic distance between distributions on feasible paths. When the prior is reversible, it shown that solutions to this discrete time and space steering problem are reversible as well. A notion of temperature is defined for Boltzmann distributions on networks, and problems analogous to cooling (in this case, for evolutions in discrete space and time) are discussed.

Index Terms—Controlled Markov chain, Schrödinger Bridge, Reversibility, Regularized Optimal Mass Transport

1 Introduction

We consider an optimal steering problem for networks flows over a finite or infinite time horizon. Specifically, we derive discrete counterparts of our *cooling* results in [5]. The goal is to steer the Markovian evolution to a steady state with desirable properties while minimizing relative entropy, or relative entropy rate, over admissible distributions on paths. This relates to a special Markov Decision Process problem, cf. [9, Section 6] which is referred to as *Schrödinger's Bridge Problem* (SBP) or *regularized optimal mass transport* (OMT). A rich history on this circle of ideas originates from two remarkable papers by Erwin Schrödinger in 1931/32 [31], [32] who was interested in a large deviation problem for a cloud of Brownian particles, and of earlier work by Gaspar Monge in 1781 on the problem of optimally transporting mass between sites [27].

Important contributions on the existence question in SBP, left open by Schrödinger, were provided over time by Fortet, Beurling, Jamison and Föllmer [2], [19], [20], [22]. It should be remarked that Fortet's proof in 1940 is algorithmic, establishing convergence of a (rather complex) iterative scheme. This predates by more than twenty years the contribution of Sinkhorn [34] who established convergence in a special case of the discrete problem The latter proof is much simpler than in the continuous (time and space) problem solved by Fortet. Thus, these algorithms should be called Fortet-IPF-Sinkhorn, where IPF stands for the Iterative Proportional Fitting algorithm proposed in 1940 without proof of convergence in [16]. These problems admit a "static" and a "dynamic" formulation. While the static, discrete space problem was studied by many, starting from Sinkhorn, see [14], [29] and references therein, the dynamic, discrete problem was considered in [11], [12], [13], [21], [28]. We provide in this paper a new fluid-dynamic derivation of the Schrödinger system on which the iteration is based. Convergence of the iterative scheme in a suitable projective

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This topic lies nowadays at the crossroads of many fields of science such as probability, statistical physics, optimal mass transport, machine learning, computer graphics, statistics, stochastic control, image processing, etc. Several survey papers have appeared over time emphasizing different aspects of the subject, see [8], [9], [10], [23], [29], [37].

The paper is outlined as follows. In Section 2, we present background on the discrete-time and space Schrödinger bridge problem while emphasizing its "fluid dynamic" formulation (the original proof of a key well-known result is deferred to the Appendix). In Section 3, we introduce the corresponding infinite-horizon steering problem by minimizing the entropy rate with respect to the prior measure. We then discuss existence for the one-step Schrödinger system leading to existence for the steering problem. Section 4 is devoted to an interesting result linking optimality in the steering problem to reversibility of the solution. The final Section 5 applies all the previous results to cooling, where the goal is to optimally steer the Markov chain to a steady state corresponding to a lower *effective* temperature.

2 DISCRETE-TIME DYNAMIC BRIDGES: BACK-GROUND

We begin by discussing a paradigm of great significance in network flows. It amounts to designing probabilistic transitions between nodes, and thereby probability laws on path spaces, so as to reconcile marginal distributions with priors that reflect on the structure of the network and objectives on transferance of resourses across the network. The basic formulation we discuss amounts to the so called Schrödinger bridge problem in discrete-time. This dynamic formulation echoes the fluid dynamic formulation of the classical (continuous time and space) Schrödinger bridge problem. Certain proofs that we present are mildly new.

We consider a directed, strongly connected, aperiodic graph $\mathbf{G} = (\mathcal{X}, \mathcal{E})$ with vertex set $\mathcal{X} = \{1, 2, \dots, n\}$ and edge set $\mathcal{E} \subseteq \mathcal{X} \times \mathcal{X}$, and we consider trajectories/paths on this graph over the time set $\mathcal{T} = \{0, 1, \dots, N\}$. The family of

feasible paths $x=(x_0,\ldots,x_N)$ of length N, namely paths such that $x_ix_{i+1}\in\mathcal{E}$ for $i=0,1,\ldots,N-1$, is denoted by $\mathcal{F}P_0^N\subseteq\mathcal{X}^{N+1}$. We seek a probability distribution \mathfrak{P} on the space of paths $\mathcal{F}\mathcal{P}_0^N$ with prescribed initial and final marginals $\nu_0(\cdot)$ and $\nu_N(\cdot)$, respectively, and such that the resulting random evolution is closest to a "prior" measure \mathfrak{M} on $\mathcal{F}\mathcal{P}_0^N$ in a suitable sense.

The prior law for our problem is a Markovian evolution

$$\mu_{t+1}(x_{t+1}) = \sum_{x_t \in \mathcal{X}} \mu_t(x_t) m_{x_t x_{t+1}}(t) \tag{1}$$

with nonnegative distributions $\mu_t(\cdot)$ over \mathcal{X} , $t \in \mathcal{T}$, and weights $m_{ij}(t) \geq 0$ for all indices $i, j \in \mathcal{X}$ and all times. In accordance with the topology of the graph, $m_{ij}(t) = 0$ for all t whenever $ij \notin \mathcal{E}$. Often, but not always, the matrix

$$M(t) = [m_{ij}(t)]_{i,j=1}^{n}$$
 (2)

does not depend on t. Here, m_{ij} plays the same role as that of the heat kernel in continuous-time. However, herein, the transition matrix M(t) may not represent a *probability* transition matrix in that the rows of M(t) do not necessarily sum up to one. Thus, the "total transported mass" is not necessarily preserved, in that $\sum_{x_t \in \mathcal{X}} \mu_t(x_t)$ may be afunction of time. A particular case of interest is when M is the *adjacency matrix* of the graph that encodes the topological structure of the network.

The evolution (1), together with measure $\mu_0(\cdot)$, which we assume positive on \mathcal{X} , i.e.,

$$\mu_0(x) > 0 \text{ for all } x \in \mathcal{X},$$
 (3)

induces a measure $\mathfrak M$ on \mathcal{FP}_0^N as follows. It assigns to a path $x=(x_0,x_1,\ldots,x_N)\in\mathcal{FP}_0^N$ the value

$$\mathfrak{M}(x_0, x_1, \dots, x_N) = \mu_0(x_0) m_{x_0 x_1}(0) \cdots m_{x_{N-1} x_N}(N-1),$$
(4)

and gives rise to a flow of one-time marginals

$$\mu_t(x_t) = \sum_{x_{\ell \neq t}} \mathfrak{M}(x_0, x_1, \dots, x_N), \quad t \in \mathcal{T}.$$

Definition 1. We denote by $\mathcal{P}(\nu_0, \nu_N)$ the family of probability distributions on \mathcal{FP}_0^N having the prescribed marginals $\nu_0(\cdot)$ and $\nu_N(\cdot)$.

We seek a distribution in this set which is closest to the prior $\mathfrak M$ in *relative entropy* (divergence, Kullback-Leibler index) defined by

$$\mathfrak{D}(\mathfrak{P}\|Q) := \left\{ \begin{array}{ll} \sum_x \mathfrak{P}(x) \log \frac{\mathfrak{P}(x)}{\mathfrak{M}(x)}, & \operatorname{Supp}(\mathfrak{P}) \subseteq \operatorname{Supp}(\mathfrak{M}), \\ +\infty, & \operatorname{Supp}(\mathfrak{P}) \not\subseteq \operatorname{Supp}(\mathfrak{M}), \end{array} \right.$$

Here, by definition, $0 \cdot \log 0 = 0$. The value of $\mathfrak{D}(\mathfrak{P}||\mathfrak{M})$ may turn out to be negative due to the different total masses in the case when \mathfrak{M} is not a probability measure. The optimization problem, however, poses no challenge as the relative entropy is (jointly) convex over this larger domain and is bounded below. This brings us to the so-called *Schrödinger Bridge Problem* (SBP):

Problem 2. Determine

$$\mathfrak{P}^*[\nu_0, \nu_N] := \operatorname{argmin} \{ \mathfrak{D}(\mathfrak{P} || \mathfrak{M}) \mid \mathfrak{P} \in \mathcal{P}(\nu_0, \nu_N) \}.$$
 (5)

By analyzing the contribution to the entropy functional of transitions along edges, in a sequential manner, we arive at a formulation that parallels the fluid-dynamic formulation of the Schrödinger problem in continuous time¹, considered in [23, Section 4] and [6].

Suppose we restrict our search in Problem 2 to Markovian \mathfrak{P} 's. In analogy to (2), we then have

$$\mathfrak{P}(x_0, x_1, \dots, x_N) = \nu_0(x_0) \pi_{x_0 x_1}(0) \cdots \pi_{x_{N-1} x_N}.$$
 (6)

Also let p_t be the one-time marginals of \mathfrak{P} . i.e.

$$p_t(x_t) = \sum_{x_{\ell \neq t}} \mathfrak{P}(x_0, x_1, \dots, x_N), \quad t \in \mathcal{T}.$$

We finally have the update mechanism

$$p_{t+1}(x_{t+1}) = \sum_{x_t \in \mathcal{X}} p_t(x_t) \pi_{x_t x_{t+1}}(t)$$
 (7)

which, in vector form, is

$$p_{t+1} = \Pi'(t)p_t. \tag{8}$$

Here $\Pi = [p_{ij}(t)]_{i,j=1}^n$ is the transition matrix and prime denotes transposition. Using (4)-(6) we obtain

$$\mathfrak{D}(\mathfrak{P}||\mathfrak{M}) = \mathfrak{D}(\nu_0||\mu_0) + \sum_{t=0}^{N-1} \sum_{x_t} \mathfrak{D}(\pi_{x_t x_{t+1}}(t)||m_{x_t x_{t+1}}(t))p_t(x_t).$$

Since $\mathfrak{D}(\nu_0 \| \mu_0)$ is invariant over $\mathcal{P}(\nu_0, \nu_N)$, we can now have the following equivalent (fluid dynamic) formulation:

Problem 3.

$$\min_{(p,\pi)} \left\{ \sum_{t=0}^{N-1} \sum_{x_t} \mathfrak{D} \left(\pi_{x_t x_{t+1}}(t) \| m_{x_t x_{t+1}}(t) \right) p_t(x_t) \right) \right\},\,$$

subject to

$$p_{t+1}(x_{t+1}) = \sum_{x_t \in \mathcal{X}} p_t(x_t) \pi_{x_t x_{t+1}}(t), \tag{9}$$

$$\sum_{x_{t+1}} \pi_{x_t x_{t+1}}(t) = 1, \ \forall x_t \in \mathcal{X}, \ \text{and}$$
 (10)

$$p_0(x_0) = \nu_0(x_0), \quad p_N(x_N) = \nu_N(x_N), \quad (11)$$

for
$$t \in \{0, 1, \dots, N-1\}$$
. (12)

Here $p=\{p_t;t=0,1,\ldots,N\}$ is a flow of probability distributions on \mathcal{X} (corresponds to the flow of densities ρ_t in the continuous setting) and $\pi=\{\pi_{x_tx_{t+1}}(t);t=0,1,\ldots,N-1\}$ is a flow of transition probabilities (corresponds to the flow of the drifts). The relative entropy $\mathfrak{D}\left(\pi_{x_tx_{t+1}}(t)\|m_{x_tx_{t+1}}(t)\right)$ between transition laws, corresponds to the square of the modulus of the velocity field in the continuous setting [6], so that $\mathfrak{D}\left(\pi_{x_tx_{t+1}}(t)\|m_{x_tx_{t+1}}(t))p_t(x_t)\right)$ in fact corresponds to kinetic energy.

We do not impose explicitly the non-negativity constraint on the p_t and $\pi_{x_t x_{t+1}}(t)$ as it will be automatically satisfied (due to the fact that the relative entropy grows unbounded at the boundary of the admissible distributions

1. The fluid dynamic reformulation of Schrödinger's bridge problem in continuous space/time drew important connections with Monge-Kantorovich optimal mass transport (OMT) [1] –the latter seen as a limit when the stochastic excitation reduces to zero [23]. In particular, it pointed to a time-symmetric formulation of Schrödinger's bridges [6].

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and transition probabilities). We have the following theorem:

Theorem 4. Suppose there exists a pair of nonnegative functions $(\varphi, \hat{\varphi})$ defined on $[0, T] \times \mathcal{X}$ and satisfying the system

$$\varphi(t, x_t) = \sum_{x_{t+1}} m_{x_t x_{t+1}}(t) \varphi(t+1, x_{t+1}), \tag{13}$$

$$\hat{\varphi}(t+1, x_{t+1}) = \sum_{x_t} m_{x_t x_{t+1}}(t) \hat{\varphi}(t, i), \qquad (14)$$

for $0 \le t \le (T-1)$, as well as the boundary conditions

$$\varphi(0, x_0) \cdot \hat{\varphi}(0, x_0) = \nu_j(x_0), \ \varphi(T, x_T) \cdot \hat{\varphi}(T, x_T) = \nu_T(x_T),$$
(15)

for $x_t \in \mathcal{X}$ and $t \in \{0, T\}$, accordingly. Suppose moreover that $\varphi(t, i) > 0$, $\forall 0 \le t \le T, \forall i \in \mathcal{X}$. Then, the Markov distribution \mathfrak{P}^* in $\mathcal{P}(\nu_0, \nu_N)$ having transition probabilities

$$\pi_{x_t x_{t+1}}^*(t) = m_{x_t x_{t+1}}(t) \frac{\varphi(t+1, x_{t+1})}{\varphi(t, x_t)}$$
 (16)

solves Problem 3.

Remark 5. Notice that if $(\varphi, \hat{\varphi})$ satisfy (13)-(14)-(15), so does the pair $(c\varphi, \frac{1}{c}\hat{\varphi})$ for all c>0. Hence, uniqueness for the Schrödinger system is always intended as uniqueness of the ray.

The proof of Theorem 4 is deferred to Appendix A. Our derivation there of the Schrödinger system appears original and alternative to the two usual approaches. The first one uses Lagrange multipliers for the constraints involving the marginals [21] very much as in Schrödinger's original spirit. The second uses a "completion of the relative entropy" argument, see [28, Section IV]. Let $M(t) = (m_{ij}(t))$. Under the assumption that the entries of the matrix product

$$G := M(0)M(1)\cdots M(N-2)M(N-1)$$
 (17)

are all positive, there exists a (unique in the projective geometry sense) solution to the system (13)-(15) which can be computed through a Fortet-IPF-Sinkhorn iteration [14], [16], [20], [21], [34].

3 OPTIMAL STEERING TO A STEADY STATE

Consider a given prior transition rate between the vertices of the graph, represented by a matrix M as in (2), which at present we assume as being time-invariant. Suppose π is a desired stationary probability distribution that we wish to maintain over the state space $\mathcal X$ for the distribution of resources, goods, packets, vehicles, etc. at steady state. We address below the following basic question: How can we modify M so that the new evolution is close to the prior in relative entropy while at the same time it admits π as invariant distribution? We address the above question next and provide a partial answer to the complementary question on what conditions ensure that any given π can be rendered the stationary distribution with a transition law compatible with the topology of the graph.

3.1 Minimizing the relative entropy rate

We consider the following problem inspired by [15]. Given a (prior) measure $\mathfrak{M} \in \mathcal{FP}_0^N$ as in Section 2, corresponding to a constant transition matrix M, and a probability vector π on \mathcal{X} , we are seeking a (row) stochastic matrix Π such that

$$\Pi'\pi=\pi$$

while the corresponding (time-invariant) measure \mathfrak{P} on $\mathcal{X} \times \mathcal{X} \times \cdots$ is close to \mathfrak{M} in a suitable sense. Our interest here focuses on the infinite horizon case where N is arbitrarily large.

To this, we let \mathcal{P} be the family of probability distributions on \mathcal{FP}_0^N , and consider the following problem.

Problem 6.

$$\begin{aligned} \min_{\mathfrak{P}\in\mathcal{P}} \lim_{N\to\infty} \frac{1}{N} \mathfrak{D}\left(\mathfrak{P}_{[0,N]} \| \mathfrak{M}_{[0,N]} \right) \\ \text{subject to} \qquad \Pi'\pi = \pi, \\ \Pi\mathbb{1} = \mathbb{1}, \end{aligned}$$

where $\mathbb{1}$ is the vector with all entries equal to 1.

By formula (18) in [28], which applies to general (not necessarily mass preserving) Markovian evolutions, we have the following representation for the relative entropy between Markovian measures

$$\mathfrak{D}\left(\mathfrak{P}_{[0,N]} \| \mathfrak{M}_{[0,N]}\right) = \mathfrak{D}(\pi \| m_0) + \sum_{k=0}^{N-1} \sum_{i_k} \mathfrak{D}(\pi_{i_k i_{k+1}} \| m_{i_k i_{k+1}}) \pi(i_k).$$

Thus, Problem 6 reduces to the *stationary* Schrödinger bridge problem:

Problem 7.

$$\min_{(\pi_{ij})} \sum_{i,j \in \mathcal{X}} \mathfrak{D}(\pi_{ij} || m_{ij}) \pi(i),$$
subject to
$$\sum_{i \in \mathcal{X}} \pi_{ij} \pi(i) = \pi(j), \quad j \in \mathcal{X},$$
$$\sum_{j \in \mathcal{X}} \pi_{ij} = 1, \quad i \in \mathcal{X}.$$

Note that in the above we have ignored enforcing the nonnegativity of the π_{ij} . This problem can readily be shown to be equivalent to a standard *one-step* Schrödinger bridge problem for the joint distributions p(i,j) and m(i,j) at times $t \in \{0,1\}$ with the two marginals equal to π . Indeed, a straightforward calculation gives

$$\sum_{ij} \log \frac{\pi(i,j)}{m(i,j)} \pi(i,j) = \sum_{ij} \log \frac{\pi_{ij}\pi(i)}{m_{ij}m_0(i)} \pi_{ij}\pi(i)$$
$$= \sum_{i} \mathfrak{D}(\pi_{ij} \| m_{ij}) \pi(i) + \mathfrak{D}(\pi \| m_0). \tag{18}$$

Following Theorem 4, suppose there exist two vectors

$$(\varphi(t,\cdot),\hat{\varphi}(t,\cdot)), \text{ for } t \in \{0,1\},$$

with nonnegative entries, satisfying the Schrödinger system

$$\varphi(0,i) = \sum_{j} m_{ij} \varphi(1,j), \qquad (19a)$$

$$\hat{\varphi}(1,j) = \sum_{i} m_{ij} \hat{\varphi}(0,i), \qquad (19b)$$

$$\hat{\varphi}(1,j) = \sum_{i} m_{ij} \hat{\varphi}(0,i), \qquad (19b)$$

$$\varphi(0,i) \cdot \hat{\varphi}(0,i) = \pi(i), \tag{19c}$$

$$\varphi(1,j) \cdot \hat{\varphi}(1,j) = \pi(j). \tag{19d}$$

Thence, we conclude that

$$\pi_{ij}^* = \frac{\varphi(1,j)}{\varphi(0,i)} m_{ij} \tag{20}$$

satisfies both constraints of Problem 7. The corresponding measure $\mathfrak{P}^* \in \mathcal{P}$ solves Problem 6. There is, however, a difficulty. The assumption on the matrix G in (17), which guarantees existence for the Schrödinger system, becomes here the fact that M must have all positive elements. The latter property is typically not satisfied since M must comply with the topology of the graph. There exists, fortunately, a reasonable condition on M which ensures existence of solutions for (19).

3.2 Existence for the one-step Schrödinger system

Definition 8. [18] A square matrix $A = (a_{ij})$ is called indecomposable if no permutation matrix P exists such that

$$A = P \left[\begin{array}{cc} A_{11} & 0 \\ A_{21} & A_{22} \end{array} \right] P'$$

where A_{11} and A_{22} are nonvacuous square matrices. A is called *fully indecomposable* if there exist no pair of permutation matrices P and Q such that

$$A = P \begin{bmatrix} A_{11} & 0 \\ A_{21} & A_{22} \end{bmatrix} Q \tag{21}$$

where A_{11} and A_{22} are nonvacuous square matrices.

Remark 9. A square, indecomposable matrix A has a real positive simple eigenvalue equal to its spectral radius [35]. Let $A = (a_{ij})$ be the adjacency matrix of the graph G = $(\mathcal{X}, \mathcal{E})$, namely

$$a_{ij} = \begin{cases} 1, & (i,j) \in \mathcal{E}, \\ 0, & (i,j) \notin \mathcal{E}. \end{cases}$$

Then A is indecomposable if and only if $G = (\mathcal{X}, \mathcal{E})$ is strongly connected [18, p.608].

Proposition 10. Suppose M is fully indecomposable and π has all positive components. Then there exists a solution to (19) with $\varphi(0,\cdot)$ and $\varphi(1,\cdot)$ with positive components which is unique in the sense of Remark 5.

Proof 1. Let $\varphi_0 = \varphi(0,\cdot)$ and $\varphi_1 = \varphi(1,\cdot)$. Observe that (19a)-(19b)-(20) admit the matricial form

$$\varphi_0 = M\varphi_1, \tag{22a}$$

$$\hat{\varphi}_1 = M' \hat{\varphi}_0, \tag{22b}$$

$$\Pi^* = \text{Diag}(\varphi_0)^{-1} M \text{Diag}(\varphi_1). \tag{22c}$$

$$\Pi^* = \operatorname{Diag}(\varphi_0)^{-1} M \operatorname{Diag}(\varphi_1). \tag{22c}$$

The proof can now be constructed along the lines of [26, Theorem 5].

Another interesting question is the following: Given the graph G, what distributions π admit at least one stochastic matrix compatible with the topology of the graph for which they are invariant? Clearly, if all self loops are present $((i,i) \in \mathcal{E}, \forall i \in \mathcal{X})$, any distribution is invariant with respect to the identity matrix which is compatible. Without such a strong assumption, a partial answer is provided by the following result.

Proposition 11. Let π be a probability distribution supported on all of \mathcal{X} , i.e. $\pi(i) > 0, \forall i \in \mathcal{X}$. Assume that the adjacency matrix of $G = (\mathcal{X}, \mathcal{E})$ is fully indecomposable. Then, there exist stochastic matrices Π compatible with the topology of the graph G such that

$$\Pi'\pi=\pi.$$

Proof 2. Take, in Problem 7, $M = A = [a_{ij}]$ the adjacency matrix of the graph G. By Theorem 4 and Proposition 10, Problem 7 has a solution which admits π as invariant distribution.

One final interesting question is the following: Assume that the adjacency matrix of the graph G is fully indecomposable. Let \mathcal{Q}_{π} be the non empty set of stochastic matrices Qcompatible with the topology of **G** and such that $Q'\pi = \pi$. Clearly Q is a convex set. Can we characterize the matrix in Q which induces a maximum entropy rate measure on the feasible paths? We already know the answer to this question. Indeed, consider the formulation of Problem 7 with the distribution of the edges of formula (18). Recall that maximizing entropy (rate) is equivalent to minimizing relative entropy (rate) from the uniform. If we take as prior the uniform distribution on the edges, M is just a positive scalar times the adjacency matrix A of the graph. Thus, the solution to Problem 7 with A as prior transition provides the maximum entropy rate.

REVERSIBILITY

In [5, Corollary 2], we have shown that, in the case of a reversible prior (Boltzmann density) for a stochastic oscillator, the solution of the continuous countepart of Problem 6 (minimizing the expected input power) is reversible. We prove next that the same remarkable property holds here in the discrete setting.

Theorem 12. Let the transition matrix M of the prior measure $\mathfrak M$ be time invariant. Assume that M is reversible with respect to $\mu_0 = \mu$, i.e.

$$Diag(\mu)M = M'Diag(\mu). \tag{23}$$

Then, then the solution Π^* of Problem 7 is also reversible with respect to π .

Proof 3. Reversibility of M with respect to μ is equivalent to the statement that $\Sigma := \operatorname{Diag}(\mu)M$ is symmetric, as noted. Define the vectors

$$\hat{\psi}_0 = \operatorname{Diag}(\mu)^{-1} \hat{\varphi}_0, \quad \psi_0 = \operatorname{Diag}(\mu) \varphi_0.$$

Then, the first two equations in system (22) supplemented with the marginal conditions read

$$\psi_0 = \Sigma \varphi_1, \tag{24a}$$

$$\hat{\varphi}_1 = \Sigma' \hat{\psi}_0 = \Sigma \hat{\psi}_0, \tag{24b}$$

$$\psi_0 \circ \hat{\psi}_0 = \varphi_1 \circ \hat{\varphi}_1 = \pi, \tag{24c}$$

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where the operation \circ in (24c) represents componentwise between vectors. Due to the symmetry of Σ and the uniqueness in the sense of Remark 5, we have that $\hat{\psi}_0 = c\varphi_1$ and $\psi_0 = \frac{1}{c}\hat{\varphi}_1$ for some positive scalar c. It readily follows that

$$\begin{aligned} \operatorname{Diag}(\pi)\Pi^* &= \operatorname{Diag}(\pi)\operatorname{Diag}(\varphi_0)^{-1}M\operatorname{Diag}(\varphi_1) \\ &= \operatorname{Diag}(\hat{\varphi}_0)M\operatorname{Diag}(\varphi_1) \\ &= \operatorname{Diag}(\hat{\psi}_0)\operatorname{Diag}(\mu)M\operatorname{Diag}(\varphi_1) \\ &= \operatorname{Diag}(\hat{\psi}_0)M'\operatorname{Diag}(\mu)\operatorname{Diag}(\varphi_1) \\ &= \operatorname{Diag}(\hat{\psi}_0)M'\operatorname{Diag}(\varphi_0)^{-1}\operatorname{Diag}(\psi_0)\operatorname{Diag}(\varphi_1) \\ &= \operatorname{Diag}(\varphi_1)M'\operatorname{Diag}(\varphi_0)^{-1}\operatorname{Diag}(\hat{\varphi}_1)\operatorname{Diag}(\varphi_1) \\ &= \Pi'\operatorname{Diag}(\pi). \end{aligned}$$

Returning now to the question raised at the end of Subsection 3.2, in the case when A is symmetric, we can take $\pi_A := A1$.

COOLING 5

In several advanced applications such as atomic force microscopy and microresonators, it is often important to dampen stochastic excitations (due to vibrations, molecular dynamics, etc.) affecting experimental apparatuses. This is often accomplished through feedback, steering the system to a desired steady state corresponding to an effective temperature which is lower than that of the environment (e.g., fluid), see for instance [4], [17], [24], [25], [33], [36]. Optimal asymptotic and fast cooling of stochastic oscillators was studied in [5]. We show next how the results of Section 3 permit to derive corresponding results in the context of discrete space and time considered herein.

Optimal fast cooling

Consider the setting of the previous section where the transition matrix of the prior measure M is time invariant. Let us introduce a *Boltzmann distribution* π_T on \mathcal{X}

$$\pi_T(i) := Z(T)^{-1} \exp\left[\frac{-E_i}{kT}\right], \quad Z(T) = \sum_i \exp\left[\frac{-E_i}{kT}\right],$$
(25)

corresponding to the "energy function" E_x , for $x \in \mathcal{X}$, and let us assume that π_T is invariant for M = P(T), that is,

$$P(T)'\pi_T = \pi_T.$$

One such class of transition matrices is given by $P(T,Q) = (p_{ij}(T,Q))$ with

$$p_{ij}(T,Q) = \left\{ \begin{array}{ll} q_{ij} \min \left(\exp \left(\frac{E_i - E_j}{kT} \right), 1 \right), & i \neq j, \\ 1 - \sum_{l,l \neq i} q_{il} \min \left(\exp \left(\frac{E_i - E_l}{kT} \right), 1 \right), & i = j. \end{array} \right. \text{ APPENDIX}$$

where $Q = (q_{ij})$ is any symmetric transition matrix of an irreducible chain compatible with the topology of G^2 . Let $T_{\rm eff} < T$ be a desired lower temperature. Given any prior, such as the Ruelle-Bowen measure [11] or the invariant path space measure $\mathfrak{P}(T)$ with transition P(T) and marginals

2. As is well-known, this (Metropolis) chain is actually reversible with respect to the Boltzmann distribution.

 π_T and a sufficiently long time interval [0, N], we can use a standard Schrödinger bridge (see Section 2) to steer optimally the network flow from any initial distribution ν_0 to $\nu_N = \pi_{T_{\rm eff}}$ at time N. At time N, however, we need to change the transition mechanism to keep the chain in the steady state $\pi_{T_{\rm eff}}$. This is accomplished in the next subsection using the results of Section 3.

5.2 Optimal asymptotic cooling

Consider once again the case where the prior transition M =P(T) remains constant over time and has the Boltzmann distribution (25) as initial, invariant measure. Consider the equivalent Problems 6 and 7.

Theorem 13. Assume that P(T) is fully indecomposable. Then, the solution to Problem 7 is given by

$$\Pi^* = \operatorname{Diag}(\varphi_0)^{-1} P(T) \operatorname{Diag}(\varphi_1). \tag{26}$$

where

$$\varphi_0 = P(T)\varphi_1, \tag{27a}$$

$$\hat{\varphi}_1 = P(T)'\hat{\varphi}_0, \tag{27b}$$

$$\varphi_0 \circ \hat{\varphi}_0 = \varphi_1 \circ \hat{\varphi}_1 = \pi_{T_{\text{eff}}}.$$
 (27c)

As earlier, o denotes componentwise multiplication of vectors. Moreover, if P(T) is reversible with respect to π_T , so is Π^* with respect to $\pi_{T_{\text{eff}}}$.

Proof 4. The result follows from Theorem 4, Proposition 10 and Theorem 12.

CONCLUSION

The key point of this paper has been to explore analogues, in the setting of discrete space and time, for Markovian evolutions that match specified marginals and echo wellknown results in the continuous time setting for Schödinger bridges. Specifically, a key result is to show reversibility of the transition rates under the assumption that this is a property of the prior. We consider both, transitioning between marginals over a specified time window as well as the problem to secure a stationary distribution. Both cases are accomplished by suitably adjusting the transition rates from a given prior, while keeping the distance of the new law closest to that corresponding to the prior in the relative entropy sense. Application of the results in the context regulating the flow of resources over a network is contemplated. A notion of temperature when distributions are expressed as Boltzmann distributions with respect to an energy function is brought up, and the problem to transition between distributions corresponding to different temperatures considered, in analogy to the problem of cooling in continuous time and space.

PROOF OF THEOREM 4

We form the Lagrangian for Problem 3:

$$\mathcal{L}(p,\pi;\lambda) = \sum_{t=0}^{N-1} \sum_{x_t} \mathfrak{D}(\pi_{x_t x_{t+1}}(t) \| m_{x_t x_{t+1}}(t)) p_t(x_t)$$

$$+ \sum_{t=0}^{N-1} \sum_{x_{t+1}} \lambda_t(x_{t+1}) \left[p_{t+1}(x_{t+1}) - \sum_{x_t} p_t(x_t) \pi_{x_t x_{t+1}}(t) \right]$$

We now use discrete integration by parts:

$$\sum_{t=0}^{N-1} \sum_{x_{t+1}} \lambda_t(x_{t+1}) p_{t+1}(x_{t+1})$$

$$= \sum_{t=0}^{N-1} \sum_{x_t} \lambda_{t-1}(x_t) p_t(x_t)$$

$$+ \sum_{x_N} \lambda_{N-1}(x_N) \nu_N(x_N) - \sum_{x_0} \lambda_{-1}(x_0) \nu_0(x_0).$$

Thus, the Lagrangian reads

$$\mathcal{L}(p,\pi;\lambda) = \sum_{t=0}^{N-1} \sum_{x_t} \mathfrak{D}(\pi_{x_t x_{t+1}}(t) \| m_{x_t x_{t+1}}(t)) p_t(x_t)$$

$$+ \sum_{t=0}^{N-1} \sum_{x_t} \left[\lambda_{t-1}(x_t) - \sum_{x_{t+1}} \lambda_t(x_{t+1}) \pi_{x_t x_{t+1}}(t) \right] p_t(x_t)$$

$$+ \sum_{x_N} \lambda_{N-1}(x_N) \nu_N(x_N) - \sum_{x_0} \lambda_{-1}(x_0) \nu_0(x_0).$$

Observe that the last two terms are invariant over pairs (p,π) satisfying (9)-(11) and can therefore be discarded. Since we are minimizing over pairs satisfying the nonnegativity requirement and with π satisfying (10), we can multiply $\lambda_{t-1}(x_t)$ by $\sum_{x_{t+1}} \pi_{x_t x_{t+1}}(t)$ and subtract $N = \sum_{t=0}^{N-1} \sum_{x_t} \sum_{x_{t+1}} \pi_{x_t x_{t+1}}(t) p_t(x_t)$ to get

$$\mathcal{L}(p, \pi; \lambda) = \sum_{t=0}^{N-1} \sum_{x_t} \mathfrak{D}(\pi_{x_t x_{t+1}}(t) || m_{x_t x_{t+1}}(t)) p_t(x_t)$$

$$+ \sum_{t=0}^{N-1} \sum_{x_t} \sum_{x_{t+1}} \pi_{x_t x_{t+1}}(t) \left[\lambda_{t-1}(x_t) - \lambda_t(x_{t+1}) \right] p_t(x_t)$$

$$- \sum_{t=0}^{N-1} \sum_{x_t} \sum_{x_{t+1}} \pi_{x_t x_{t+1}}(t) p_t(x_t).$$

Next, we perform two-stage unconstrained minimization of the Lagrangian: For fixed flow $p=\{p_t\}$ (and fixed multipliers), we optimize the strictly convex function $L(p,\cdot;\lambda)$ at each time t. We get the optimality conditions:

$$\left[1 + \log \pi_{x_t x_{t+1}}^*(t) - \log m_{x_t x_{t+1}}(t) + \lambda_{t-1}(x_t) - \lambda_t(x_{t+1}) - 1\right] p_t(x_t) = 0.$$

or

$$\pi_{x_t,x_{t+1}}^*(t) = m_{x_t,x_{t+1}}(t) \exp\left[\lambda_t(x_{t+1}) - \lambda_{t-1}(x_t)\right].$$
 (28)

Define the positive function

$$\varphi(t+1, x_{t+1}) = \exp\left[\lambda_t(x_{t+1})\right].$$

Then (28) becomes

$$\pi_{x_t x_{t+1}}^*(t) = m_{x_t x_{t+1}}(t) \frac{\varphi(t+1, x_{t+1})}{\varphi(t, x_t)}.$$

Let us impose condition (10) on π^* . We get that π^* satisfies such condition if and only if φ satisfies the reverse-time recursion

$$\varphi(t, x_t) = \sum_{x_{t+1}} m_{x_t x_{t+1}}(t) \varphi(t+1, x_{t+1}),$$

$$\forall x_t \in \mathcal{X}, \quad t = 0, 1, \dots, N-1$$

Observe now that

$$\mathcal{L}(p, \pi^*; \log \varphi) = \sum_{t=0}^{N-1} \sum_{x_t} \sum_{x_{t+1}} \left[-m_{x_t x_{t+1}}(t) \frac{\varphi(t+1, x_{t+1})}{\varphi(t, x_t)} \right] p_t(x_t)$$

$$= -\sum_{t=0}^{N-1} \sum_{x_t} p_t(x_t) = -N,$$

which is independent of p. Thus, we can choose p^* defined by

$$p_{t+1}^*(x_{t+1}) = \sum_{x_t} p_t^*(x_t) \pi_{x_t x_{t+1}}^*(t), \quad p_0(x_0) = \nu(x_0),$$

so as to satisfy constraint (9) and the first of (11). Define

$$\hat{\varphi}(t, x_t) := \frac{p_t^*(x_t)}{\varphi(t, x_t)}.$$

We get

$$\hat{\varphi}(t+1, x_{t+1}) = \frac{p_{t+1}^*(x_{t+1})}{\varphi(t+1, x_{t+1})}
= \frac{\sum_{x_t} p_t^*(x_t) \pi_{x_t x_{t+1}}^*(t)}{\varphi(t+1, x_{t+1})}
= \frac{\sum_{x_t} p_t^*(x_t) m_{x_t x_{t+1}}(t) \frac{\varphi(t+1, x_{t+1})}{\varphi(t, x_t)}}{\varphi(t+1, x_{t+1})}
= \sum_{x_t} m_{x_t x_{t+1}}(t) \frac{p_t^*(x_t)}{\varphi(t, x_t)}
= \sum_{x_t} m_{x_t x_{t+1}}(t) \hat{\varphi}(t, i),$$

namely $\hat{\varphi}(t, x_t)$ is space-time co-harmonic.

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REFERENCES

- [1] J. Benamou and Y. Brenier, A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem, *Numerische Mathematik*, **84**, no. 3, 2000, 375-393.
- [2] A. Beurling, An automorphism of product measures, Ann. Math. 72 (1960), 189-200.
- [3] D. Bertsekas, Dynamic Programming and Optimal Control, vol 2. MA: Athena, 1995.
- [4] Y. Braiman, J. Barhen, and V. Protopopescu, Control of Friction at the Nanoscale, *Phys. Rev. Lett.* 90, (2003), 094301.
- [5] Y. Chen, T.T. Georgiou and M. Pavon, Fast cooling for a system of stochastic oscillators, *J. Math. Phys.*, **56(11)**: 113302, 2015.
- 6] Y. Chen, T.T. Georgiou and M. Pavon, On the relation between optimal transport and Schrödinger bridges: A stochastic control viewpoint, J. Optim. Theory and Applic., 169(2): 671-691, 2016.
- [7] Y. Chen, T.T. Georgiou and M. Pavon, Entropic and displacement interpolation: a computational approach using the Hilbert metric, SIAM Journal on Applied Mathematics, 76 (6), 2375-2396, 2016.
- [8] Y. Chen, T.T. Georgiou and M. Pavon, Stochastic control liaisons: Richard Sinkhorn meets Gaspard Monge on a Schrödinger bridge, ArXiv e-prints, arXiv: 2005.10963, SIAM Review, to appear.
- [9] Y. Chen, T.T. Georgiou and M. Pavon, Optimal Transport in Systems and Control, Annual Review of Control, Robotics, and Autonomous Systems, published online at https://www.annualreviews.org/doi/abs/10.1146/annurev-control-070220-100858, to appear in vol. 4, May 2021.

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[10] Y. Chen, T.T. Georgiou and M. Pavon, Controlling Uncertainty: Schrödinger's Inference Method and the Optimal Steering of Probability Distributions, June 2020, IEEE Control Systems Magazine, to appear.

- [11] Y. Chen, T.T. Georgiou, M. Pavon and A. Tannenbaum, Robust transport over networks, *IEEE Trans. Aut. Control*, 62, n.9, 4675-4682, 2017
- [12] Y. Chen, T.T. Georgiou, M. Pavon and A. Tannenbaum, Efficient-robust routing for single commodity network flows, *IEEE Trans. Aut. Control*, 63(7): 2287-2294, 2018.
- [13] Y. Chen, T.T. Georgiou, M. Pavon and A. Tannenbaum, Relaxed Schroödinger bridges and robust network routing, *IEEE Trans. on Control of Network Systems*, 7(2): 923-931, 2020.
- [14] M.Cuturi, "Sinkhorn Distances: Lightspeed Computation of Optimal Transport", Advances in Neural Information Processing Systems, 2292-2300, 2013.
- [15] J.-C. Delvenne and A.-S. Libert, Centrality measures and thermodynamic formalism for complex networks, *Physical Review E*, 83 (4), 046117, 2011.
- [16] W. E. Deming and F. F. Stephan, On a least squares adjustment of a sampled frequency table when the expected marginal totals are known, Ann. Math. Statist., 11 (4), (1940), 427-444.
- [17] M. Doi and S. F. Edwards, The Theory of Polymer Dynamics, Oxford University Press, New York, 1988.
- [18] T. I. Fenner and G. Loizou, On fully indecomposable matrices, J. Computer and System Sciences, 5, 1971, 607-622.
- [19] H. Föllmer, Random fields and diffusion processes, in: Ècole d'Ètè de Probabilitès de Saint-Flour XV-XVII, edited by P. L. Hennequin, Lecture Notes in Mathematics, Springer-Verlag, New York, 1988, vol.1362,102-203.
- [20] R. Fortet, Résolution d'un système d'equations de M. Schrödinger, J. Math. Pure Appl. IX (1940), 83-105.
- [21] T. T. Georgiou and M. Pavon, Positive contraction mappings for classical and quantum Schrödinger systems, J. Math. Phys., 56, 033301 (2015).
- [22] B. Jamison, The Markov processes of Schrödinger, Z. Wahrscheinlichkeitstheorie verw. Gebiete 32 (1975), 323-331.
- [23] C. Léonard, A survey of the Schroedinger problem and some of its connections with optimal transport, *Discrete Contin. Dyn. Syst.* A, 2014, 34 (4): 1533-1574.
- [24] S. Liang, D. Medich, D. M. Czajkowsky, S. Sheng, J. Yuan, and Z. Shao, *Ultramicroscopy*, 84 (2000), p.119.
- [25] F. Marquardt and S. M. Girvin, Optomechanics, Physics 2, 40 (2009).
- [26] A. W. Marshall and I. Olkin, Scaling of matrices to achieve specified row and column sums, *Numerische Mathematik*, 12, 1968, 83-90.
- [27] G. Monge, Mémoire sur la théorie des déblais et des remblais, Histoire de l'Academie royale des sciences avec les mémoires de mathématique et de physique tirés des registres de cette Académie, De l'Imprimerie Royale, 1781, 666-704.
- [28] M. Pavon and F. Ticozzi, Discrete-time classical and quantum Markovian evolutions: Maximum entropy problems on path space, J. Math. Phys., 51, 042104-042125 (2010).
- [29] G. Peyré and M. Cuturi, Computational Optimal Transport, Foundations and Trends in Machine Learning, 11, no. 5-6,1-257, 2019.
- [30] M. L. Puterman, Markov Decision Processes, Wiley, 1994.
- [31] E. Schrödinger, Über die Umkehrung der Naturgesetze, Sitzungsberichte der Preuss Akad. Wissen. Berlin, Phys. Math. Klasse, 10, 144-153, 1931.
- [32] E. Schrödinger, Sur la théorie relativiste de l'électron et l'interpretation de la mécanique quantique, Ann. Inst. H. Poincaré 2, 269 (1932).
- [33] K. C. Schwab and M. L. Roukes, Phys. Today 58, No. 7, 36 (2005).
- [34] R. Sinkhorn, A relationship between arbitrary positive matrices and doubly stochastic matrices, Ann. Math. Statist., 35 (2)(1964), 876-879.
- [35] R. S. Varga, Matrix Iterative Analysis, Prentice-Hall, 1962.
- [36] A. Vinante, M. Bignotto, M. Bonaldi et al., Feedback Cooling of the Normal Modes of a Massive Electromechanical System to Submillikelvin Temperature, *Physical Review Letters* 101 (2008), 033601.
- [37] A. Wakolbinger, Schroedinger bridges from 1931 to 1991, in *Proc.* of the 4th Latin American Congress in Probability and Mathematical Statistics, Mexico City 1990, Contribuciones en probabilidad y estadistica matematica, 3 (1992), 61-79.