Controlled Markov chains for controlled n-level quantum systems

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***Abstract*— We develop the theory of Schrödinger bridges for continuous-time Markov chains. We then investigate the possibility of employing the Nelson-Guerra stochastic mechanics, jointly with the Schrödinger bridges, as a tool for state preparation for n-level systems.**

I. SCHRÖDINGER MARVELOUS BRIDGES

In 1931/32 [20], [21], Erwin Schrödinger studied the following problem. Consider N Brownian particles in $\mathbb{R}^3$ evolving in time. This cloud of particles has been observed having at time t_0 an empirical distribution equal to $\rho_0(x)dx$. At some later time t_1, we observe an empirical distribution equal to $\rho_1(x)dx$ which considerably differs from what it should be according to the law of large numbers (N is large, say of the order of Avogadro's number), namely

$$\int_{t_0}^{t_1} p(t_0, y, t_1, x)\rho_0(y)dy,$$

where

$$p(s, y, t, x) = [2\pi(t-s)]^{-\frac{n}{2}} \exp\left[-\frac{|x-y|^2}{2(t-s)}\right], \quad s < t.$$

is the transition density of the Wiener process. Namely, $p(t_0, y, t_1, x)\rho_0(y)dy$ is the probability that the Brownian particle be found in x at time t_1 given that it was in the volume dy at time t_0. It is apparent that the particles have been transported in an unlikely way. But of the many unlikely ways in which this could have happened, which one is the most likely? In modern probabilistic language, this is a problem of large deviations of the empirical distribution [6]. By discretization and passing to the limit, Schrödinger computed the most likely intermediate empirical distribution as $N \to \infty$. It turned out that the optimal random evolution, the *Schrödinger bridge* from ρ_0 to ρ_1 over Brownian motion, had at each time a density $\rho(\cdot, t)$ that factored as $\rho(x,t) = \phi(x,t)\hat{\phi}(x,t)$, where ϕ and $\hat{\phi}$ are a p-harmonic and a p-coharmonic functions, respectively. That is

$$\phi(t, x) = \int p(t, x, t_1, y)\phi(t_1, y)dy, \tag{1}$$

$$\hat{\phi}(t, x) = \int p(t_0, y, t, x)\hat{\phi}(t_0, y)dy. \tag{2}$$

The existence and uniqueness of a pair $(\phi, \hat{\phi})$ satisfying (1)-(2) and the boundary conditions $\phi(x, t_0)\hat{\phi}(x, t_0) = \rho_0(x)$, $\phi(x, t_1)\hat{\phi}(x, t_1) = \rho_1(x)$ was guessed by Schrödinger on the basis of his intuition. He was later shown to be quite right in various degrees of generality by Fortet [7], Beurling [3], Jamison [11], Föllmer [6]. Jamison showed, in particular, that the Schrödinger bridge is the unique Markov process $\{x(t)\}$ in the class of *reciprocal processes* (one-dimensional Markov fields) introduced by Bernstein [2] having as two-sided transition density

$$q(s, x; t, y; u, z) = \frac{p(s, x; t, y)p(t, y; u, z)}{p(s, x; u, z)}, \quad s < t < u,$$

namely $q(s, x; t, y; u, z)dy$ is the probability of finding the process x in the volume dy at time t given that $x(s) = x$ and $x(u) = z$. Schrödinger was struck by the following remarkable property of the solution: The Schrödinger bridge from ρ_1 to ρ_0 over Brownian motion is just the time reversal of the Schrödinger bridge from ρ_0 to ρ_1. In Schrödinger's words: "Abnorm states have arisen with high probability by an exact time reversal of a proper diffusion process". This led him to entitle [20]: "On the reversal of natural laws". A few years later, Kolmogorov wrote a paper on the subject with a very similar title [13]. Moreover, the fact that the Schrödinger bridge has density $\rho(x,t) = \phi(x,t)\hat{\phi}(x,t)$ resembles the fact that in quantum mechanics the density may be expressed as $\rho(x,t) = \psi(x,t)\bar{\psi}(x,t)$. The Kullback-Leibler pseudo-distance between two probability densities $p(\cdot)$ and $q(\cdot)$ is defined by

$$H(p, q) := \int_{\mathbb{R}^n} \log \frac{p(x)}{q(x)} p(x)dx.$$

Given $P \in \mathbb{D}$, we consider the following problem:

$$\text{Minimize} \quad H(Q, P) \quad \text{over} \quad \mathbb{D}(\rho_0, \rho_1).$$

This problem is connected through Sanov's theorem [6] to a problem of large deviations of the empirical distribution, according to Schrödinger original motivation. If there is at least one Q in $\mathbb{D}(\rho_0, \rho_1)$ such that $H(Q, P) < \infty$, it may be shown that there exists a unique minimizer Q^* in $\mathbb{D}(\rho_0, \rho_1)$ called *the Schrödinger bridge* from ρ_0 to ρ_1 over P. Q^* can be seen as a controlled version of P where the control modifies the forward drift as follows. If (the coordinate process under) P is Markovian with forward drift field $b_+^P(x,t)$ and transition density $p(\sigma, x, \tau, y)$, then Q^* is also Markovian with forward drift field

$$b_+^{Q^*}(x,t) = b_+^P(x,t) + \nabla \log \phi(x,t),$$

where the (everywhere positive) function ϕ solves together with another function $\hat{\phi}$ the system (1)-(2) with boundary

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conditions

$$\phi(x,t_0)\hat\phi(x,t_0)=\rho_0(x), \quad \phi(x,t_1)\hat\phi(x,t_1)=\rho_1(x).$$

Moreover, $\rho(x,t)=\phi(x,t)\hat\phi(x,t), \forall t\in[t_0,t_1]$. This result has been suitably extended to the case where P is non-Markovian in [18]. For a survey and an extended bibliography on Schródinger bridges see [22].

II. Elements of Nelson's stochastic mechanics

Let $\{\psi(x,t); t_0\le t\le t_1\}$ be the solution of the *Schrödinger equation*

$$\frac{\partial\psi}{\partial t}=\frac{i\hbar}{2m}\Delta\psi-\frac{i}{\hbar}V(x)\psi, \tag{3}$$

with initial condition $\psi_0(x)$. Assume that

$$||\nabla\psi||_2^2\in L^1_{\rm loc}[t_0,+\infty). \tag{4}$$

This is Carlen's *finite action condition*. Under these hypotheses, the Nelson measure P may be constructed on path space, [5], [4, Chapter IV], and references therein. Namely, letting $\Omega:=\mathcal{C}([t_0,t_1],\mathbb{R}^n)$ the n-dimensional continuous functions on $[t_0,t_1]$, under the probability measure P, the canonical coordinate process $x(t,\omega)=\omega(t)$ is an n-dimensional Markov diffusion process $\{x(t); t_0\le t\le t_1\}$, called *Nelson's process*, having (forward) Ito differential

$$dx(t)=\left[\frac{\hbar}{m}\nabla\left(\Re\log\psi+\Im\log\psi\right)\right](x(t),t)dt+\sqrt{\frac{\hbar}{m}}dw(t),$$

where w is a standard, n-dimensional Wiener process. Moreover, the probability density $\rho(\cdot,t)$ of $x(t)$ satisfies

$$\rho(x,t)=|\psi(x,t)|^2, \quad \forall t\in[t_0,t_1]. \tag{5}$$

III. Steering a quantum systems over a Schrödinger bridge

We now show that the theory of Schrödinger bridges can be employed, jointly with the Nelson-Guerra stochastic mechanics [15], [16], [8], [9], [5], [17], [4],, to attack the steering problem for quantum systems. First of all, observe that everything we said about Schrödinger bridges continues to hold if we consider finite-energy diffusions with diffusion coefficient equal to $\frac{\hbar}{m}$ rather than 1. Let ψ_0 and ψ_1 be the given initial and final quantum states. Let $V_i(x)$ be the ambient (internal) potential, and consider a *reference* quantum evolution $\{\psi(x,t); t_0\le t\le t_1\}$ solving the Schrödinger equation

$$\frac{\partial\psi}{\partial t}=\frac{i\hbar}{2m}\Delta\psi-\frac{i}{\hbar}V_i(x)\psi,$$

and satisfying Carlen's finite action condition (4). Let $P\in\mathbb{D}$ be the Markovian measure of the Nelson process associated to $\{\psi(x,t)\}$ as in (5). Hence, in particular, the probability density satisfies $\rho(x,t)=|\psi(x,t)|^2$. Thus, if we write

$$\psi(x,t)=\exp[R(x,t)+\frac{i}{\hbar}S(x,t)], \tag{6}$$

the forward drift of the Nelson process is then given by

$$b_+^P(x,t)=\frac{1}{m}\nabla S(x,t)+\frac{\hbar}{m}\nabla R(x,t).$$

As it was noticed already at the beginning of wave mechanics [14], R and S satisfy the system of nonlinear p.d.e.'s

$$\frac{\partial R}{\partial t}+\frac{1}{m}\nabla R\cdot\nabla S+\frac{1}{2m}\Delta S=0, \tag{7}$$

$$\frac{\partial S}{\partial t}+\frac{1}{2m}\nabla S\cdot\nabla S+V_i-\frac{\hbar^2}{2m}\left[\nabla R\cdot\nabla R+\Delta R\right]=0. \tag{8}$$

We then have the following result [1].

Theorem 1: Let Q^* be the *Schrödinger bridge* from $|\psi_0|^2$ to $|\psi_1|^2$ over P (see previous section). Then, Q^* has forward drift field

$$b_+^{Q^*}(x,t)=\frac{1}{m}\nabla S(x,t)+\frac{\hbar}{m}\nabla R(x,t)+\frac{\hbar}{m}\nabla\log\phi(x,t), \tag{9}$$

where the function ϕ solves together with another function $\hat\phi$ the system

$$\frac{\partial\phi}{\partial t}+(\frac{1}{m}\nabla S+\frac{\hbar}{m}\nabla R)\cdot\nabla\phi+\frac{\hbar}{2m}\Delta\phi=0, \tag{10}$$

$$\frac{\partial\hat\phi}{\partial t}+\nabla\cdot\left[(\frac{1}{m}\nabla S+\frac{\hbar}{m}\nabla R)\hat\phi\right]-\frac{\hbar}{2m}\Delta\hat\phi=0, \tag{11}$$

with the boundary conditions

$$\phi(x,t_0)\hat\phi(x,t_0)=|\psi_0|^2(x), \quad \phi(x,t_1)\hat\phi(x,t_1)=|\psi_1|^2(x).$$

The one-time probability density of Q^* satisfies

$$\tilde\rho(x,t)=\phi(x,t)\hat\phi(x,t). \tag{12}$$

Define, for $t\in[t_0,t_1]$,

$$\tilde S(x,t)=S(x,t)+\hbar R(x,t)+\frac{\hbar}{2}\log\frac{\phi(x,t)}{\hat\phi(x,t)}, \tag{13}$$

$$\tilde R(x,t)=\frac{1}{2}\log\tilde\rho(x,t). \tag{14}$$

Let $\{\tilde\psi(x,t); t_0\le t\le t_1\}$ be defined by

$$\tilde\psi(x,t)=\exp[\tilde R(x,t)+\frac{i}{\hbar}\tilde S(x,t)].$$

Then, $\{\tilde\psi(x,t)\}$ satisfies the controlled Schrödinger equation

$$\frac{\partial\tilde\psi}{\partial t}=\frac{i\hbar}{2m}\Delta\tilde\psi-\frac{i}{\hbar}[V_i(x)+V_c(x,t)]\tilde\psi, \tag{15}$$

with controlling potential function $V_c(x,t)$ given by

$$V_c(x,t)=\frac{\hbar^2}{m}\left[\frac{\Delta\sqrt{\tilde\rho(x,t)}}{\sqrt{\tilde\rho(x,t)}}-\frac{\Delta\sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}}\right], \tag{16}$$

and we have

$$|\tilde\psi(x,t_0)|=|\psi_0(x)|, \quad |\tilde\psi(x,t_1)|=|\psi_1(x)|.$$

Moreover, the *Schrödinger bridge* Q^* is indeed the Nelson process associated to the new quantum evolution $\{\tilde\psi(x,t); t_0\le t\le t_1\}$.

Remark 1: The quantum evolution $\{\tilde\psi(x,t); t_0\le t\le t_1\}$ has the desired absolute value at t_0 and t_1. In order to obtain also the correct initial and final phase, we can use the freedom we have in choosing the reference evolution. Namely, we can choose the ambient potential $V_i(x)$ so that this procedure yields the desired phases. Examples are provided in [1].

IV. Kinematics for Markov chains

Let us consider a continuous-time Markov chain $\{q(t); t_0 \le t \le t_1\}$ with state space $\mathcal{X} = \{1, 2, \dots, N\}$. We denote by $\rho_j(t) := \mathbb{P}[q(t) = j]$ the probability of occupying the site j at time t. Let us also introduce the *transition probabilities*

$$p(s, j, t, k) := \mathbb{P}[q(t) = k | q(s) = j], \quad t_0 \le s < t \le t_1.$$

Notice that we do not assume the *time homogeneity* property ($p(s, j, t, k) = p_1(j, k, t-s)$) since we shall consider *controlled* Markov chains. We have the evolution equation

$$\rho_k(t) = \sum_j p(s, j, t, k)\rho_j(s), \quad s < t. \tag{17}$$

(Here and in the following summations run from 1 to N). Transition probabilities satisfy

$$\begin{aligned} & p(s, j, t, k) \ge 0, \\ & \sum_k p(s, j, t, k) = 1, \\ & \lim_{t \searrow s} p(s, j, t, k) = \delta_{jk} = p(t, j, t, k), \\ & \sum_k p(s, j, t, k) p(t, k, u, l) = p(s, j, u, l). \end{aligned} \tag{18}$$

Let us introduce the infinitesimal generator

$$a^+_{jk}(t) := \lim_{\Delta t \searrow 0} \frac{p(t, j, t+\Delta t, k) - \delta_{jk}}{\Delta t}.$$

We have

$$\begin{aligned} & a^+_{jk}(t) \ge 0, \quad j \ne k, \\ & \sum_k a^+_{jk}(t) = 0. \end{aligned} \tag{19}$$

It follows that $a^+_{jj} \le 0$ is completely determined by the other $a^+_{jk}, k \ne j$. We get the *forward* equation

$$\frac{\partial}{\partial t} p(s, j, t, k) = \sum_l a^+_{lk}(t) p(s, j, t, l). \tag{20}$$

From this and (18), we get the *backward* equation

$$\frac{\partial}{\partial s} p(s, j, t, k) = -\sum_l a^+_{jl}(s) p(s, l, t, k) \tag{21}$$

Moreover, (17) gives immediately that also the one-time distributions satisfy the forward equation (Fokker-Planck equation)

$$\frac{\partial}{\partial t}\rho_k(t) = \sum_l a^+_{lk}(t)\rho_l(t). \tag{22}$$

Let us also introduce the *reverse-time transition probabilities*

$$\bar{p}(t, j, s, i) := \mathbb{P}[q(s) = i | q(t) = j], \quad t_0 \le s < t \le t_1.$$

The two transition mechanisms, for $s < t$, are related through

$$\mathbb{P}[q(s) = i, q(t) = j] = p(s, i, t, j)\rho_i(s) = \bar{p}(t, j, s, i)\rho_j(t).$$

When $\rho_j(t) > 0, \forall j, \forall t$, we get

$$\bar{p}(t, j, s, i) = \frac{\rho_i(s)}{\rho_j(t)} p(s, i, t, j). \tag{23}$$

V. Schrödinger bridges for Markov chains

Suppose now we consider Schrödinger's problem of Section 1 after the phase space has undergone some "coarse graining". Then the *a priori* model is indeed given by a continuous time Markov chain $\{q(t); t_0 \le t \le t_1\}$ as considered above. Denote by ρ^0 and ρ^1 the given initial and final distributions, respectively.We outline the solution steps (details will be provided elsewhere [19]). By decomposing relative entropy on path space as in [6, p.161], one can show that the solution process is characterized by the two following properties:

1) it has the same "three times" transition probabilities as the original process

$$q(s, i; t, j; u, k) = \frac{p(s, i; t, j) p(t, j; u, k)}{p(s, i; u, k)}, \quad s < t < u; \tag{24}$$

2) the joint probability of the initial and final time $q^*(i, j)$ minimizes the relative entropy

$$\sum_i \sum_j \log \frac{q(i, j)}{p(i, j)} q(i, j),$$

subject to the constraints

$$\sum_j q(i, j) = \rho^0_i, \quad i \in \mathcal{X}, \tag{25}$$

$$\sum_i q(i, j) = \rho^1_j, \quad j \in \mathcal{X}. \tag{26}$$

Here $p(i, j) = \rho_i(t_0) p(t_0, i, t_1, j)$ is the joint probability of initial and final time of the reference process. The solution of the latter constrained optimization problem may be obtained with the aid of Lagrange multipliers. The Lagrangian function has the form

$$\mathcal{L}(q) = \sum_i \sum_j \log \frac{q(i, j)}{p(i, j)} q(i, j) + \sum_i \lambda(i) \left[\sum_j q(i, j) - \rho^0_i\right] + \sum_j \mu(j) \left[\sum_i q(i, j) - \rho^1_j\right].$$

We get the optimality condition

$$1 + \log q(i, j) - \log p(t_0, i, t_1, j) - \log \rho_i(t_0) + \lambda(i) + \mu(j) = 0.$$

Hence, the optimal $q^*(\cdot, \cdot)$ has the form $q^*(i, j) = \hat{\varphi}(i) p(t_0, i, t_1, j) \varphi(j)$, where φ and $\hat{\varphi}$ are determined by

$$\hat{\varphi}(i) \sum_j p(t_0, i, t_1, j)\varphi(j) = \rho^0_i, \tag{27}$$

$$\varphi(j) \sum_i p(t_0, i, t_1, j)\hat{\varphi}(i) = \rho^1_j. \tag{28}$$

Let us introduce the *space-time harmonic* function

$$\varphi(t,i) := \sum_j p(t,i,t_1,j)\varphi(j),$$

and the *space-time co-harmonic* function

$$\hat{\varphi}(t,j) := \sum_j p(t_0,i,t,j)\hat{\varphi}(i).$$

Because of (21)-(20), φ and $\hat{\varphi}$ satisfy the backward and forward equation, respectively,

$$\frac{\partial}{\partial t}\varphi(t,j) + \sum_l a^+_{jl}\varphi(t,l) = 0, \quad (29)$$

$$\frac{\partial}{\partial t}\hat{\varphi}(t,j) = \sum_l a^+_{lj}\hat{\varphi}(t,l). \quad (30)$$

Let q^*_t denote the distribution of the Schrödinger bridge at time t. We get

$$q^*_t(j) = \sum_i\sum_k q(t_0,i,t,j,t_1,k)q^*(i,k) = \quad (31)$$

$$\sum_i\sum_k \frac{p(t_0,i;t,j)p(t,j;t_1,k)}{p(t_0,i;t_1,k)}\hat{\varphi}(i)p(t_0,i,t_1,k)\varphi(k) \quad (32)$$

$$= \hat{\varphi}(t,j)\cdot\varphi(t,j). \quad (33)$$

Similarly, one gets for the transition probabilities

$$q^*(s,j,t,k) = p(s,j,t,k)\frac{\varphi(t,k)}{\varphi(s,j)}. \quad (34)$$

Notice, in particular, that the Schrödinger bridge is also a *Markov chain*. Notice, moreover, that the property

$$\sum_k q^*(s,j,t,k) = 1$$

follows from the fact that φ satisfies the backward equation

$$\varphi(s,j) := \sum_k p(s,j,t,k)\varphi(t,k).$$

Let us compute the infinitesimal generator $b^+_{jk}(t)$ of the Schrödinger bridge. From (34) one gets

$$b^+_{jk}(t) = a^+_{jk}(t)\frac{\varphi(t,k)}{\varphi(t,j)}, j\neq k. \quad (35)$$

VI. Stochastic mechanics of n-level quantum systems

Consider an n-level quantum system, namely a system where states are represented by unit vectors in a complex, n-dimensional Hilbert space $\mathcal{H}$. The pure states evolution is then given by

$$i\hbar\partial_t\psi = H\psi, \quad (36)$$

where H is the *Hamiltonian* operator. Let $\{\varphi_1,\ldots,\varphi_n\}$ be an orthonormal basis of $\mathcal{H}$. For $\psi\in\mathcal{H}$ with $\|\psi\|=1$, write $\psi_j := \langle\varphi_j,\psi\rangle$. We can then replace (36) with the system

$$i\hbar\partial_t\psi_j = \sum_k g_{jk}\exp\left(\frac{i}{\hbar}a_{jk}\right)\psi_k, \quad j=1,\ldots,n. \quad (37)$$

In the right-hand side of (37), the elements $h_{jk} = g_{jk}\exp\left(\frac{i}{\hbar}\alpha_{jk}\right)$ are such that $g_{jk}\geq 0$. By self-adjointness of the Hamiltonian, $g_{jk}=g_{kj}$ and $\alpha_{jk}=-\alpha_{kj}$. Write each component as

$$\psi_j = \rho_j^{1/2}\exp\left(\frac{i}{\hbar}S_j\right).$$

Then the complex system (37) turns into a real one

$$\dot{\rho}_j = \sum_k \frac{2g_{jk}}{\hbar}\sqrt{\rho_j\rho_k}\sin\beta_{jk}, \quad (38)$$

$$\dot{S}_j = -\sum_k g_{jk}\sqrt{\frac{\rho_k}{\rho_j}}\cos\beta_{jk}, \quad (39)$$

where

$$\beta_{jk} = \frac{\alpha_{jk}+S_k-S_j}{\hbar}, \quad \beta_{jk}=-\beta_{kj}, \quad \beta_{jj}=0.$$

Notice that (38) is a continuity equation implying conservation of the probability mass at each time

$$\sum_j \rho_j(t) = 1.$$

In the Nelson-Guerra *stochastic mechanics* [10], to each quantum evolution $\{\psi(t); t\geq t_0\}$, it is associated a jump Markov process (a continuous-time Markov chain) $\{q(t); t\geq t_0\}$ taking values in $\mathcal{X}=\{1,2,\ldots,n\}$. The probability of occupying the site j at time t is given by $\rho_j(t)=|\psi_j(t)|^2$. The infinitesimal generator of the Nelson process is given by

$$a^+_{jk} = \frac{g_{kj}}{\hbar}\sqrt{\frac{\rho_k}{\rho_j}}\left(\sin\left(\frac{\alpha_{kj}+S_j-S_k}{\hbar}\right)+1\right). \quad (40)$$

Consider the steering problem for the n-level system with ψ^0_j, $j=1,\ldots,n$ and ψ^1_j, $j=1,\ldots,n$ the given initial and final quantum states. Let q=$\{q(t); t_0\leq t\leq t_1\}$ be the Nelson jump Markov process associated to a quantum evolution (36). Consider the Schrödinger bridge problem for the process q with initial and final marginals $|\psi^0_j|^2$, $j=1,\ldots,n$ and $|\psi^1_j|^2$, $j=1,\ldots,n$, respectively. Then, to the solution of this problem q^* has infinitesimal generator that is related to the previous one as in (35). The new process may be viewed as the Nelson process of another quantum evolution, details will be provided in [19]. The new quantum evolution has the correct initial and final absolute values. Finally, in order to adjust the initial and final phases, one can use the freedom we have in picking the initial reference quantum evolution.

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