

# A Variational Approach to Sampling in Diffusion Processes

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**Abstract**—We revisit the work of Mitter and Newton on an information-theoretic interpretation of Bayes' formula through the Gibbs variational principle. This formulation allowed them to pose nonlinear estimation for diffusion processes as a problem in stochastic optimal control, so that the posterior density of the signal given the observation path could be sampled by adding a drift to the signal process. We show that this control-theoretic approach to sampling provides a common mechanism underlying several distinct problems involving diffusion processes, specifically importance sampling using Feynman–Kac averages, time reversal, and Schrödinger bridges.

Dedicated to the memory of Sanjoy K. Mitter (1933-2023)

## I. INTRODUCTION

In a remarkable paper [1], Mitter and Newton showed that the Kallianpur–Striebel formula, a core ingredient in the theory of nonlinear filtering for diffusion processes, can be derived from the Gibbs variational principle pertaining to the minimization of a certain free energy functional on the space of probability measures over paths. Among other things, this variational formulation provided an information-theoretic explanation of the fact that the PDE for the logarithm of the filtering density has the form of the Hamilton–Jacobi–Bellman equation for the value function of a particular stochastic control problem, a coincidence that had been noted earlier in several works [2]–[4]. Moreover, Mitter and Newton have shown that one can obtain exact samples from the filtering density by the addition of a drift term to the signal process, where the drift is of the state feedback form and is equal to the negative gradient of the value function.

In this paper, we show that a variational formulation based on free energy minimization underlies a broad circle of questions pertaining to diffusion processes which include, in addition to path estimation, such problems as time reversal [5]–[7], the Schrödinger bridge problem [7], [8], and importance sampling via Feynman–Kac averages [9]. In fact, this variational interpretation was implicit in some of the existing treatments of these problems; our aim here is to provide a unifying perspective and to draw attention to the fact that the particular constructions that emerge in the solutions of these problems can all be viewed as instances of stochastic optimal control of diffusion processes, in the spirit of the original work of Mitter and Newton. Due to space limitations, most technical details have been omitted; see [10].

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## II. THE GIBBS VARIATIONAL PRINCIPLE

Let  $(X, \mathcal{X})$  be a standard Borel space. Let  $\mathcal{P}(X)$  and  $\mathcal{H}(X)$  be the space of all probability measures on  $(X, \mathcal{X})$  and the space of all measurable functions  $H : X \rightarrow (-\infty, +\infty]$ , respectively. Let  $P, \tilde{P} \in \mathcal{P}(X)$  and  $H \in \mathcal{H}(X)$  be given. Then we define the following quantities:

$$D(\tilde{P} \| P) := \int_X \log \left( \frac{d\tilde{P}}{dP} \right) d\tilde{P} \text{ if } \tilde{P} \ll P, \quad (1)$$

+ ∞ otherwise,

$$i(H) := -\log \left( \int_X \exp(-H) dP \right) \quad (2)$$

if  $0 < \int_X \exp(-H) dP < \infty$ ,

− ∞ otherwise,

$$\langle H, \tilde{P} \rangle := \int_X H d\tilde{P} \text{ if the integral is finite,} \quad (3)$$

+ ∞ otherwise.

The quantity in eq. (1) is the relative entropy of  $P$  with respect to  $\tilde{P}$ . In the context of statistical physics,  $X$  acquires the interpretation of the state (or configuration) space of some physical system,  $P$  is some base (or reference) probability measure on the state space, and  $H$  is the energy (or Hamiltonian) function. Under this interpretation, the quantity  $i(H)$  defined in eq. (2) is the equilibrium free energy (at unit temperature), while the quantity  $\langle H, \tilde{P} \rangle$  is the average energy under an alternative probability measure  $\tilde{P}$ . The *Gibbs variational principle* [1], [11] states that  $i(H)$  is the minimum value of the *free energy*

$$F(\tilde{P}) := \langle H, \tilde{P} \rangle + D(\tilde{P} \| P) \quad (4)$$

among all  $\tilde{P}$ , and characterizes the unique minimizer of  $F(\cdot)$ :

**Proposition 1.** *Let  $P \in \mathcal{P}(X)$  and  $H \in \mathcal{H}(X)$  be such that*

$$-\int_X H \exp(-H) dP < \infty,$$

*with the convention  $+\infty \cdot \exp(-\infty) = 0$ . Then the probability measure  $P^* \in \mathcal{P}(X)$  defined by*

$$\frac{dP^*}{dP} = \frac{\exp(-H)}{\int_X \exp(-H) dP}$$

*is the unique minimizer of eq. (4), and  $i(H) = F(P^*) = \min_{\tilde{P} \in \mathcal{P}(X)} F(\tilde{P})$ .*

In many cases,  $(X, \mathcal{X})$  has the product structure  $(X_0 \times \bar{X}, \mathcal{X}_0 \otimes \bar{\mathcal{X}})$ , and we are interested in minimizing the free energy  $F(\cdot)$  subject to constraints on the marginal probability

law of  $X_0$ , where  $X$  splits into  $(X_0, \bar{X})$ . That is, we disintegrate the reference measure  $P$  as  $P(\cdot) = \int_{X_0} \mu(dx_0) P^{x_0}(\cdot)$ , where  $\mu$  is the marginal law of  $X_0$  under  $P$  and  $P^{x_0}$  is the regular conditional probability law of  $X$  given  $X_0 = x_0$ , and then minimize the free energy  $F(\tilde{P})$  over all  $\tilde{P} \in \mathcal{P}(X_0 \times \bar{X})$ , possibly subject to a constraint of the form  $\tilde{\mu} \in \mathcal{C}$ , where  $\tilde{\mu}$  is the marginal law of  $X_0$  under  $\tilde{P}$  and  $\mathcal{C}$  is some subset of  $\mathcal{P}(X_0)$ . We can use the chain rule for the relative entropy and Fubini's theorem to decompose the free energy as

$$\begin{aligned} F(\tilde{P}) &= \langle H, \tilde{P} \rangle + D(\tilde{P} \| P) \\ &= D(\tilde{\mu} \| \mu) + \int_{X_0} \tilde{\mu}(dx_0) F(x_0, \tilde{P}^{x_0}), \end{aligned} \quad (5)$$

where we have denoted by  $F(x_0, \tilde{P}^{x_0})$  the free energy of  $\tilde{P}^{x_0}$  with respect to the energy function  $H(x_0, \cdot)$  and the reference measure  $P^{x_0}$ . Then, applying Proposition 1 conditionally on  $x_0$ , we have  $F(\tilde{P}) \geq \langle v, \tilde{\mu} \rangle + D(\tilde{\mu} \| \mu)$ , where  $v(x_0) := -\log \int_{\bar{X}} e^{-H(x_0, \cdot)} dP^{x_0}$  is the minimum value of  $F(x_0, \cdot)$  achieved uniquely by  $dP^{*,x_0} \propto \exp -H(x_0, \cdot) dP^{x_0}$ . We conclude that

$$\min_{\tilde{P} \in \mathcal{P}(X): \tilde{\mu} \in \mathcal{C}} F(\tilde{P}) = \min_{\tilde{\mu} \in \mathcal{C}} (\langle v, \tilde{\mu} \rangle + D(\tilde{\mu} \| \mu)).$$

In particular, if  $\mathcal{C} = \{\mu\}$ , then the minimum is attained uniquely by the Gibbs mixture  $P^{*,\mu}(\cdot) := \int_{X_0} \mu(dx_0) P^{*,x_0}(\cdot)$ . If, on the other hand,  $\mathcal{C} = \mathcal{P}(X_0)$  (i.e., the marginal  $\tilde{\mu}$  is completely unconstrained), then we apply the Gibbs variational principle again to get

$$\min_{\tilde{P} \in \mathcal{P}(X)} F(\tilde{P}) = -\log \int_X e^{-H(x)} P(dx),$$

where the minimum is achieved uniquely by the mixture  $P^{*,\mu_*}$  with

$$\frac{d\mu_*}{d\mu} = \frac{\exp(-v)}{\int_{X_0} \exp(-v) d\mu}.$$

The problem of interest is how to generate samples from  $P^*$  (or from  $P^{*,\mu_*}$ ) when we have the means to generate samples from the reference measure  $P$ . In general, this runs into issues of computational tractability. However, in some specific instances it may be possible to exploit additional structure of the problem to deduce the existence of a measurable mapping  $\Phi: X \rightarrow X$ , such that  $P^* = P \circ \Phi^{-1}$ —in other words, we first obtain a sample  $X$  from  $P$  and then transform it into a sample  $\Phi(X)$  from  $P^*$ . As we shall see next, this is indeed possible when  $P$  is a sufficiently regular probability law of a diffusion process.

### III. THE PROBLEM SET-UP

We now particularize the setting of Section II to the case when  $(X, \mathcal{X})$  is the space  $(C([0, T]; \mathbb{R}^n), \mathcal{B}_T)$  of continuous paths  $x: [0, T] \rightarrow \mathbb{R}^n$ , where  $\mathcal{B}_T$  is the Borel  $\sigma$ -algebra induced by the uniform norm topology. The reference measure  $P$  is the probability law of the diffusion process governed by the Itô integral equation

$$\begin{aligned} X_t &= X_0 + \int_0^t b(X_s, s) ds + \int_0^t \sigma(X_s, s) dW_s, \\ X_0 &\sim \mu, \quad 0 \leq t \leq T \end{aligned} \quad (6)$$

where  $X_t$  takes values in  $\mathbb{R}^n$  and  $W_t$  takes values in  $\mathbb{R}^m$ . Here, the Borel probability law  $\mu$  and the mappings  $b(\cdot, \cdot)$  and  $\sigma(\cdot, \cdot)$  are assumed to satisfy enough regularity conditions for eq. (6) to have a unique strong solution. In the latter case, we will have a filtered probability space  $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$  that carries an  $\mathbb{R}^n$ -valued random variable  $X_0$  and an  $m$ -dimensional standard Brownian motion process  $W$  independent of  $X_0$ , as well as a measurable map  $\Phi: \mathbb{R}^n \times C([0, T]; \mathbb{R}^m) \rightarrow X$ , such that  $(X_t = \Phi_t(X_0, W); 0 \leq t \leq T)$  is an  $(\mathcal{F}_t)$ -adapted semimartingale satisfying eq. (6). The following conditions, imposed in [1], suffice for our purposes as well:

(R1) there exists a constant  $c > 0$ , such that

$$\int_{\mathbb{R}^n} \exp(c|z|^2) \mu(dz) < \infty;$$

(R2) there exists a constant  $K > 0$ , such that  $b$  and  $\sigma$  satisfy

$$\begin{aligned} |b(x, t) - b(\bar{x}, t)| + |\sigma(x, t) - \sigma(\bar{x}, t)| &\leq K|x - \bar{x}|, \\ |b(x, t)| &\leq K(1 + |x|), \\ |\sigma(x, t)| &\leq K \end{aligned}$$

for all  $x, \bar{x} \in \mathbb{R}^n$  and all  $0 \leq t \leq T$ , where we use  $|\cdot|$  to denote the Euclidean norm for vectors and the Hilbert–Schmidt norm for matrices;

Next, we assume that the Hamiltonian function  $H: X \rightarrow \mathbb{R}$  is of the form

$$H(X) = \int_0^T f(X_t, t) dt + g(X_T), \quad (7)$$

and the functions  $f(\cdot, \cdot)$  and  $g(\cdot)$  satisfy the following:

(H1)  $f$  and  $g$  are bounded from below, continuously differentiable, and there exists a constant  $C > 0$ , such that

$$\begin{aligned} |f(0, t)| &\leq C, \\ \sum_{i=1}^n \left| \frac{\partial}{\partial x_i} f(0, t) \right| &\leq C \end{aligned}$$

for all  $0 \leq t \leq T$ ;

(H2) the derivatives of  $f$  and  $g$  are Lipschitz continuous: there exists a constant  $M > 0$ , such that

$$\begin{aligned} \sum_{i=1}^n \left| \frac{\partial}{\partial x_i} f(x, t) - \frac{\partial}{\partial x_i} f(\bar{x}, t) \right| &\leq M|x - \bar{x}|, \\ \sum_{i=1}^n \left| \frac{\partial}{\partial x_i} g(x) - \frac{\partial}{\partial x_i} g(\bar{x}) \right| &\leq M|x - \bar{x}| \end{aligned}$$

for all  $x, \bar{x} \in \mathbb{R}^n$  and all  $0 \leq t \leq T$ .

The above assumptions ensure that  $\mathbf{E}[\exp(-H(X))] < \infty$  and  $-\mathbf{E}[H(X) \exp(-H(X))] \leq \mathbf{E}[\exp(-2H(X))] < \infty$ , where  $\mathbf{E}[\cdot]$  denotes expectation with respect to  $P$  [1]. It is also straightforward to verify that, under (H1) and (H2),  $f$  and  $g$  are of at most quadratic growth in  $x$  and their derivatives are of at most linear growth in  $x$ , uniformly in  $t$ .

We will need to consider the case when the initial condition  $X_0$  is nonrandom, i.e.,  $\mu$  in eq. (6) is a Dirac measure centered at some  $z \in \mathbb{R}^n$ . It is convenient, just as in [1], to define for each  $z \in \mathbb{R}^n$  and each  $0 \leq s \leq T$  the process

$(X_t^{z,s} : s \leq t \leq T)$  as the solution of (6) on the time interval  $s \leq t \leq T$  with initial condition  $X_s^{z,s} = z$ . Then we will denote by  $P^z$  the probability law of the process  $X^{z,0}$ . We also define the measurable maps

$$H: [0, T] \times \mathbb{R}^n \times \mathbb{X} \rightarrow \mathbb{R},$$

$$H(s, z, X^{z,s}) := \int_s^T f(X_t^{z,s}, t) dt + g(X_T^{z,s}) \quad (8)$$

[so that, in particular,  $H(X^{z,0}) = H(0, z, X^{z,0})$ ] and

$$v: \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R},$$

$$v(z, s) := -\log \mathbf{E} \exp(-H(s, z, X^{z,s})), \quad (9)$$

which is the equilibrium free energy of  $P^{z,s}$  corresponding to the Hamiltonian function  $H(s, z, \cdot)$ .

#### IV. THE OPTIMAL CONTROL PROBLEM

We now consider the controlled equation

$$\tilde{X}_t = z + \int_0^t \left( b(\tilde{X}_s, s) + a(\tilde{X}_s, s)u(\tilde{X}_s, s) \right) ds$$

$$+ \int_0^t \sigma(\tilde{X}_s, s) d\tilde{W}_s, \quad (10)$$

where  $a(x, s) := \sigma(x, s)\sigma(x, s)^T$ , and where the measurable function  $u: \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^n$  is the control. Let  $\mathbf{U}$  denote the set of all  $u$  with the following properties:

- (U1)  $u$  is continuous;
- (U2)  $\mathbf{E} Z^u = 1$ , where

$$Z^u := \exp \left( \int_0^T u^T \sigma(X_t^{z,0}, t) dW_t \right.$$

$$\left. - \frac{1}{2} \int_0^T |\sigma^T u(X_t^{z,0}, t)|^2 dt \right), \quad (11)$$

where the objects  $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$ ,  $W$ , and  $X^{z,0}$  are as above.

Following Beneš [12], we will refer to  $u \in \mathbf{U}$  as *admissible controls*, the maps  $(x, s) \mapsto b(x, s) + a(x, s)u(x, s)$  as *admissible drifts*, and to  $Z^u$  in eq. (11) as *attainable densities*. The problem, then, is to show that the Gibbs density

$$\frac{dP^{*,z}}{dP^z} = \frac{\exp(-H)}{\int_X \exp(-H) dP^z} = \frac{\exp(-H(0, z, \cdot))}{\int_X \exp(-H(0, z, \cdot)) dP^z}. \quad (12)$$

is an attainable density and to identify the admissible control  $u_* \in \mathbf{U}$ , such that  $\frac{dP^{*,z}}{dP^z} = Z^{u_*}$ . Let  $(\tilde{\Omega}, \tilde{\mathcal{F}}, (\tilde{\mathcal{F}}_t), \tilde{\mathbb{P}}, \tilde{X}, \tilde{W})$  be a weak solution of eq. (10) corresponding to an admissible control  $u \in \mathbf{U}$ . Let  $\tilde{P}$  denote the probability law of  $\tilde{X}$ . We then define the control cost of  $u$  by

$$J(u, z) := \langle H, \tilde{P} \rangle + D(\tilde{P} \| P^z)$$

$$= \tilde{\mathbf{E}} \left[ \int_0^T \left( f(\tilde{X}_t, t) + \frac{1}{2} |\sigma^T u(\tilde{X}_t, t)|^2 \right) dt + g(\tilde{X}_T) \right]. \quad (13)$$

The optimal control that attains the minimum of  $J(u, z)$  is given by the following theorem, in the spirit of [1, Thm. 4.2]:

**Theorem 1.** Suppose that  $b$ ,  $\sigma$ ,  $f$ , and  $g$  satisfy (R2), (H1), (H2). Define the function  $u_*: \mathbb{R}^n \times [0, T] \rightarrow \mathbb{R}^n$  by

$$u_*(x, t) := - \left( \frac{\partial v}{\partial x}(x, t) \right)^T, \quad (14)$$

where  $v$  is defined in eq. (9). Then  $u_*$  is an admissible control, and for all  $z \in \mathbb{R}^n$  and all  $\tilde{P} \in \mathcal{P}(\mathbb{X})$  (not necessarily arising from an admissible control),

$$J(u_*, z) \leq D(\tilde{P} \| P^z) + \langle H(0, z, \cdot), \tilde{P}_X \rangle. \quad (15)$$

We now turn to the case when the initial condition is random. To that end, consider the controlled process

$$\tilde{X}_t = \tilde{X}_0 + \int_0^t \left( b(\tilde{X}_s, s) + a(\tilde{X}_s, s)u(\tilde{X}_s, s) \right) ds$$

$$+ \int_0^t \sigma(\tilde{X}_s, s) d\tilde{W}_s, \quad (16)$$

for  $0 \leq t \leq T$ , with  $\tilde{X}_0 \sim \tilde{\mu}$ . We thus find ourselves in the situation described at the end of Section II involving minimization over both the admissible controls  $u$  and the initial condition  $\tilde{\mu}$ , possibly subject to additional constraints on  $\tilde{\mu}$ . Let  $\tilde{P}$  denote the distribution of  $\tilde{X}$  for a given pair  $(\tilde{\mu}, u)$ . Then, specializing the decomposition (5) to the present setting, we can write

$$F(\tilde{P}) = D(\tilde{\mu} \| \mu) + \langle J(u, \cdot), \tilde{\mu} \rangle,$$

which is minimized by the choice of  $u = u_*$  and of  $\tilde{\mu}$  as any minimizer of the functional  $\tilde{\mu} \mapsto D(\tilde{\mu} \| \mu) + \langle J(u_*, \cdot), \tilde{\mu} \rangle$  subject to the given constraint  $\tilde{\mu} \in \mathcal{C}$ . We will primarily consider the setting when (R1) holds for every element of  $\mathcal{C}$  for some constant  $c > 0$ .

#### V. CONSEQUENCES

We now examine several problems pertaining to diffusion processes through the control-theoretic lens of Theorem 1.

##### A. Feynman–Kac averages

Due to the structure of the Hamiltonian function  $H$  in (7), the Gibbs measures  $P^{*,z}$  in (12) are of the *Feynman–Kac type* [13]. Thus, the problem of generating samples from  $P^{*,z}$  is synonymous with the problem of computing (or estimating) Feynman–Kac averages of the form

$$\langle F, P^{*,z} \rangle = \frac{1}{\int_X \exp(-H) dP^z} \int_X F \exp(-H) dP^z \quad (17)$$

for bounded measurable functions  $F: \mathbb{X} \rightarrow \mathbb{R}$  on the path space  $\mathbb{X} = C([0, T]; \mathbb{R}^n)$ , provided we have a mechanism for generating random paths under the reference measure  $P^z$ . In some special cases, a sampling procedure can be built based on the ‘killing’ interpretation of Feynman–Kac averages [14]: If  $f$  is everywhere positive and  $g \equiv 0$ , then we can think of a particle following a path in the  $P^z$ -ensemble that gets ‘killed’ at a point  $(x, t)$  and in time interval  $[t, t + dt]$  with probability  $f(x, t) dt$ . Then the average of  $F$  over the paths that have ‘survived’ at time  $T$  is exactly the Feynman–Kac average (17). This procedure amounts to a reweighting of sample paths generated according to the reference measure.

To the best of the author's knowledge, the first explicit construction of an alternative sampling method relying, instead of killing, on the addition of a drift to the reference process was given by Ezawa, Klauder, and Shepp [9] in the special case when the reference process is an  $n$ -dimensional Brownian motion starting at  $z$  at  $t = 0$  and when  $g \equiv 0$  in (7). In fact, the drift constructed in [9] is exactly the optimal control  $u_*$  defined in (14), where the function  $\rho = \exp(-v)$  is given as a solution of a certain (linear) PDE. Following the ideas of Fleming [15], we can view this linear PDE as related to Hamilton–Jacobi–Bellman PDE for the value function  $v$  via the logarithmic (or Cole–Hopf) transformation  $v = -\log \rho$ . No such control-theoretic interpretation was given in the original paper [9], although it was pointed out in later works by other authors [16], [17].

### B. Reciprocal Markov processes and the Schrödinger bridge

Let two Borel probability measures  $\mu, \mu'$  on  $\mathbb{R}^n$  be given. Consider the controlled process (16) with  $\tilde{X}_0 \sim \mu$ . We wish to find an admissible drift  $u \in \mathcal{U}$  such that the ‘energy’

$$\frac{1}{2} \tilde{\mathbf{E}} \int_0^T \frac{1}{2} |\sigma^T u(\tilde{X}_t, t)|^2 dt$$

is minimized subject to the constraint  $\tilde{X}_T \sim \mu'$ . This problem, going back to the work of Schrödinger and Bernstein on so-called reciprocal Markov processes, is now commonly referred to as the *Schrödinger bridge* problem [7]. A control-theoretic treatment was given by Dai Pra [8]. Here, we revisit it from the free energy minimization perspective and, in particular, explicitly identify the corresponding Gibbs measure on the path space.

We assume that, in addition to (R1) and (R2),  $z^T a(\tilde{z}, t) z \geq c|z|^2$  holds with some constant  $c > 0$  for all  $z, \tilde{z} \in \mathbb{R}^n$  and all  $t \in [0, T]$ , so that the reference process (6) is nondegenerate, as in [8]. This ensures the existence of everywhere positive transition densities  $p(z, y; s, t)$  for  $0 \leq s \leq t \leq T$  and  $z, y \in \mathbb{R}^n$ , so that

$$\mathbf{E} h(X_t^{z,s}) = \int_{\mathbb{R}^n} h(y) p(z, y; s, t) dy$$

for all bounded, measurable  $h : \mathbb{R}^n \rightarrow \mathbb{R}$ . We will denote by  $\tilde{\mu}'$  the probability law of  $X_T$  under the reference process (6) when  $X_0 \sim \mu$ , i.e.,

$$\tilde{\mu}'(A) = \int_A \left( \int_{\mathbb{R}^n} p(z, y; 0, T) \mu(dz) \right) dy$$

for any Borel set  $A \subseteq \mathbb{R}^n$ ; in particular,  $\tilde{\mu}'$  has a density with respect to the Lebesgue measure. We assume henceforth that  $\mu'$  is absolutely continuous w.r.t.  $\tilde{\mu}'$ .

Following [8], we will make essential use of the following key structural result of Beurling [18] and Jamison [19]: Given  $\mu, \mu'$ , and  $p$ , there exist two unique  $\sigma$ -finite Borel measures  $\nu$  and  $\nu'$  on  $\mathbb{R}^n$ , such that the measure

$$\pi(E) := \int_E p(z, y; 0, T) \nu(dz) \nu'(dy) \quad (18)$$

on  $\mathbb{R}^n \times \mathbb{R}^n$  has marginals  $\mu$  and  $\mu'$ , i.e.,

$$\pi(\cdot \times \mathbb{R}^n) = \mu(\cdot), \quad \pi(\mathbb{R}^n \times \cdot) = \mu'(\cdot); \quad (19)$$

moreover,  $\mu \sim \nu$  and  $\mu' \sim \nu'$ , where  $\sim$  indicates equivalence (mutual absolute continuity) of measures. Since  $\tilde{\mu}'$  has a density w.r.t. the Lebesgue measure, so does  $\nu'$ . Denoting the latter density by  $q$ , let us define

$$\rho(z, t) := \mathbf{E}[q(X_T^{z,t})] = \int_{\mathbb{R}^n} p(z, y; t, T) q(y) dy.$$

Then  $\rho(z, T) = q(z)$ , and it follows from (18) and (19) that

$$\rho(z, 0) = \int_{\mathbb{R}^n} p(z, y; 0, T) q(y) dy = \frac{d\mu}{d\nu}(z).$$

For a nonrandom initial condition  $\tilde{X}_0 = z$ , consider the Gibbs measure  $P^{*,z}$  with

$$\frac{dP^{*,z}}{dP^z} = \frac{q(X_T^z)}{\rho(z, 0)} = \frac{\exp(-H(X^z))}{\mathbf{E}_{P^z} \exp(-H(X^z))}$$

corresponding to  $H(X^z) = -\log q(X_T^z)$ , i.e., we take  $f \equiv 0$  and  $g = -\log q$  in (7). Assuming  $g$  is such that (H1) and (H2) are satisfied, Theorem 1 tells us that we can obtain samples from  $P^{*,z}$  using the admissible control

$$u_*(x, t) = - \left( \frac{\partial v}{\partial x}(x, t) \right)^T$$

with  $v(x, t) = -\log \rho(x, t)$ ; the same control also yields the optimal solution for the random initial condition  $\mu$ , and in that case the law of the corresponding controlled process  $(\tilde{X}_t^*; 0 \leq t \leq T)$  is given by the Gibbs mixture

$$P^{*,\mu} = \int_{\mathbb{R}^n} \mu(dz) P^{*,z} \quad (20)$$

(cf. the discussion following the proof of Theorem 1). It is readily verified that  $\tilde{X}_T^*$  has the prescribed law  $\mu'$ : For any bounded and measurable  $h : \mathbb{R}^n \rightarrow \mathbb{R}$ , we have

$$\begin{aligned} \mathbf{E} h(\tilde{X}_T^*) &= \int_{\mathbb{R}^n \times \mathbb{R}^n} h(y) p(z, y; 0, T) \frac{q(y)}{\rho(z, 0)} \mu(dz) dy \\ &= \int_{\mathbb{R}^n \times \mathbb{R}^n} h(y) p(z, y; 0, T) \nu(dz) \nu'(dy) \\ &= \int_{\mathbb{R}^n} h(y) \mu'(dy). \end{aligned}$$

The corresponding free energies (or minimum expected costs) can be computed as follows. First, for the nonrandom initial condition  $\tilde{X}_0 = z$ , we have

$$\begin{aligned} F(z, P^{*,z}) &= \frac{1}{2} \mathbf{E} \int_0^T |\sigma^T u_*(\tilde{X}_t^{z,z}, t)|^2 dt - \mathbf{E}[\log q(\tilde{X}_T^{z,z})] \\ &= -\log \rho(z, 0) = -\log \frac{d\mu}{d\nu}(z); \end{aligned}$$

then, under (20),

$$F(P^{*,\mu}) = \int_{\mathbb{R}^n} F(z, P^{*,z}) \mu(dz) = -D(\mu \parallel \nu),$$

where we have extended the definition (1) of the relative entropy  $D(\cdot \parallel \cdot)$  to any pair of  $\sigma$ -finite Borel measures (recall

that  $\mu \sim \nu$ ). Using these, we can recover the following expression for the ‘minimum control effort’ from [8]:

$$\frac{1}{2} \mathbf{E} \int_0^T |\sigma^T u_*(\tilde{X}_t^*)|^2 dt = D(\mu' \|\tilde{\nu}') - D(\mu \|\nu),$$

where  $\tilde{\nu}'(A) := \int_A \left( \int_{\mathbb{R}^n} p(z, y; 0, T) \nu(dz) \right) dy$ .

In general, the determination of the Beurling–Jamison measures  $\nu$  and  $\nu'$  in (18) and (19) is not straightforward, and can be done using a forward-backward successive approximation scheme going back to the seminal work of Fortet, cf. [20] and references therein. However, an explicit solution can be given when  $\mu = \delta_0$  (the Dirac measure at  $z = 0$ ) and when the reference process is a standard  $n$ -dimensional Brownian motion ( $W_t; 0 \leq t \leq T$ ) [7]. In that case,  $\tilde{\mu}'$  is the Gaussian measure  $\gamma_T$  with mean 0 and covariance matrix  $T I_n$ ,  $\nu = \mu = \delta_0$ , and  $q = \frac{d\mu'}{d\gamma_T}$ . The value function is then given by  $v(x, t) = -\log \mathbf{E}[q(x + W_T - W_t)]$ , and the optimal control  $u_*(x, t) = -\left(\frac{\partial v}{\partial x}(x, t)\right)^T$  (the so-called *Föllmer drift*) attains the minimum energy

$$\frac{1}{2} \mathbf{E} \int_0^T |u_*(\tilde{X}_t^*)|^2 dt = D(\mu' \|\gamma_T).$$

### C. Time reversal of diffusions

A closely related problem is the following [5], [6]: Consider an  $n$ -dimensional diffusion process

$$X_t = X_0 + \int_0^t b(X_s, s) ds + \int_0^t \sigma(X_s, s) dW_s, 0 \leq t \leq T \quad (21)$$

(where, as before,  $W_t$  is an  $m$ -dimensional standard Brownian motion) and define its time reversal  $\bar{X}_t := X_{T-t}$  for  $0 \leq t \leq T$ . The question is to determine whether  $\bar{X}_t$  is itself a diffusion process, so that it can be expressed as

$$\bar{X}_t = \bar{X}_0 + \int_0^t \bar{b}(\bar{X}_s, s) ds + \int_0^t \bar{\sigma}(\bar{X}_s, s) d\bar{W}_s \quad (22)$$

for some  $\bar{b}$ ,  $\bar{\sigma}$  and for some  $m$ -dimensional Brownian motion  $\bar{W}$ . Haussmann and Pardoux [6] showed that, under certain regularity conditions, there exists an  $m$ -dimensional Brownian motion process  $\bar{W}$ , such that (22) holds with

$$\begin{aligned} \bar{b}_i(x, t) &= -b_i(x, T-t) \\ &+ p(x, T-t)^{-1} \sum_{j=1}^n \frac{\partial}{\partial x_j} (a_{ij}(x, T-t) p(x, T-t)), \\ \bar{\sigma}_{ik}(x, t) &= \sigma_{ik}(x, T-t), \bar{a}_{ij}(x, t) = a_{ij}(x, T-t) \end{aligned} \quad (23)$$

for  $i, j = 1, \dots, n$  and  $k = 1, \dots, m$ . As in [6], we adopt the convention that the term involving  $p(x, T-t)^{-1}$  is set to zero if  $p(x, T-t) = 0$ . We now derive the result of [6] as a consequence of Theorem 1.

To that end, we first rewrite the drift  $\bar{b}$  in (23) as

$$\bar{b}(x, t) = \hat{b}(x, t) + \bar{a}(x, t) \left( \frac{\partial}{\partial x} \log \bar{p}(x, t) \right)^T, \quad (24)$$

where

$$\hat{b}_i(x, t) := -b_i(x, T-t) + \sum_{j=1}^n \frac{\partial}{\partial x_j} \bar{a}_{ij}(x, t), i = 1, \dots, n \quad (25)$$

and  $\bar{p}(x, t) := p(x, T-t)$ . Let  $P$  denote the probability law of the process

$$\hat{X}_t = \hat{X}_0 + \int_0^t \hat{b}(\hat{X}_s, s) ds + \int_0^t \bar{\sigma}(\hat{X}_s, s) d\bar{W}_s \quad (26)$$

with  $\hat{X}_0$  having density  $\bar{p}(\cdot, 0) \equiv p(\cdot, T)$ . This will be our reference process. The processes  $\{\hat{X}_t^{z,s} : s \leq t \leq T\}$  for  $z \in \mathbb{R}^n$  and  $0 \leq s \leq T$  are defined in the same way as before, and  $P^z$  will denote the probability law of  $\hat{X}^{z,0}$ . We will next show that the second term on the right-hand side of (24) arises as an optimal control for an appropriately defined Hamiltonian, the controlled process now taking the form

$$\begin{aligned} \tilde{X}_t &= \tilde{X}_0 + \int_0^t \left( \hat{b}(\tilde{X}_s, s) + \bar{a}(\tilde{X}_s, s) u(\tilde{X}_s, s) \right) ds \\ &+ \int_0^t \bar{\sigma}(\tilde{X}_s, s) d\tilde{W}_s \end{aligned} \quad (27)$$

with random initialization  $\tilde{X}_0$  having density  $\bar{p}(\cdot, 0)$ .

Under appropriate regularity conditions [10], (R2) holds for  $\hat{b}$  and  $\bar{\sigma}$ , and (H1)–(H2) hold for the Hamiltonian

$$H(\hat{X}) = \int_0^T f(\hat{X}_t, t) dt + g(\hat{X}_T)$$

with

$$f(x, t) := \sum_{i=1}^n \frac{\partial}{\partial x_i} \hat{b}_i(x, t), \quad g(x) := -\log p(x, 0). \quad (28)$$

Moreover, the density  $p(x, t)$  of  $X_t$  in (21) is a classical solution of the forward Kolmogorov equation

$$\begin{aligned} \frac{\partial}{\partial t} p(x, t) &= - \sum_{i=1}^n \frac{\partial}{\partial x_i} (b_i(x, t) p(x, t)) \\ &+ \frac{1}{2} \sum_{i,j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} (a_{ij}(x, t) p(x, t)) \end{aligned}$$

for  $(x, t) \in \mathbb{R}^n \times [0, T]$  (see, e.g., [21]). It is then readily verified that the time-reversed density  $\bar{p}(x, t)$  is a solution of the Cauchy problem

$$\frac{\partial}{\partial t} \bar{p}(x, t) + \hat{L} \bar{p}(x, t) - f(x, t) \bar{p}(x, t) = 0 \text{ on } \mathbb{R}^n \times [0, T]$$

subject to  $\bar{p}(x, T) = p(x, 0)$ , where

$$\hat{L} = \sum_i \hat{b}_i(\cdot, t) \frac{\partial}{\partial x_i} + \frac{1}{2} \sum_{i,j} \bar{a}_{ij}(\cdot, t) \frac{\partial^2}{\partial x_i \partial x_j}$$

is the generator of the reference process (26). The Feynman–Kac formula gives the following expression:

$$v(x, t) := -\log \bar{p}(x, t) = -\log \mathbf{E} \exp(-H(t, x, \hat{X}^{x,t})),$$

where, analogously to (8), we have defined

$$H(t, x, \hat{X}^{x,t}) := \int_t^T f(\hat{X}_s^{x,t}, s) ds + g(\hat{X}_T^{x,t})$$

with  $f$  and  $g$  given in (28). Theorem 1 then says that

$$u_*(x, t) = - \left( \frac{\partial v}{\partial x}(x, t) \right)^T = \left( \frac{\partial}{\partial x} \log \bar{p}(x, t) \right)^T$$

minimizes the expected cost

$$J(u, z) = \tilde{\mathbf{E}} \left[ \int_0^T \left( \frac{1}{2} |\bar{\sigma}^T u(\tilde{X}_t, t)|^2 + \sum_{i=1}^n \frac{\partial}{\partial x_i} \hat{b}_i(\tilde{X}_t, t) \right) dt - \log p(\tilde{X}_T, 0) \right]$$

over all admissible controls for (27) with nonrandom initial condition  $\tilde{X}_0 = z$ , and also attains the Gibbs measure  $dP^{*,z} \propto \exp(-H(\tilde{X}^{z,0})) dP^z$ . As a consequence, we obtain the following variational representation of  $-\log p(\cdot, t)$ :

$$\begin{aligned} & -\log p(z, t) \\ &= \min_u \tilde{\mathbf{E}} \left[ \int_{T-t}^T \left( \frac{1}{2} |\bar{\sigma}^T u(\tilde{X}_s, s)|^2 + \sum_{i=1}^n \frac{\partial}{\partial x_i} \hat{b}_i(\tilde{X}_s, s) \right) ds - \log p(\tilde{X}_T; 0) \middle| \tilde{X}_{T-t} = z \right], \end{aligned}$$

where the minimization is over all admissible controls for (27). The second term in the integrand is the divergence of the drift vector field  $\hat{b}$ , which depends on  $b$  and on the derivatives of  $a$  w.r.t.  $x$ , cf. (25). The special case of  $\sigma$  depending only on  $t$  was worked out in [22] and, recently, in [23] in the context of probabilistic generative models.

The same control  $u_*$  also works for the random initial condition  $\tilde{X}_0$  with density  $\bar{p}(\cdot, 0) \equiv p(\cdot, T)$ , and the probability law of the corresponding process  $\{\tilde{X}_t^* : 0 \leq t \leq T\}$  with  $\tilde{X}_t^*$  sampled from  $p(\cdot, T)$  is the Gibbs mixture  $P^{*,p(\cdot,T)} = \int_{\mathbb{R}^n} p(z, T) P^{*,z} dz$ . This is also the probability law of the process  $\{\tilde{X}_t : 0 \leq t \leq T\}$ , the time reversal of  $X_t$  in (21). The minimum value of the free energy is given by

$$F(P^{*,p(\cdot,T)}) = - \int_{\mathbb{R}^n} p(z, T) \log p(z, T) dz,$$

the differential entropy of the density  $p(\cdot, T)$  [24, Sec. 1.3], which is finite because  $p(\cdot, T)$  has finite second moments.

## VI. CONCLUSIONS

We have revisited the work of Mitter and Newton [1] which used an information-theoretic interpretation of the Bayes' formula to develop an optimal control approach to sampling from conditional densities of diffusion processes. While variational formulations of the Bayes' formula as free energy minimization can be found in other works (see, e.g., Zellner [25] and Walker [26]), the stochastic control formulation in [1] leads to an alternative procedure for conditional sampling not based on iterative methods like Markov chain Monte Carlo. We have shown that free energy minimization provides a natural framework for a number of

other problems arising in the context of diffusion processes, and that the stochastic optimal control viewpoint can be used to explain the structure of the solutions to these problems.

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