

## I. RESTATEMENT OF THE MAIN RESULT AND ITS PROOF

We restate Theorem 1 below which now includes the pde formulation as well.

**Theorem 1.** *Consider the variational problem (11)-(14).*

(i) *For the probabilistic form (11) of the variational problem, the optimal control  $U_t^* = e^{\alpha_t - \gamma_t} Y_t$ , where the optimal trajectory  $\{(X_t, Y_t)\}_{t \geq 0}$  evolves according to the Hamilton's odes:*

$$\frac{dX_t}{dt} = U_t^* = e^{\alpha_t - \gamma_t} Y_t, \quad X_0 \sim \rho_0 \quad (\text{I.1a})$$

$$\frac{dY_t}{dt} = -e^{\alpha_t + \beta_t + \gamma_t} \nabla_\rho F(\rho_t)(X_t), \quad Y_0 = \nabla \phi_0(X_0) \quad (\text{I.1b})$$

where  $\phi_0$  is a convex function, and  $\rho_t = \text{Law}(X_t)$ .

(ii) *For the pde form (14) of the variational problem, the optimal control is  $u_t^* = e^{\alpha_t - \gamma_t} \nabla \phi_t(x)$ , where the optimal trajectory  $\{(\rho_t, \phi_t)\}_{t \geq 0}$  evolves according to the Hamilton's pdes:*

$$\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\underbrace{\rho_t e^{\alpha_t - \gamma_t} \nabla \phi_t}_{u_t^*}), \quad \text{initial condn. } \rho_0 \quad (\text{I.2a})$$

$$\frac{\partial \phi_t}{\partial t} = -e^{\alpha_t - \gamma_t} \frac{|\nabla \phi_t|^2}{2} - e^{\alpha_t + \gamma_t + \beta_t} \nabla_\rho F(\rho) \quad (\text{I.2b})$$

(iii) *The solutions of the two forms are equivalent in the following sense:*

$$\text{Law}(X_t) = \rho_t, \quad U_t = u_t(X_t), \quad Y_t = \nabla \phi_t(X_t)$$

(iv) *Suppose additionally that the functional  $F$  is displacement convex and  $\rho_\infty$  is its minimizer.*

*Define*

$$V(t) = \frac{1}{2} \mathbb{E}(|X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)|^2) + e^{\beta_t} (F(\rho) - F(\rho_\infty)) \quad (\text{I.3})$$

where the map  $T_{\rho_t}^{\rho_\infty} : \mathbb{R}^d \rightarrow \mathbb{R}^d$  is the optimal transport map from  $\rho_t$  to  $\rho_\infty$ . Assume the dimension  $d = 1$ . Consequently, the following rate of convergence is obtained along the optimal trajectory

$$F(\rho_t) - F(\rho_\infty) \leq O(e^{-\beta_t}), \quad \forall t \geq 0$$

*Proof.* (i) The Hamiltonian function defined in (12) is equal to

$$H(t, x, \rho, y, u) = y \cdot u - e^{\gamma_t - \alpha_t} \frac{1}{2} |u|^2 + e^{\alpha_t + \gamma_t + \beta_t} \tilde{F}(\rho, x)$$

after inserting the formula for the Lagrangian. According to the maximum principle in probabilistic form for (mean-field) optimal control problems (see [1, Sec. 6.2.3]), the optimal control law  $U_t^* = \arg \min_v H(t, X_t, \rho_t, Y_t, v) = e^{\alpha_t - \gamma_t} Y_t$  and the Hamilton's equations are

$$\begin{aligned} \frac{dX_t}{dt} &= +\nabla_y H(t, X_t, \rho_t, Y_t, U_t^*) = U_t^* = e^{\alpha_t - \gamma_t} Y_t \\ \frac{dY_t}{dt} &= -\nabla_x H(t, X_t, \rho_t, Y_t, U_t^*) - \tilde{E}[\nabla_\rho H(t, \tilde{X}_t, \rho_t, \tilde{Y}_t, \tilde{U}_t^*)(X_t)] \end{aligned}$$

where  $\tilde{X}_t, \tilde{Y}_t, \tilde{U}_t^*$  are independent copies of  $X_t, Y_t, U_t^*$ . The derivatives

$$\begin{aligned} \nabla_x H(t, x, \rho, y, u) &= e^{\alpha_t + \beta_t + \gamma_t} \nabla_x \tilde{F}(\rho, x) \\ \nabla_\rho H(t, x, \rho, y, u) &= e^{\alpha_t + \beta_t + \gamma_t} \nabla_\rho \tilde{F}(\rho, x) \end{aligned}$$

It follows that

$$\frac{dY_t}{dt} = -e^{\alpha_t + \beta_t + \gamma_t} (\nabla_x \tilde{F}(\rho_t, X_t) + \tilde{E}[\nabla_\rho \tilde{F}(\rho_t, \tilde{X}_t)(X_t)]) = -e^{\alpha_t + \beta_t + \gamma_t} \nabla_\rho F(\rho)(X_t)$$

where we used the definition  $F(\rho) = \int \tilde{F}(x, \rho) \rho(x) dx$  and the identity [1, Sec. 5.2.2 Example 3]

$$\nabla_\rho F(\rho)(x) = \nabla_x \tilde{F}(\rho, x) + \int \nabla_\rho \tilde{F}(\rho, \tilde{x})(x) \rho(\tilde{x}) d\tilde{x}$$

(ii) The Hamiltonian function defined in (15) is equal to

$$\mathcal{H}(t, \rho, \phi, u) = \int \left[ \nabla \phi(x) \cdot u(x) - \frac{1}{2} e^{\gamma_t - \alpha_t} |u(x)|^2 \right] \rho(x) dx + e^{\alpha_t + \gamma_t + \beta_t} F(\rho)$$

after inserting the formula for the Lagrangian. According to the maximum principle for pde formulation of mean-field optimal control problems (see [1, Sec. 6.2.4]) the optimal control vector field is  $u_t^* = \arg \min_v \mathcal{H}(t, \rho_t, \phi_t, v) = e^{\alpha_t - \gamma_t} \nabla \phi_t$  and the Hamilton's equations are:

$$\begin{aligned} \frac{\partial \rho_t}{\partial t} &= +\frac{\partial \mathcal{H}}{\partial \phi}(t, \rho_t, \phi_t, u_t) = -\nabla \cdot (\rho_t \nabla u_t^*) \\ \frac{\partial \phi_t}{\partial t} &= -\frac{\partial \mathcal{H}}{\partial \rho}(t, \rho_t, \phi_t, u_t) = -(\nabla \phi \cdot u^* - e^{\gamma_t - \alpha_t} \frac{1}{2} |u_t^*|^2 + e^{\alpha_t + \gamma_t + \beta_t} \frac{\partial F}{\partial \rho}(\rho_t)) \end{aligned}$$

inserting the formula  $u_t^* = e^{\alpha_t - \gamma_t} \nabla \phi_t$  concludes the result.

(iii) Consider the  $(\rho_t, \phi_t)$  defined from (I.2). The distribution  $\rho_t$  is identified with a stochastic process  $\tilde{X}_t$  such that  $\frac{d\tilde{X}_t}{dt} = e^{\alpha_t - \gamma_t} \nabla \phi_t(\tilde{X}_t)$  and  $\text{Law}(\tilde{X}_t) = \rho_t$ . Then define  $\tilde{Y}_t = \nabla \phi_t(\tilde{X}_t)$ . Taking the time derivative shows that

$$\begin{aligned} \frac{d\tilde{Y}_t}{dt} &= \frac{d}{dt} \nabla \phi_t(\tilde{X}_t) = \nabla^2 \phi_t(\tilde{X}_t) \frac{d\tilde{X}_t}{dt} + \nabla \frac{\partial \phi_t}{\partial t}(X_t) \\ &= e^{\alpha_t - \gamma_t} \nabla^2 \phi_t(\tilde{X}_t) \nabla \phi_t(\tilde{X}_t) - e^{\alpha_t - \gamma_t} \nabla^2 \phi_t(\tilde{X}_t) \nabla \phi_t(X_t) - e^{\alpha_t + \beta_t + \gamma_t} \nabla \frac{\partial F}{\partial \rho}(\rho_t)(\tilde{X}_t) \\ &= -e^{\alpha_t + \beta_t + \gamma_t} \nabla \frac{\partial F}{\partial \rho}(\rho_t)(\tilde{X}_t) \\ &= -e^{\alpha_t + \beta_t + \gamma_t} \nabla_\rho F(\rho_t)(\tilde{X}_t) \end{aligned}$$

with the initial condition  $\tilde{Y}_0 = \nabla \phi_0(\tilde{X}_0)$ , where we used the identity  $\nabla_x \frac{\partial F}{\partial \rho}(\rho) = \nabla_\rho F(\rho)$  [1, Prop. 5.48]. Therefore the equations for  $\tilde{X}_t$  and  $\tilde{Y}_t$  are identical. Hence one can identify  $(X_t, Y_t)$  with  $(\tilde{X}_t, \tilde{Y}_t)$ .

(iv) The energy functional

$$V(t) = \frac{1}{2} \underbrace{\mathbb{E} [ |X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)|^2 ]}_{\text{first term}} + \underbrace{e^{\beta_t} (F(\rho) - F(\rho_\infty))}_{\text{second term}}$$

Then the derivative of the first term is

$$\mathbb{E} \left[ (X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)) \cdot (e^{\alpha_t - \gamma_t} Y_t - \dot{\gamma}_t e^{-\gamma_t} Y_t - e^{\alpha_t + \beta_t} \nabla_\rho F(\rho_t)(X_t) + \xi(T_{\rho_t}^{\rho_\infty}(X_t))) \right]$$

where  $\xi(T_{\rho_t}^{\rho_\infty}(X_t)) := \frac{d}{dt} T_{\rho_t}^{\rho_\infty}(X_t)$ . Using the scaling condition  $\dot{\gamma}_t = e^{\alpha_t}$  the derivative of the first term simplifies to

$$\mathbb{E} \left[ (X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)) \cdot (-e^{\alpha_t + \beta_t} \nabla_\rho F(\rho_t)(X_t) + \xi(T_{\rho_t}^{\rho_\infty}(X_t))) \right]$$

We claim that when the dimension  $d = 1$ , the expectation

$$\mathbb{E}[(X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)) \cdot \xi(T_{\rho_t}^{\rho_\infty}(X_t))] = 0 \quad (\text{I.4})$$

We present the proof for the claim at the end. Assuming that the claim is true, the derivative of the first term simplifies to

$$\mathbb{E} \left[ (X_t + e^{-\gamma_t} Y_t - T_{\rho_t}^{\rho_\infty}(X_t)) \cdot (-e^{\alpha_t + \beta_t} \nabla_\rho F(\rho_t)(X_t)) \right]$$

The derivative of the second term is

$$\begin{aligned} \frac{d}{dt} (\text{second term}) &= \dot{\beta}_t e^{\beta_t} (F(\rho_t) - F(\rho_\infty)) + e^{\beta_t} \frac{d}{dt} F(\rho_t) \\ &= e^{\alpha_t + \beta_t} (F(\rho_t) - F(\rho_\infty)) + e^{\beta_t} \mathbb{E}[\nabla_\rho F(\rho_t)(X_t) e^{\alpha_t - \gamma_t} Y_t] \end{aligned}$$

where we used the scaling condition  $\beta_t = e^{\alpha_t}$  and the chain-rule for the Wasserstein gradient [2, Ch. 10, E. Chain rule]. Adding the derivative of the first and second term yields:

$$\frac{dV}{dt}(t) = e^{\alpha_t + \beta_t} (F(\rho_t) - F(\rho_\infty) - E[(X_t - T_{\rho_t}^{\rho_\infty}(X_t)) \cdot \nabla_\rho F(\rho_t)(X_t)])$$

which is negative by variational inequality characterization of the displacement convex function  $F(\rho)$  [2, Eq. 10.1.7].

We now present the proof of the claim (I.4) under the assumption that  $d = 1$ . According to Brenier theorem [3], there exists a convex function  $\psi_t$  such that  $T_{\rho_t}^{\rho_\infty}(x) = \nabla \psi_t(x)$  and  $T_{\rho_\infty}^{\rho_t}(x) = \nabla \psi_t^*(x)$  where  $\psi_t^*$  is the convex conjugate of  $\psi_t$ . Because  $\rho_\infty$  is the push-forward of  $\rho_t$  under the map  $\nabla \psi_t$ , we have

$$E[g(\nabla \psi_t(X_t))] = \int g(x) \rho_\infty(x) dx,$$

for all measurable functions  $g$ . Upon taking the derivative with respect to time,

$$\frac{d}{dt} E[g(\nabla \psi_t(X_t))] = \frac{d}{dt} \int g(x) \rho_\infty(x) dx = 0$$

Hence by application of the dominated convergence theorem (DCT) and interchanging the expectation and the derivative,

$$E\left[\frac{d}{dt} g(\nabla \psi_t(X_t))\right] = E[\nabla g(\nabla \psi_t(X_t)) \cdot \xi(\nabla \psi_t(X_t))] = 0 \quad (\text{I.5})$$

Letting  $g(x) = \psi^*(x) - e^{-\gamma} \int_{-\infty}^x \nabla \phi_t(\nabla \psi^*(z)) dz - \frac{1}{2}|x|^2$  where  $\phi_t$  is defined in part-(ii) of the theorem 1 concludes

$$\begin{aligned} 0 &= E[\nabla g(\nabla \psi_t(X_t)) \cdot \xi(\nabla \psi_t(X_t))] = E[X_t - e^{-\gamma} \nabla \phi_t(X_t) - \nabla \psi_t(X_t) \cdot \xi(\nabla \psi_t(X_t))] \\ &= E[X_t - e^{-\gamma} Y_t - \nabla \psi_t(X_t) \cdot \xi(\nabla \psi_t(X_t))] \end{aligned}$$

where we used  $Y_t = \nabla \phi_t(X_t)$  from part-(iii) of Theorem 1. This concludes the proof of the claim. Note that the application of DCT in (I.5) follows from smoothness of  $g(x)$  and assuming  $T_{\rho_t}^{\rho_\infty}(x)$  is differentiable with respect to time. Showing  $T_{\rho_t}^{\rho_\infty}(x)$  is differentiable with respect to time is technical out of the scope of this work. □

## II. WASSERSTEIN GRADIENT AND GÂTEAUX DERIVATIVE

This section contains definitions of the Wasserstein gradient and Gâteaux derivative [2], [1].

Let  $F : \mathcal{P}_{ac,2}(\mathbb{R}^d) \rightarrow \mathbb{R}$  be a (smooth) functional on the space of probability distributions.

**Gâteaux derivative:** The Gâteaux derivative of  $F$  at  $\rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d)$  is a real-valued function on  $\mathbb{R}^d$  denoted as  $\frac{\partial F}{\partial \rho}(\rho) : \mathbb{R}^d \rightarrow \mathbb{R}$ . It is defined as a function that satisfies the identity

$$\left. \frac{d}{dt} F(\rho_t) \right|_{t=0} = \int_{\mathbb{R}^d} \frac{\partial F}{\partial \rho}(\rho)(x) (-\nabla \cdot (\rho(x)u(x))) dx$$

for all path  $\rho_t$  in  $\mathcal{P}_{ac,2}(\mathbb{R}^d)$  such that  $\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t u)$  with  $\rho_0 = \rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d)$ .

**Wasserstein gradient:** The Wasserstein gradient of  $F$  at  $\rho$  is a vector-field on  $\mathbb{R}^d$  denoted as  $\nabla_{\rho} F(\rho) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ . It is defined as a vector-field that satisfies the identity

$$\left. \frac{d}{dt} F(\rho_t) \right|_{t=0} = \int_{\mathbb{R}^d} \nabla_{\rho} F(\rho)(x) \cdot u(x) \rho(x) dx$$

for all path  $\rho_t$  in  $\mathcal{P}_{ac,2}(\mathbb{R}^d)$  such that  $\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t u)$  with  $\rho_0 = \rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d)$ .

The two definitions imply the following relationship [1, Prop. 5.48]:

$$\nabla_{\rho} F(\rho)(\cdot) = \nabla_x \frac{\partial F}{\partial \rho}(\rho)(\cdot)$$

**Example:** Let  $F(\rho) = \int \log\left(\frac{\rho(x)}{\rho_{\infty}(x)}\right) \rho(x) dx$  be the relative entropy functional. Consider a path  $\rho_t$  in  $\mathcal{P}_{ac,2}(\mathbb{R}^d)$  such that  $\frac{\partial \rho_t}{\partial t} = -\nabla \cdot (\rho_t u)$  with  $\rho_0 = \rho \in \mathcal{P}_{ac,2}(\mathbb{R}^d)$ . Then

$$\begin{aligned} \frac{d}{dt} F(\rho_t) &= \int \log\left(\frac{\rho_t(x)}{\rho_{\infty}(x)}\right) \frac{\partial \rho_t}{\partial t}(x) dx + \int \frac{\partial \rho_t}{\partial t}(x) dx \\ &= - \int \log\left(\frac{\rho_t(x)}{\rho_{\infty}(x)}\right) \nabla \cdot (\rho_t(x)u(x)) dx \\ &= \int \nabla_x \log\left(\frac{\rho_t(x)}{\rho_{\infty}(x)}\right) \cdot u(x) \rho_t(x) dx \end{aligned}$$

where the divergence theorem is used in the last step. The definitions of the Gâteaux derivative and Wasserstein gradient imply

$$\begin{aligned} \frac{\partial F}{\partial \rho}(\rho)(x) &= \log\left(\frac{\rho(x)}{\rho_{\infty}(x)}\right) \\ \nabla_{\rho} F(\rho)(x) &= \nabla_x \log\left(\frac{\rho(x)}{\rho_{\infty}(x)}\right) \end{aligned}$$

### III. RELATIONSHIP WITH THE UNDER-DAMPED LANGEVIN EQUATION

A basic form of the under-damped (or second order) Langevin equation is given in [4]

$$\begin{aligned} dX_t &= v_t dt \\ dv_t &= -\gamma v_t dt - \nabla f(X_t) dt + \sqrt{2} dB_t \end{aligned} \tag{III.1}$$

where  $\{B_t\}_{t \geq 0}$  is the standard Brownian motion.

Consider next, the the accelerated flow (19). Denote  $v_t := e^{\alpha_t - \gamma t} Y_t$ . Then, with an appropriate choice of scaling parameters (e.g.  $\alpha_t = 0$ ,  $\beta_t = 0$  and  $\gamma_t = -\gamma t$ ):

$$\begin{aligned} dX_t &= v_t dt \\ dv_t &= -\gamma v_t dt - \nabla f(X_t) dt - \nabla_x \log(\rho_t(X_t)) \end{aligned} \tag{III.2}$$

The scaling parameters are chosen here for the sake of comparison and do not satisfy the ideal scaling conditions of [5].

The sdes (III.1) and (III.2) are similar except that the stochastic term  $\sqrt{2} dB_t$  in (III.1) is replaced with a deterministic term  $-\nabla_x \log(\rho_t(X_t))$  in (III.2). Because of this difference, the resulting distributions are different. Let  $p_t(x, v)$  denote the joint distribution on  $(X_t, v_t)$  of (III.1) and let  $q_t(x, v)$  denote the joint distribution on  $(X_t, v_t)$  of (III.2). Then the corresponding Fokker-Planck equations are:

$$\begin{aligned} \frac{\partial p}{\partial t}(x, v) &= -\nabla_x \cdot (p_t(x, v)v) + \nabla_v \cdot (p_t(x, v)(\gamma v + \nabla f(x))) + \Delta_v p_t(x, v) \\ \frac{\partial q}{\partial t}(x, v) &= -\nabla_x \cdot (q_t(x, v)v) + \nabla_v \cdot (q_t(x, v)(\gamma v + \nabla f(x))) + \nabla_v \cdot (q_t(x, v) \nabla_x \log(\rho_t(x))) \end{aligned}$$

where  $\rho_t(x) = \int q_t(x, v) dv$  is the marginal of  $q_t(x, v)$  on  $x$ . The final term in the Fokker-Planck equations are clearly different. The joint distributions are different as well.

The situation is in contrast to the first order Langevin equation, where the stochastic term  $\sqrt{2} dB_t$  and  $-\nabla \log(\rho_t(X_t))$  are equivalent, in the sense that the resulting distributions have the same marginal distribution as a function of time. To illustrate this point, consider the following two forms of the Langevin equation:

$$dX_t = -\nabla f(X_t) dt + \sqrt{2} dB_t \tag{III.3}$$

$$dX_t = -\nabla f(X_t) dt - \nabla \log(\rho_t(X_t)) \tag{III.4}$$

Let  $p_t(x)$  denote the distribution of  $X_t$  of (III.3) and let  $q_t(x)$  denote the distribution of  $X_t$  of (III.4). The corresponding Fokker-Planck equations are as follows

$$\begin{aligned}\frac{\partial p}{\partial t}(x) &= -\nabla \cdot (p_t(x)\nabla f(x)) + \Delta p_t(x) \\ \frac{\partial q}{\partial t}(x) &= -\nabla \cdot (q_t(x)\nabla f(x)) + \nabla \cdot (q_t(x)\nabla \log(\rho_t(x))) \\ &= -\nabla \cdot (q_t(x)\nabla f(x)) + \nabla \cdot (q_t(x)\nabla \log(q_t(x))) \\ &= -\nabla \cdot (q_t(x)\nabla f(x)) + \Delta q_t(x)\end{aligned}$$

where we used  $\rho_t(x) = q_t(x)$ . In particular, this implies that the marginal probability distribution of the stochastic process  $X_t$  are the same for first order Langevin sde (III.3) and (III.4) .

## REFERENCES

- [1] R. Carmona and F. Delarue, Probabilistic Theory of Mean Field Games with Applications I-II. Springer, 2017.
- [2] L. Ambrosio, N. Gigli, and G. Savaré, Gradient flows: in metric spaces and in the space of probability measures. Springer Science & Business Media, 2008.
- [3] C. Villani, Topics in optimal transportation. American Mathematical Soc., 2003, no. 58.
- [4] X. Cheng, N. S. Chatterji, P. L. Bartlett, and M. I. Jordan, “Underdamped langevin mcmc: A non-asymptotic analysis,” arXiv preprint arXiv:1707.03663, 2017.
- [5] A. Wibisono, A. C. Wilson, and M. I. Jordan, “A variational perspective on accelerated methods in optimization,” Proceedings of the National Academy of Sciences, p. 201614734, 2016.