SUPPLEMENTARY MATERIALS: A SUPERVISED LEARNING SCHEME FOR COMPUTING HAMILTON–JACOBI EQUATION VIA DENSITY COUPLING*

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SM1. Proof of Lemma 2.1 . In order to prove Lemma 2.1, we first prove the following result.

LEMMA SM1.1. *Suppose* $f \in \mathcal{C}^2(\mathbb{R}^d)$*, and* $\alpha I \preceq \nabla^2 f \preceq LI$ *with* $L \geq \alpha > 0$*. Then* $\nabla f : \mathbb{R}^d \to \mathbb{R}^d$ *is invertible, if we denote* $(\nabla f)^{-1}$ *as the inverse function of* ∇f*, we have* $(\nabla f)^{-1} \in \mathcal{C}^1(\mathbb{R}^d; \mathbb{R}^d)$*, and* $\nabla((\nabla f)^{-1}) = (\nabla^2 f \circ \nabla f^{-1})^{-1}$*.*

Proof. We first prove that ∇f is invertible. For arbitrary $p \in \mathbb{R}^d$, consider $g(x) = -p \cdot x + f(x)$, then g is $\alpha-$strongly convex. There exists unique $x' \in \mathbb{R}^d$ s.t. $\nabla g(x') = 0$, i.e., $\nabla f(x') = p$; furthermore, for any x'' such that $\nabla f(x'') = p$ we have $\nabla g(x'') = 0$, the uniqueness yields $x'' = x'$. This proves that ∇f is a bijective map on $\mathbb{R}^d$. We denote $(\nabla f)^{-1}$ as the inverse map of ∇f. To show the continuity of $(\nabla f)^{-1}$, for any $\epsilon > 0$, choose $\delta < \alpha\epsilon$. For fixed $p \in \mathbb{R}^d$, consider any q with $\|q - p\| < \delta$, denote $x = \nabla f^{-1}(p)$, $y = \nabla f^{-1}(q)$, from $\alpha-$strongly convexity, we have $\|\nabla f(y) - \nabla f(x)\| \geq \alpha\|y - x\|$, this yields $\|\nabla f^{-1}(q) - \nabla f^{-1}(p)\| \leq \frac{\|q-p\|}{\alpha} < \epsilon$. This verifies the continuity of ∇f^{-1}.

We then show $(\nabla f)^{-1}$ is differentiable. Since $f \in \mathcal{C}^2$, $\nabla f \in \mathcal{C}^1$. So ∇f is differentiable, which indicates that for any $x, y \in \mathbb{R}^d$,

$$\nabla f(y) - \nabla f(x) = \nabla^2 f(x)(y - x) + r(x, y),$$

where $r : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is certain vector function satisfying $\lim_{y \to x} \frac{\|r(x,y)\|}{\|y-x\|} = 0$. Denote $p = \nabla f(x), q = \nabla f(y)$, the above equation yields,

$$q - p = \nabla^2 f(x)(\nabla f^{-1}(q) - \nabla f^{-1}(p)) + r(x, y).$$

This is

$$\nabla f^{-1}(q) - \nabla f^{-1}(p) = (\nabla^2 f(x))^{-1}(q - p) - (\nabla^2 f(x))^{-1} r(x, y). \quad \text{(SM1.1)}$$

Denote $\hat{r}(q, p) = -(\nabla^2 f(x))^{-1} r(x, y)$, we have

$$\|\hat{r}(q, p)\| \leq \|\nabla^2 f(x))^{-1}\| \cdot \frac{\|r(x, y)\|}{\|y - x\|} \cdot \frac{\|y - x\|}{\|q - p\|} \cdot \|q - p\|.$$

Since $\|\nabla^2 f(x)^{-1}\| \leq \frac{1}{\alpha}$, and $\frac{\|y-x\|}{\|q-p\|} = \frac{\|y-x\|}{\|\nabla f(y) - \nabla f(x)\|} \leq \frac{1}{L}$. This yields

$$\|\hat{r}(q, p)\| \leq \frac{1}{\alpha L} \frac{\|r(x, y)\|}{\|y - x\|} \cdot \|q - p\|.$$

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Now send $q \to p$, due to the continuity of ∇f^{-1}, we know $y \to x$. The above inequality yields $r(q,p) = o(\|q-p\|)$, which verifies the differentiability of ∇f^{-1}. Furthermore, by (SM1.1), we know the Jacobian of ∇f^{-1} is $\nabla(\nabla f^{-1})(p) = (\nabla^2 f(\nabla f^{-1}(p)))^{-1}$, which is continuous. This verifies $\nabla f^{-1} \in \mathcal{C}^1$. ∎

Proof of Lemma 2.1. By Lemma SM1.1, we know ∇f is bijective, and we denote $\nabla f^{-1} \in \mathcal{C}^1$ as its inverse. According to the definition of Legendre transformation,

$$f^*(p) = \sup_{\xi \in \mathbb{R}^d} \{\xi \cdot p - f(\xi)\},$$

since $\xi \cdot p - f(\xi)$ is $\alpha-$strongly concave as a function of ξ, for any $p \in \mathbb{R}^d$, there is a unique maximizer ξ_*, which solves $\nabla f(\xi_*) = p$, i.e., $\xi_* = (\nabla f)^{-1}(p)$. Thus $f^*(p) = (\nabla f)^{-1}(p) \cdot p - f((\nabla f)^{-1}(p))$, since $\nabla f^{-1} \in \mathcal{C}^1$, f^* is at least $\mathcal{C}^1$, use $\nabla(\nabla f^{-1}(p)) = (\nabla^2 f(\nabla f^{-1}(p)))^{-1}$, we have

$$\nabla f^*(p) = \nabla((\nabla f)^{-1}(p))p + \nabla f^{-1}(p) - f(\nabla f^{-1}(p)) = \nabla f^{-1}(p).$$

Since $\nabla f^{-1} \in \mathcal{C}^1$, we know $\nabla f^* \in \mathcal{C}^1$, this leads to $f^* \in \mathcal{C}^2$.

Furthermore, we have $\nabla^2 f^*(p) = \nabla(\nabla f^{-1}(p)) = [\nabla^2 f(\nabla f^{-1}(p))]^{-1}$, this yields $\frac{1}{L} I \preceq \nabla^2 f^* \preceq \frac{1}{\alpha} I$.

On the other hand, recall that $\xi_* = \nabla f^{-1}(p) = \nabla f^*(p)$, we have $f^*(p) = \nabla f^*(p) \cdot p - f(\nabla f^*(p))$. Thus,

$$\begin{aligned}
f(q) + f^*(p) - q \cdot p &= f(q) + \nabla f^*(p) \cdot p - f(\nabla f^*(p)) - q \cdot p \\
&= f(q) - f(\nabla f^*(p)) - p \cdot (q - \nabla f^*(p)) \\
&= f(q) - f(\nabla f^*(p)) - \nabla f(\nabla f^*(p)) \cdot (q - \nabla f^*(p)) \\
&= D_f(q : \nabla f^*(p)).
\end{aligned}$$

For the third equality, we use the fact that $\nabla f^*(p) = (\nabla f)^{-1}(p)$ for any $p \in \mathbb{R}^d$.

To prove the fact that $f(q) + f^*(p) - q \cdot p = D_{f^*}(p : \nabla f(q))$, one only needs to treat $g = f^* \in \mathcal{C}^2(\mathbb{R}^d)$ with $\frac{1}{L} I \preceq \nabla^2 g \preceq \frac{1}{\alpha} I$, and $g^* = f^{**} = f$,* and then apply the above argument to g. ∎

SM2. Proof of Theorem 2.1.

Proof of Theorem 2.1. Given the Lipschitz condition on the vector field $(\frac{\partial}{\partial x} H^\top, \frac{\partial}{\partial p} H^\top)^\top$, it is known that the underlying Hamiltonian system considered admits a unique solution with continuous trajectories for arbitrary initial condition $(\boldsymbol{X}_0, \nabla g(\boldsymbol{X}_0))$.

Let us recall the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ used to describe the randomness of the Hamiltonian system. Since

$$\mathbb{E}_\omega \left[\int_0^T D_{H,x}(\nabla \widehat{\psi}(\boldsymbol{X}_t(\omega), t) : \boldsymbol{P}_t(\omega)) \, dt \right] = 0,$$

then by the fact that Bregman divergence $D_{H,x}$ is always non-negative, we obtain

$$\int_0^T D_{H,x}(\nabla \widehat{\psi}(\boldsymbol{X}_t(\omega), t) : \boldsymbol{P}_t(\omega)) \, dt = 0, \quad \mathbb{P}\text{-almost surely.}$$

*This is true for any $f \in \mathcal{C}(\mathbb{R}^d)$ that is convex, c.f. Chapter 11 of [SM1].

Thus, there exists a measurable subset $\Omega' \subset \Omega$ with $\mathbb{P}(\Omega') = 1$ such that

$$\int_0^T D_{H,x}(\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) : \boldsymbol{P}_t(\omega'))\, dt = 0, \quad \forall\, \omega' \in \Omega'.$$

By using the continuity and non-negativity of $D_{H,x}(\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) : \boldsymbol{P}_t(\omega'))$ with respect to t, we have

$$\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) = \boldsymbol{P}_t(\omega') \quad \text{for } \ 0 \le t \le T. \tag{SM2.1}$$

When $t = 0$, we have $\nabla\widehat{\psi}(\boldsymbol{X}_0(\omega'),0) = \boldsymbol{P}_0(\omega')$. Recall the initial condition of the Hamiltonian System, we have $\boldsymbol{P}_0(\omega') = \nabla g(\boldsymbol{X}_0(\omega'))$. This yields $\nabla\widehat{\psi}(\boldsymbol{X}_0(\omega'),0) = \nabla g(\boldsymbol{X}_0(\omega'))$ for any $\omega' \in \Omega'$, which yields

$$\nabla\widehat{\psi}(x,0) = \nabla g(x) \quad \text{for all } x \in \operatorname{Spt}(\rho_0). \tag{SM2.2}$$

On the other hand, for $t \in (0,T]$, by differentiating on both sides of (SM2.1) w.r.t. t, we obtain

$$\frac{\partial}{\partial t}\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) + \nabla^2\widehat{\psi}(\boldsymbol{X}_t(\omega'),t)\dot{\boldsymbol{X}}_t(\omega') = \dot{\boldsymbol{P}}_t(\omega'). \tag{SM2.3}$$

Recall that we have

$$\dot{\boldsymbol{X}}_t = \frac{\partial}{\partial p}H(\boldsymbol{X}_t,\boldsymbol{P}_t) = \frac{\partial}{\partial p}H(\boldsymbol{X}_t,\nabla\widehat{\psi}(\boldsymbol{X}_t,t)),$$

$$\dot{\boldsymbol{P}}_t = -\frac{\partial}{\partial x}H(\boldsymbol{X}_t,\boldsymbol{P}_t) = -\frac{\partial}{\partial x}H(\boldsymbol{X}_t,\nabla\widehat{\psi}(\boldsymbol{X}_t,t)).$$

Plugging these into (SM2.3) yields

$$\frac{\partial}{\partial t}\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) + \nabla^2\widehat{\psi}(\boldsymbol{X}_t(\omega'),t)\frac{\partial}{\partial p}H(\boldsymbol{X}_t(\omega'),\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t))$$

$$= -\frac{\partial}{\partial x}H(\boldsymbol{X}_t(\omega'),\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t)),$$

which leads to

$$\nabla\left(\frac{\partial}{\partial t}\widehat{\psi}(\boldsymbol{X}_t(\omega'),t) + H(x,\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega'),t))\right) = 0, \quad \forall\, \omega' \in \Omega'.$$

Since the probability density distribution of $\boldsymbol{X}_t$ is ρ_t, we have proved that

$$\nabla\left(\frac{\partial}{\partial t}\widehat{\psi}(x,t) + H(x,\nabla\widehat{\psi}(x,t))\right) = 0, \quad \forall \ \ x \in \operatorname{Spt}(\rho_t). \tag{SM2.4}$$

Combining (SM2.2) and (SM2.4) proves this theorem.

On the other hand, if $\mathscr{L}^{|\cdot|^2}_{\rho_0,g,T}(\widehat{\psi}) = 0$. By using the fact that $|\nabla\widehat{\psi}(\boldsymbol{X}_t(\omega),t) - \boldsymbol{P}_t(\omega)|^2$ is continuous and non-negative for a.s. $\omega \in \Omega$, we can repeat the previous proof to show the same assertion still holds. ∎

SM3. Proof of Lemma 2.2.

Proof of Lemma 2.2. Let us first consider the term

$$\int_{\mathbb{R}^d} \psi(x,t)\rho_t(x)dx = \mathbb{E}_{\boldsymbol{X}_t}\psi(\boldsymbol{X}_t,t). \tag{SM3.1}$$

By differentiating (SM3.1) w.r.t. time t, we obtain

$$\frac{d}{dt}\left(\int_{\mathbb{R}^d} \psi(x,t)\rho_t(x)dx\right) = \mathbb{E}\left[\nabla\psi(\boldsymbol{X}_t,t)\cdot\dot{\boldsymbol{X}}_t + \frac{\partial\psi(\boldsymbol{X}_t,t)}{\partial t}\right].$$

The right-hand side of the above equation equals

$$\begin{aligned}&\mathbb{E}_{\boldsymbol{X}_t,\boldsymbol{P}_t}\nabla\psi(\boldsymbol{X}_t,t)\cdot\frac{\partial}{\partial p}H(\boldsymbol{X}_t,\boldsymbol{P}_t) + \mathbb{E}_{\boldsymbol{X}_t}\left[\frac{\partial\psi(\boldsymbol{X}_t,t)}{\partial t}\right]\\ &= \int_{\mathbb{R}^{2d}}\nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p)\ d\mu_t(x,p) + \int_{\mathbb{R}^d}\frac{\partial\psi(x,t)}{\partial t}\rho_t(x)dx.\end{aligned}$$

Combining the above equations, we have

$$\int_{\mathbb{R}^d} -\partial_t\psi(x,t)d\rho_t(x) = \int_{\mathbb{R}^{2d}}\nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p)\ d\mu_t(x,p) - \frac{d}{dt}\left(\int_{\mathbb{R}^{2d}}\psi(x,t)\rho_t(x)dx\right). \tag{SM3.2}$$

Plugging (SM3.2) into the formula of $\mathscr{L}_{\rho_0,g,T}(\psi)$ yields that

$$\begin{aligned}&\mathscr{L}_{\rho_0,g,T}(\psi)\\ &= \int_0^T\left(\int_{\mathbb{R}^{2d}}\nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p)\ d\mu_t(x,p) - \frac{d}{dt}\left(\int_{\mathbb{R}^{2d}}\psi(x,t)\rho_t(x)dx\right)\right)\ dt\\ &\quad + \int_0^T\int_{\mathbb{R}^d} -H(x,\nabla\psi(x,t))\rho_t(x)\ dx\ dt\\ &\quad + \int_{\mathbb{R}^d}\psi(x,T)\rho_t(x)\ dx - \int_{\mathbb{R}^d}\psi(x,0)\rho_0(x)\ dx.\\ &= \int_0^T\int_{\mathbb{R}^{2d}}(\nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p) - H(x,\nabla\psi(x,t)))\ d\mu_t(x,p)dt\\ &= \int_0^T\int_{\mathbb{R}^{2d}}(\nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p) - H(x,\nabla\psi(x,t)) - H^*(x,\frac{\partial}{\partial p}H(x,p)))\ d\mu_t(x,p)dt\\ &\quad + \int_0^T\int_{\mathbb{R}^{2d}}H^*(x,\frac{\partial}{\partial p}H(x,p))\ d\mu_t(x,p)dt.\end{aligned} \tag{SM3.3}$$

The second equality is obtained by integrating the time-derivative of (SM3.1) on $[0,T]$ as well as by using the fact that $\rho_t(\cdot)$ is the density of $\boldsymbol{X}-$marginal of μ_t.

Based on Lemma 2.1, choosing f as H^* and f^* as the Hamiltonian H, and letting $q = \frac{\partial}{\partial p}H(x,p)$ and $p = \nabla\psi(x,t)$, we obtain

$$\begin{aligned}&H^*(x,\frac{\partial}{\partial p}H(x,p)) + H(x,\nabla\psi(x,t)) - \nabla\psi(x,t)\cdot\frac{\partial}{\partial p}H(x,p)\\ &= D_{H,x}(\nabla\psi(x,t):\nabla_v H^*(x,\frac{\partial}{\partial p}H(x,p))).\end{aligned}$$

Since $\frac{\partial}{\partial v}H^*(x,\cdot) = (\frac{\partial}{\partial p}H(x,\cdot))^{-1}$, the right-hand side of the above equality leads to $D_{H,x}(\nabla\psi(x,t):p)$. Plugging this back to (SM3.3) proves Lemma 2.2. ∎

SM4. Discussion on the dependence on ρ_0. We give a brief discussion about the dependence on ρ_0 for the computed solution ψ_θ via an example with the classical Hamiltonian $H(x,p) = \frac{1}{2}|p|^2 + V(x)$. Assume that the solution ψ_θ exists for any initial density and is regular enough in time and space. For simplicity, we ignore the numerical error caused by symplectic integrator and consider the difference between $\psi_{\theta,\rho_{0,1}}$ and $\psi_{\theta,\rho_{0,2}}$ with different initial densities $\rho_{0,1}$ and $\rho_{0,2}$..

Then by remark 2.1, one can verify for any test function $f \in \mathcal{C}^1([0,T]\times\mathbb{R}^d)$

$$\int_0^T \int_{\mathbb{R}^d} \Big(\nabla\psi_{\theta,\rho_{0,i}}(x,t) - \bar{p}_i(x,t)\Big)\nabla f(x,t)\rho_i(x,t)dxdt = 0. \tag{SM4.1}$$

Here $i \le 2$, $\rho_i(x,t)$ is the marginal density of the position of the particle X_t^i with different initial data $x_0^{(i)}$, and $\bar{p}_i(x,t) = \int_{\mathbb{R}^d} pd\mu_t^{(i)}(p|x)$ with $\mu_t^{(i)}(p|x)$ being the conditional distribution of the joint distribution $\mu_t^{(i)}(x,p)$.

In particular, when the characteristic lines do not intersect, by (SM4.1) one can infer that $\nabla\psi_{\theta,\rho_{0,1}}(x,t) = \nabla\psi_{\theta,\rho_{0,2}}(x,t)$ in the intersection of the supports of $\rho_{0,1}(t,\cdot)$ and $\rho_{0,2}(t,\cdot)$. Moreover, in this case $\bar{p}_i(x,t) = P_t^i$ with the initial value $(X_t^{(i)})^{-1}(x), \nabla g\big((X_t^{(i)})^{-1}(x)\big)$ as the initial value of the underlying Hamiltonian ODE. Since characteristic lines do not intersect, it is not hard to see that

$$|\bar{p}_i(x,t)| \le C \sup_{x\in supp(\rho_{0,i})} |\nabla g(x)|,\ i \le 2, \tag{SM4.2}$$

$$\bar{p_1}(x,t) = \bar{p_2}(x,t),\ \text{for any fixed } (x,t).$$

By subtracting (SM4.1) for $i = 1, 2$, one further has that

$$\begin{aligned}
&\int_0^T \int_{\mathbb{R}^d} \Big(\nabla\psi_{\theta,\rho_{0,1}}(x,t) - \nabla\psi_{\theta,\rho_{0,2}}(x,t)\Big)\nabla f(x,t)\rho_1(x,t)dxdt \\
&+ \int_0^T \int_{\mathbb{R}^d} \nabla\psi_{\theta,\rho_{0,2}}(x,t)\nabla f(x,t)(\rho_2(x,t) - \rho_1(x,t))dxdt \\
&- \int_0^T \int_{\mathbb{R}^d} \Big(\bar{p_1}(x,t) - \bar{p_2}(x,t)\Big)\nabla f(x,t)\rho_1(x,t)dxdt \\
&- \int_0^T \int_{\mathbb{R}^d} \bar{p_2}(x,t)\nabla f(x,t)(\rho_1(x,t) - \rho_2(x,t))dxdt = 0.
\end{aligned} \tag{SM4.3}$$

Taking $f = \psi_{\theta,\rho_{0,1}}(x,t) - \psi_{\theta,\rho_{0,2}}(x,t)$ and using Young's inequality, by the symmetry of $\rho_{0,i}$ and (SM4.2), one can obtain

$$\begin{aligned}
&\sup_{i\le 2}\int_0^T \int_{\mathbb{R}^d} |\nabla\psi_{\theta,\rho_{0,1}}(x,t) - \nabla\psi_{\theta,\rho_{0,2}}(x,t)|^2\rho_i(x,t)dxdt \\
&\le C\int_0^T \int_{\mathbb{R}^d} \Big(1 + |\nabla\psi_{\theta,\rho_{0,1}}(x,t)|^2 + |\nabla\psi_{\theta,\rho_{0,1}}(x,t)|^2\Big)|\rho_1(x,t) - \rho_2(x,t)|dxdt \\
&+ C\int_0^T \int_{\mathbb{R}^d} \Big(1 + |\bar{p_1}(x,t)|^2 + \bar{p_2}(x,t)|^2\Big)|\rho_1(x,t) - \rho_2(x,t)|dxdt.
\end{aligned}$$

This, together with the fact that $\rho_i(t,\cdot)$ is continuous w.r.t. the initial density, implies that the approximate solution ψ_θ is continuous w.r.t. the initial density.

After the characteristic lines intersect, the analysis is more complicate and relies on the properties of conditional distribution $\mu_t^{(i)}(p|x)$ and the averaged momentum $\bar{p}_i(t,x)$. It is beyond the scope of this current work. We hope to address and study this issue in the future.

SM5. A stronger version of Theorem 3.1.

THEOREM SM5.1. *Under the condition of Theorem 3.1, in addition assume that the classical solution of HJ PDE exists. Then with the probability $1-\epsilon$, the neural network ψ_θ satisfies*

$$\int_{\mathbb{R}^d} \left|\nabla\left(\frac{\partial}{\partial t}\psi_\theta(x,t_i)+H(x,\nabla\psi_\theta(x,t_i))\right)\right| \ \tilde{\rho}_{t_i}(x)dx$$

$$\leq \ C_{\theta,i}h^{r-2}+\frac{1}{N}\sum_{k=1}^{N}|\sum_{j\in N(i)} a_{ij}e_j^k\frac{1}{h}|+\nu(\theta,i)(|\nabla e_i^{(k)}|+|e_i^{(k)}|)+R(\theta,i)\sqrt{\frac{\ln M+\ln\frac{2}{\epsilon}}{2N}},$$

at $t_i=ih$, $i=1,\ldots,M$. Here, a_{ij} is the coefficient and $j\in N(i)$ denotes the node to be used in the numerical differentiation formula $I^h(f)(t_i)=\sum_{j\in N(i)} a_{ij}f(t_i)\frac{1}{h}$ of order $r_1\geq r-2$. The constants $C(\theta,i),\nu(\theta,i),R(\theta,i)$ are non-negative depending on the parameter θ, time node t_i, Hamiltonian H, initial distribution ρ_0, the exact solution of HJ PDE and the numerical solution of temporal numerical scheme.

Proof. We use the same notations as in the proof of Theorem 3.1. Let us denote the residual term of optimal neural network as

$$\mathcal{R}[\psi_\theta](x,t)=\nabla\left(\frac{\partial}{\partial t}\psi_\theta(x,t)+H(x,\nabla\psi_\theta(x))\right).$$

and the residual term of the weak solution as

$$\mathcal{R}_{exa}[\psi](x,t):=\nabla\left(\frac{\partial}{\partial t}\psi(x,t)+H(x,\nabla\psi(x,t))\right).$$

Note that if ψ is the strong solution of HJ equation, then $\mathcal{R}_{exa}[\psi](x,t)=0$.

For the sample particle $\widetilde{x}_{t_i}^{(k)}, k\leq N, i\leq M$, it holds that

$$\begin{aligned}
&\frac{1}{N}\sum_{k=1}^{N}\mathcal{R}\psi_\theta(\widetilde{x}_{t_i}^{(k)},t_i)\\
&=\frac{1}{N}\sum_{k=1}^{N}\Big(\mathcal{R}\psi_\theta(\widetilde{x}_{t_i}^{(k)},t_i)-\mathcal{R}_{exa}\psi(x_{t_i}^{(k)},t_i)\Big)\\
&=\frac{1}{N}\sum_{k=1}^{N}\Big(\mathcal{D}\psi_\theta(\widetilde{x}_{t_i}^{(k)},\widetilde{p}_{t_i}^{(k)},t_i)-\mathcal{D}\psi(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)\Big)\\
&=\frac{1}{N}\sum_{k=1}^{N}\Big(\mathcal{D}\psi_\theta(\widetilde{x}_{t_i}^{(k)},\widetilde{p}_{t_i}^{(k)},t_i)-\mathcal{D}\psi_\theta(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)\Big)\\
&+\frac{1}{N}\sum_{k=1}^{N}\Big(\mathcal{D}\psi_\theta(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)-\mathcal{D}\psi(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)\Big).
\end{aligned}$$

Next we estimate the two terms on the right hand side. First, we split the first term as

$$\begin{aligned}
&\mathcal{D}\psi_\theta(\widetilde{x}_{t_i}^{(k)},\widetilde{p}_{t_i}^{(k)},t_i)-\mathcal{D}\psi_\theta(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)\\
&=\nabla\frac{\partial}{\partial t}\psi_\theta(\widetilde{x}_{t_i}^{(k)},t_i)-\nabla\frac{\partial}{\partial t}\psi_\theta(x_{t_i}^{(k)},t_i)\\
&+\nabla^2\psi_\theta(\widetilde{x}_{t_i}^{(k)},t_i)\frac{\partial}{\partial p}H(\widetilde{x}_{t_i}^{(k)},\widetilde{p}_{t_i}^{(k)})-\nabla^2\psi_\theta(x_{t_i}^{(k)},t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)},p_{t_i}^{(k)})\\
&+\frac{\partial}{\partial x}H(\widetilde{p}_{t_i}^{(k)},\nabla\psi_\theta(x_{t_i}^{(k)},t_i)))-\frac{\partial}{\partial x}H(p_{t_i}^{(k)},\nabla\psi_\theta(x_{t_i}^{(k)},t_i))).
\end{aligned}$$

By using the finite support property of ρ_{t_i} and $\tilde{\rho}_{t_i}$ and Lipschitz property of ψ_θ on bounded domain,

$$|\nabla \frac{\partial}{\partial t}\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i) - \nabla \frac{\partial}{\partial t}\psi_\theta(x_{t_i}^{(k)}, t_i)| \leq L_{\theta,i}^A |\widetilde{x}_{t_i}^{(k)} - x_{t_i}^{(k)}|.$$

Similarly, one can obtain that

$$\begin{aligned}
&\left|\nabla^2\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(\widetilde{x}_{t_i}^{(k)}, \widetilde{p}_{t_i}^{(k)}) - \nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)})\right| \\
&\leq L_{\theta,i}^B(|\widetilde{x}_{t_i}^{(k)} - x_{t_i}^{(k)}| + |\widetilde{p}_{t_i}^{(k)} - p_{t_i}^{(k)}|)
\end{aligned}$$

and that

$$\begin{aligned}
&\left|\frac{\partial}{\partial x}H(\widetilde{p}_{t_i}^{(k)}, \nabla\psi_\theta(x_{t_i}^{(k)}, t_i))) - \frac{\partial}{\partial x}H(p_{t_i}^{(k)}, \nabla\psi_\theta(x_{t_i}^{(k)}, t_i)))\right| \\
&\qquad\leq L_{\theta,i}^C(|\widetilde{x}_{t_i}^{(k)} - x_{t_i}^{(k)}| + |\widetilde{p}_{t_i}^{(k)} - p_{t_i}^{(k)}|).
\end{aligned} \tag{SM5.1}$$

Here $L_{\theta,i}^A, L_{\theta,i}^B, L_{\theta,i}^C$ are finite depending on the support of ρ_0. Note that the global error of the numerical scheme $|\widetilde{x}_{t_i}^{(k)} - x_{t_i}^{(k)}| + |\widetilde{p}_{t_i}^{(k)} - p_{t_i}^{(k)}|$ is of order $r-1$. Thus,

$$\frac{1}{N}\sum_{k=1}^{N}\Big(\mathcal{D}\psi_\theta(\widetilde{x}_{t_i}^{(k)}, \widetilde{p}_{t_i}^{(k)}, t_i) - \mathcal{D}\psi_\theta(x_{t_i}^{(k)}, p_{t_i}^{(k)}, t_i)\Big) \sim O(h^{r-1}).$$

Notice that

$$\begin{aligned}
&\mathcal{D}\psi_\theta(x_{t_i}^{(k)}, p_{t_i}^{(k)}, t_i) - \mathcal{D}\psi(x_{t_i}^{(k)}, p_{t_i}^{(k)}, t_i) \\
&= \nabla\frac{\partial}{\partial t}\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla\frac{\partial}{\partial t}\psi(x_{t_i}^{(k)}, t_i) \\
&+ \nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) - \nabla^2\psi(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) \\
&+ \frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi_\theta(x_{t_i}^{(k)}, t_i)) - \frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi(x_{t_i}^{(k)}, t)).
\end{aligned}$$

Using the fact that $e_{t_i}^k = \nabla\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i) - \widetilde{p}_{t_i}^{(k)}$ and the mean value theorem, we get

$$\begin{aligned}
\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) &= \nabla\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i) + \nabla\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i) \\
&= \nabla\psi_\theta(\widetilde{x}_{t_i}^{(k)}, t_i) + \int_0^1 \nabla^2\psi_\theta((1-\alpha_1)\widetilde{x}_{t_i}^{(k)} + \alpha_1 x_{t_i}^{(k)}, t_i)(x_{t_i}^{(k)} - \widetilde{x}_{t_i}^{(k)})d\alpha_1 \\
&= \widetilde{p}_{t_i}^{(k)} + e_i^k + O(|\widetilde{x}_{t_i}^{(k)} - x_{t_i}^{(k)}|).
\end{aligned} \tag{SM5.2}$$

Notice that in the error estimate, directly using the fact that $\nabla\psi(\widetilde{x}_{t_i}, t_i) = \widetilde{p}_{t_i}$ and forward difference method may lead to a lower order of convergence in time for the numerical discretization since less information is known for the time derivative of $\widetilde{p}_{t_i}$. Instead, our strategy is using a high order numerical differentiation formula to approximate the time derivative first and then applying the fact that $\nabla\psi(\widetilde{x}_{t_i}, t_i) = \widetilde{p}_{t_i}$. To this end, we approximate $\frac{\partial}{\partial t}\nabla\psi_\theta$ using a high order linear numerical differential formula $I_h(\nabla\psi_\theta)$, i.e., for any sufficient smooth function f.

$$I_h(f)(t_i) = \sum_{j\in N(i)} a_{ij} f(t_j)\frac{1}{h} = f'(t_i) + O(h^{r_1}),$$

where $a_{ij} \in \mathbb{R}$ and t_j are the nodes close to t_i.

Using the numerical differentiation formula and the mean value theorem, as well as the fact that $p_t^{(k)} = \nabla\psi(x_t^{(k)}, t)$, it follows that

$$\begin{aligned}
\nabla\frac{\partial}{\partial t}\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla\frac{\partial}{\partial t}\psi(x_{t_i}^{(k)}, t_i) &= \frac{\partial}{\partial t}\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) - \frac{\partial}{\partial t}p_t^{(k)}|_{t=t_i} \\
&= I_h(\nabla\psi_\theta(x_t^{(k)}, t))|_{t=t_i} - I_h(p_t^{(k)})|_{t=t_i} + O(h^{r_1}) \\
&= I_h(\nabla\psi_\theta(x_t^{(k)}, t) - p_t^{(k)})|_{t=t_i} + O(h^{r_1}).
\end{aligned}$$

According to (5), it follows that

$$\begin{aligned}
\nabla\frac{\partial}{\partial t}\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla\frac{\partial}{\partial t}\psi(x_{t_i}^{(k)}, t_i) &= \sum_{j\in N(i)} a_{ij}(\nabla\psi_\theta(x_{t_j}^{(k)}, t_j) - p_{t_j}^k)\frac{1}{h} + O(h^{r_1}) \\
&= \sum_{j\in N(i)} a_{ij}(\widetilde{p}_{t_j}^{(k)} + e_j^k - p_{t_j}^k)\frac{1}{h} + O(h^{r-2}) + O(h^{r_1}) \\
&= \sum_{j\in N(i)} a_{ij}e_j^k\frac{1}{h} + O(h^{r-2}) + O(h^{r_1}).
\end{aligned} \tag{SM5.3}$$

Next we give the estimate for the term $\nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) - \nabla^2\psi(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)})$. By using the mean value theorem and (5) again, we obtain that

$$\begin{aligned}
&\nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) - \nabla^2\psi(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) \\
&= (\nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla p_{t_i}^{(k)})\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) \\
&= (\nabla\widetilde{p}_{t_i}^{(k)} - \nabla p_{t_i}^{(k)})\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) + \nabla e_i^k\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) + O(h^{r-1}).
\end{aligned}$$

Since the order of time integrator will not depends on the formulation of the coefficient of ODEs, one has $\nabla\widetilde{p}_{t_i}^{(k)} - \nabla p_{t_i}^{(k)} \sim O(h^{r-1})$. As a consequence, it holds that

$$\begin{aligned}
&\nabla^2\psi_\theta(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) - \nabla^2\psi(x_{t_i}^{(k)}, t_i)\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) \\
&= \nabla e_i^k\frac{\partial}{\partial p}H(x_{t_i}^{(k)}, p_{t_i}^{(k)}) + O(h^{r-1}).
\end{aligned} \tag{SM5.4}$$

It suffices to estimate the term $\frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi_\theta(x_{t_i}^{(k)}, t_i)) - \frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi(x_{t_i}^{(k)}, t))$. For this term, using the mean value theorem, (5) and the order of the numerical scheme, we get

$$\begin{aligned}
&\frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi_\theta(x_{t_i}^{(k)}, t_i)) - \frac{\partial}{\partial x}H(x_{t_i}^{(k)}, \nabla\psi(x_{t_i}^{(k)}, t)) \\
&= \int_0^1 \frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)}, \alpha_2\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) + (1-\alpha_2)\nabla\psi(x_{t_i}^{(k)}, t))(\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) - \nabla\psi(x_{t_i}^{(k)}, t_i))d\alpha_2 \\
&= \int_0^1 \frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)}, \alpha_2\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) + (1-\alpha_2)\nabla\psi(x_{t_i}^{(k)}, t))(\widetilde{p}_{t_i}^{(k)} - p_{t_i}^{(k)})d\alpha_2 + O(h^{r-1}) \\
&+ \int_0^1 \frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)}, \alpha_2\nabla\psi_\theta(x_{t_i}^{(k)}, t_i) + (1-\alpha_2)\nabla\psi(x_{t_i}^{(k)}, t))e_i^k d\alpha_2.
\end{aligned} \tag{SM5.5}$$

Combining the estimates (SM5.3)-(SM5.5), we obtain that

$$\frac{1}{N}\sum_{k=1}^{N}\mathcal{D}\psi_\theta(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)-\mathcal{D}\psi(x_{t_i}^{(k)},p_{t_i}^{(k)},t_i)$$

$$=\frac{1}{N}\sum_{k=1}^{N}\sum_{j\in N(i)}a_{ij}e_j^k\frac{1}{h}+\nabla e_i^k\frac{\partial}{\partial p}H(x_{t_i}^{(k)},p_{t_i}^{(k)})$$

$$+\int_0^1\frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)},\alpha_2\nabla\psi_\theta(x_{t_i}^{(k)},t_i)+(1-\alpha_2)\nabla\psi(x_{t_i}^{(k)},t))e_i^k d\alpha_2+O(h^{r-2})+O(h^{r_1}).$$

Taking $r_1\geq r-2$, and using (SM5.1) and the Taylor expansion, we further obtain that

$$\frac{1}{N}\sum_{k=1}^{N}\mathcal{R}\psi_\theta(\tilde{x}_{t_i}^{(k)},t_i) \tag{SM5.6}$$

$$=O(h^{r-2})+\frac{1}{N}\sum_{k=1}^{N}\Big(\sum_{j\in N(i)}a_{ij}e_j^k\frac{1}{h}+\nabla e_i^k\frac{\partial}{\partial p}H(x_{t_i}^{(k)},p_{t_i}^{(k)})$$

$$+\int_0^1\frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)},\alpha_2\nabla\psi_\theta(x_{t_i}^{(k)},t_i)+(1-\alpha_2)\nabla\psi(x_{t_i}^{(k)},t))e_i^k d\alpha_2\Big)$$

$$=O(h^{r-2})+\frac{1}{N}\sum_{k=1}^{N}|\sum_{j\in N(i)}a_{ij}e_j^k\frac{1}{h}|+\nu(\theta,i)(|\nabla e_i^{(k)}|+|e_i^{(k)}|),$$

where

$$\nu(\theta,i)=\sup_{x_{t_i}\sim\rho_{t_i}}\Big(|\frac{\partial}{\partial p}H(x_{t_i},p_{t_i})|+|\int_0^1\frac{\partial^2}{\partial x\partial p}H(x_{t_i}^{(k)},\alpha_2\nabla\psi_\theta(x_{t_i}^{(k)},t_i)$$

$$+(1-\alpha_2)\nabla\psi(x_{t_i}^{(k)},t))d\alpha_2|\Big).$$

To further estimate the expectation of the L^1-residual at all the time nodes $\{t_1,\ldots,t_T\}$, let us denote $\tilde{\rho}_{t_i}=(\tilde{\Phi}_h\circ\cdots\circ\tilde{\Phi}_h)_\sharp\rho_0$ as the probability density function of the numerical solution $\tilde{x}_{t_i}$ computed by the chosen scheme starting from $x_0\sim\rho_0$. For a fixed time t_i and samples $\{\tilde{x}_{t_i}^{(k)}\}_{1\leq k\leq N}\sim\tilde{\rho}_{t_i}$, by Hoeffding's inequality (see e.g. [SM2]), for any $0<\delta<1$, with probability $1-\delta$, we can bound the gap between the expectation and the empirical average of the L^1 residual as

$$\left|\int_{\mathbb{R}^d}\mathcal{R}[\psi_\theta](x,t_i)\tilde{\rho}_{t_i}\,dx-\frac{1}{N}\sum_{k=1}^{N}\mathcal{R}[\psi_\theta](\tilde{x}_{t_i}^{(k)},t_i)\right|\leq\underbrace{\sup_{x\in\mathrm{supp}(\tilde{\rho}_{t_i})}|\mathcal{R}[\psi_\theta](x,t_i)|}_{\text{denote as }R(\theta,i)}\sqrt{\frac{\ln\frac{2}{\delta}}{2N}}. \tag{SM5.7}$$

Similarly, for the samples $\{x_{t_i}^{(k)}\}_{1\leq k\leq N}\sim\rho_{t_i}$, for any $0<\delta<1$, with probability $1-\delta$, it holds that

$$\left|\int_{\mathbb{R}^d}\mathcal{R}_{exa}[\psi](x,t_i)\rho_{t_i}\,dx-\frac{1}{N}\sum_{k=1}^{N}\mathcal{R}_{exa}[\psi](\tilde{x}_{t_i}^{(k)},t_i)\right|\leq\underbrace{\sup_{x\in\mathrm{supp}(\rho_{t_i})}|\mathcal{R}_{exa}[\psi](x,t_i)|}_{\text{denote as }R_{exa}(i)}\sqrt{\frac{\ln\frac{2}{\delta}}{2N}}. \tag{SM5.8}$$

Since we assume that $\mathrm{supp}(\rho_0)$ is a bounded set, and the solution maps of the numerical scheme and the ODE system is continuous, then $\mathrm{supp}(\tilde{\rho}_{t_i}), \mathrm{supp}(\rho_{t_i})$ are also bounded. Thus $R(\theta, i), R_{exa}(i)$ is guaranteed to be finite. Indeed, $R_{exa}(i) = 0$ by our assumption. Combining (SM5.6), (SM5.7), and (SM5.8), and using the similar arguments as in the proof of Theorem 3.1, we obtain the desired result where $C_{\theta,i}h^{r-2}$ is the upper bound of $\mathcal{O}(h^{r-2})$. ∎

SM6. Two more numerical examples.

SM6.0.1. Example with Double Well Potential. We set potential V as a double well potential function

$$V(x) = \sum_{k=1}^{d} \frac{1}{10d}x_k^4 + \frac{8}{5d}x_k^2 + \frac{1}{2d}x_k.$$

We take the initial condition as $u(x, 0) = g(x)$ with $g(x) = \frac{1}{2}|x|^2$, the initial distribution ρ_a as the standard normal distribution.

We first test this example with $d = 2$. We solve the equation on $[0, 2]$. The phase portrait of the corresponding Hamiltonian system with the initial condition $x_0, p_0 = x_0$ is shown in Figure SM1. It can be seen from this portrait that some characteristics collide as time passes over a certain threshold T_*. (Here we mean the collision in the x space, not the phase space (x, p).) We obtain the results demonstrated in Figure SM2. As shown in these figures, our method is able to match $\nabla\psi_\theta(\cdot, t)$ well with the real momentums of particles when time t is less than 0.8. However, matching disagreements can be observed at $t = 1.2, 1.6, 2.0$, mostly near the sample boundary.

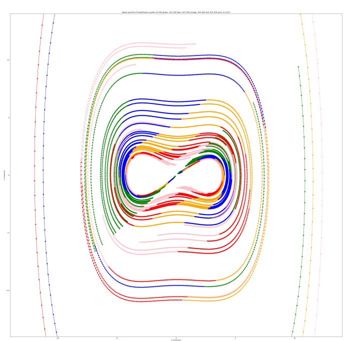
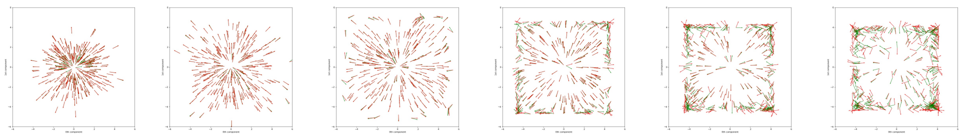


Figure SM1: Phase portrait of the Hamiltonian system associated with the double well potential. Here $0 \le t \le 5$, we use different colors to separate time intervals: green-$[0, 1)$; blue-$[1, 2)$; orange-$[2, 3)$; red-$[3, 4)$; pink-$[4, 5)$.

We also test our method on this example with $d = 20$ and solve the equation on $[0, 3]$. We demonstrate the numerical results in Figure SM3. The $\frac{1}{N}\sum_{k=1}^{N}|e_{t_i}^{(k)}|^2$-versus-$t_i$ plot is presented in Figure SM5 (left subfigure).

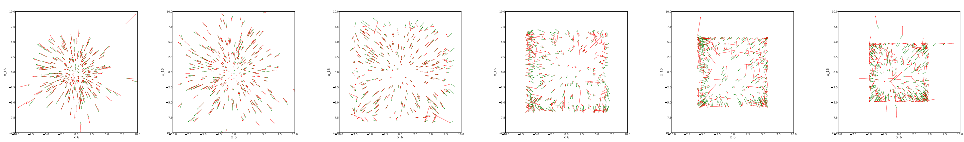
SM6.0.2. Duffing Oscillator. We consider the Duffing oscillator with $d = 2$, and the Hamiltonian

$$H(x, p) = \frac{1}{2}|p|^2 + \frac{1}{2}|x|^2 + \frac{1}{4}|x|^4.$$



(a) $t = 0.0$ (b) $t = 0.4$ (c) $t = 0.8$ (d) $t = 1.2$ (e) $t = 1.6$ (f) $t = 2.0$

Figure SM2: Plots of vector field $\nabla\psi_\theta(\cdot, t)$ (green) with momentums of samples (red) at different time stages.



(a) $t = 0.0$ (b) $t = 0.5$ (c) $t = 1.0$ (d) $t = 1.5$ (e) $t = 2.0$ (f) $t = 3.0$

Figure SM3: Plots of the vector field $\nabla\psi_\theta(\cdot, t)$ (green) with momentums of samples (red) at different time stages on the 6th $-$ 16th plane.

We select the initial condition as $g(x) = \frac{1}{2}|x|^2$. We pick $\rho_0 = \mathcal{N}(0, 2I)$ and solve the equation on $[0, 0.5]$.

The graphs of the numerical solution $\psi_\theta(\cdot, t)$ at different time stages t are shown in Figure SM4. The comparison between the learned vector field $\nabla\psi_\theta(\cdot, t)$ and the exact momentum of samples are shown in Figure SM4. They have a good agreement before time $T_* = 0.2$. The $\frac{1}{N}\sum_{k=1}^{N} |e_{t_i}^{(k)}|^2$-versus-$t_i$ plot is presented in Figure SM5 (left subfigure).

We summarize the hyperparameters used in our algorithm for each numerical example in the following table. The notations are same as in the section 4.

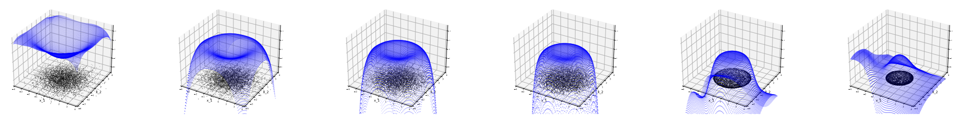
Example (dimension)	L	$\widetilde{d}$	M	M_T	N	lr	N_{Iter}
SM6.0.1 ($d = 20$)	6	50	120	1	8000	0.5×10^{-4}	8000
SM6.0.2 ($d = 2$)	7	24	100	2	2000	10^{-4}	12000

Table SM1: Hyperparameters of our algorithm for examples SM6.0.1 - SM6.0.2.

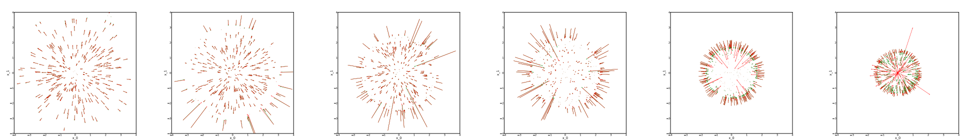
REFERENCES

[SM1] R. T. Rockafellar and R. Wets. *Variational analysis*, volume 317. Springer Science & Business Media, 2009.

[SM2] S. Shalev-Shwartz and S. Ben-David. *Understanding machine learning: From theory to algorithms*. Cambridge university press, 2014.

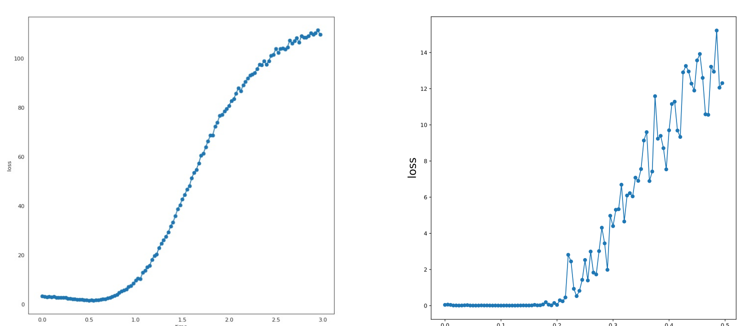


(a) $t = 0.05$ (b) $t = 0.1$ (c) $t = 0.15$ (d) $t = 0.2$ (e) $t = 0.35$ (f) $t = 0.5$



(g) $t = 0.05$ (h) $t = 0.1$ (i) $t = 0.15$ (j) $t = 0.2$ (k) $t = 0.35$ (l) $t = 0.5$

Figure SM4: (Up row) Graphs of our numerical solution ψ_θ at different time stages; (Down row) Comparison of $\nabla\psi_\theta(\cdot, t)$ (green) and the momentum of samples (red) at different time stages.



(a) Example SM6.0.1 (b) Example SM6.0.2

Figure SM5: Plots of the loss $\frac{1}{N}\sum_{k=1}^{N} |e_{t_i}^{(k)}|^2$ versus time t_i for examples SM6.0.1, SM6.0.2.