A Characteristic-Based Deep Learning Framework for Hamilton–Jacobi Equations with Application to Optimal Transport

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Outline

Hamilton-Jacobi Equations

Hamilton-Jacobi (HJ) PDE is a class of PDE of the following form:

$$\begin{cases} u_t + H(\nabla u) = 0 & \text{in } \Omega \times (0, T) \\ u = g & \text{on } \Omega \times \{t = 0\}, \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^d$ is the spatial domain, $H : \mathbb{R}^d \to \mathbb{R}$ is the Hamiltonian and $g : \Omega \to \mathbb{R}$ is the initial function.

- Non-unique
- Non-smooth, irrespective of the smoothness of the initial conditions or the Hamiltonian.

Prior Works: Classical Numerical Methods

1. Mesh-based methods, such as ENO/WENO (OS91; QS05; OS88)
   - Suffer from curse of dimensionality.

2. Hopf-formula-based causality-free method (DO16; CDOY17; CDOY19)

$$u(\mathbf{x}, t) = \inf_{\mathbf{y}} \left\{ tH^* \left(\frac{\mathbf{x} - \mathbf{y}}{t} \right) + g(\mathbf{y}) \right\}, \tag{2}$$

   where $H^*(\mathbf{z}) = \sup_{\mathbf{v} \in \mathbb{R}^d} \left\{ \mathbf{z}^{\mathrm{T}} \mathbf{v} - H(\mathbf{v}) \right\}$.
   - Suffer from computing Legendre transform.

3. PMP-based optimal control approaches (KW15; KW17)
   - Suffer from reduced practical effectiveness due to computing every single ODE trajectories.

Prior Works: Scientific ML Methods

1. Physics-Informed Neural Networks (PINNs) (DPT94; RPK19) solve the PDE by minimizing the integrated squared residual of the HJ PDE and the initial condition:

$$\mathcal{L}(u) = \int_0^T \int_\Omega \Big(u_t + H(\mathbf{x}, \nabla u)\Big)^2 + \lambda \int_\Omega (u - g)^2 .$$

   - No guarantee of obtaining the viscosity solution.

2. Specialized neural network architectures that express Hopf formulas (DLM20; DDM23)
   - Limited to specific HJ PDEs.

Method of Characteristics

Consider the HJ PDE

$$\begin{cases} u_t + H(\nabla u) = 0 & \text{in } \Omega \times (0, T) \\ u = g & \text{on } \Omega \times \{t = 0\}. \end{cases} \tag{3}$$

System of characteristic ODEs for (3) is given by the following:

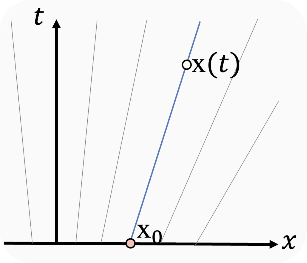
$$\begin{cases} \dot{\mathbf{x}} = \nabla H & \text{(4a)} \\ \dot{u} = q + \mathbf{p}^{\mathrm{T}} \nabla H = -H + \mathbf{p}^{\mathrm{T}} \nabla H & \text{(4b)} \\ \dot{q} = 0 & \text{(4c)} \\ \dot{\mathbf{p}} = 0, & \text{(4d)} \end{cases}$$

where the variables q and $\mathbf{p}$ are shorthand for the partial derivatives $q = u_t$ and $\mathbf{p} = \nabla u$, respectively.

Characteristic Lines

The characteristic
emanated from $\mathbf{x}(0) = \mathbf{x}_0 \in \Omega$ is a straight line

$$\mathbf{x}(t) = t\nabla H(\mathbf{p}) + \mathbf{x}_0,$$



implying that

$$\begin{aligned} u(t, \mathbf{x}(t)) &= -tH(\mathbf{p}) + t\mathbf{p}^{\mathrm{T}}\nabla H(\mathbf{p}) + u(\mathbf{x}_0, 0) \\ &= -tH(\mathbf{p}) + t\mathbf{p}^{\mathrm{T}}\nabla H(\mathbf{p}) + g(\mathbf{x}_0) \\ &= -tH(\mathbf{p}) + t\mathbf{p}^{\mathrm{T}}\nabla H(\mathbf{p}) + g(\mathbf{x} - t\nabla H(\mathbf{p})). \end{aligned}$$

Implicit Solution Formula

Substituting $\mathbf{p} = \nabla u(\mathbf{x}, t)$, we attain the following **implicit solution formula** for the HJ PDEs (3) (PO25):

$$u(\mathbf{x}, t) = -tH(\nabla u) + t\nabla u^{\mathrm{T}} \nabla H(\nabla u) + g(\mathbf{x} - t\nabla H(\nabla u)). \tag{5}$$

Theorem 1 (Convex Hamiltonian)

Assume the Hamiltonian H is differentiable and satisfies

$$\begin{cases} \mathbf{p} \mapsto H(\mathbf{p}) \ \textit{is strictly convex or concave}, \\ \lim_{|\mathbf{p}| \to \infty} \frac{H(\mathbf{p})}{|\mathbf{p}|} = +\infty, \end{cases} \tag{6}$$

and the initial function g is l.s.c. Then, the continuous function u that satisfies the implicit solution formula (5) *coincides with the* ***Hopf-Lax formula*** (2) *of* (3) *a.e.*

- Similarly, when g is convex (concave), the implicit solution formula coincides to the **Hopf formula**, representing the viscosity solution in this case.

Learning Implicit Solution with Neural Networks

Building upon the implicit solution formula, we propose the following minimization problem:

$$\min_{u} \mathcal{L}(u) \coloneqq \int_0^T \int_\Omega \Big(u + tH(\nabla u) - t\nabla u^{\mathrm{T}} \nabla H(\nabla u) - g(\mathbf{x} - t\nabla H(\nabla u)) \Big)^2 \,\mathrm{d}\mathbf{x}\,\mathrm{d}t. \tag{7}$$

- **Neural representation**: Parameterize u using a standard artificial neural network $u_\theta : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$.
- **Mesh-free**: Approximate the integral of (7) using Monte Carlo methods with randomly sampled collocation points.
- **Unsupervised Learning**: No ground truth solution data is required —the network learns the viscosity solution solely from H and g.

Algorithm

Algorithm 1 Algorithm for Learning Implicit Solution of HJ PDEs

1: Initialize the network u_θ with an initial network parameter θ_0.
2: **for** $n = 0, \cdots, N$ **do**
3: Randomly sample M collocations points $\left\{\left(\mathbf{x}_j, t_j\right)\right\}_{j=1}^{M} \sim U\left(\Omega \times [0, T]\right)$.
4: Calculate the loss by Monte Carlo integration

$$\hat{\mathcal{L}}\left(\theta_n\right) = \frac{1}{M}\sum_{j=1}^{M} \mathcal{S}\left(u_{\theta_n}\left(\mathbf{x}_j, t_j\right)\right)^2 .$$

5: Update θ_n by gradient descent with a step size $\alpha > 0$

$$\theta_{n+1} \leftarrow \theta_n - \alpha \nabla_\theta \hat{\mathcal{L}}\left(\theta_n\right) .$$

6: **end for**
7: **return** u_{θ_N} as the predicted viscosity solution to the HJ PDE (3).

Comparison with Prior Works

Question: Does this approach effectively address the key limitations of previous works?

- The curse of dimensionality associated with mesh-based methods.
  ☺ The proposed approach is **mesh-free**.
- The computational challenges of the Legendre transform in Hopf formula-based methods.
  ☺ The proposed approach **does not require the Legendre transform**.
- The inefficiency of computing single characteristic trajectories in optimal control-based methods.
  ☺ The proposed approach **does not compute individual trajectories**.

Numerical Results

- **Example 1** (Convex): $H(\mathbf{p}) = \frac{1}{2}\|\mathbf{p}\|_2^2$ and $g(\mathbf{x}) = \|\mathbf{x}\|_1$.
- **Example 2** (Concave): $H(\mathbf{p}) = -\frac{1}{2}\|\mathbf{p}\|_2^2$ and $g(\mathbf{x}) = \|\mathbf{x}\|_1$.
- **Example 3** (Level set): $H(\mathbf{p}) = \|\mathbf{p}\|_2$ and g is the signed distance function for two disjoint circles.

Table 1: The mean squared errors with the exact solution, the average computational time per epoch, and the memory usage.

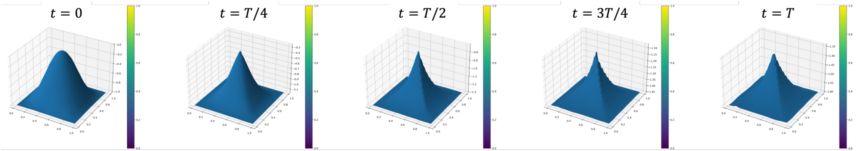
Problem	$d = 1$	$d = 10$	$d = 40$
Example 1	1.14E-7	2.56E-5	1.30E-3
Example 2	8.59E-6	1.63E-4	1.23E-3
Example 3	7.08E-6	5.57E-5	1.13E-3
Time (s) per Epoch	0.01518	0.01630	0.01864
Memory (MB)	42.648	42.648	43.623

Numerical Results

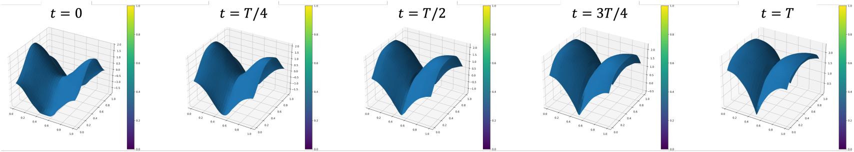
Table 2: Nonconvex examples

Problem	Hamiltonian H	Initial function g
Example 4	$-\cos\left(\sum_{i=1}^{d} u_{x_i} + 1\right)$	$-\cos\left(\frac{\pi}{d}\sum_{i=1}^{d} x_i\right)$
Example 5	$\sin\left(u_x + u_y\right)$	$\pi\left(\lvert y\rvert - \lvert x\rvert\right)$
Example 6	$u_x u_y$	$\sin(x) + \cos(y)$
Example 7	$\iint u_x + u_y + 1$	$\frac{1}{4}\left(\cos\left(2\pi x\right) - 1\right)\left(\cos\left(2\pi y\right) - 1\right) - 1$
Example 8	$-\iint u_x + u_y + 1$	$\cos\left(2\pi x\right) - \cos\left(2\pi y\right)$
Example 9	$u_x^3 - u_x$	$-\frac{1}{10}\cos\left(5x\right)$

Numerical Results



(a) Example 7 (Eikonal)



(b) Example 8 (Combustion)

Optimal Transport

For two distributions $\mu, \nu \in \mathcal{P}(\Omega)$ supported on $\Omega \subset \mathbb{R}^d$, optimal transport (OT) problem seeks a map T that transforms μ to ν whilst minimizing the cost ℓ.

Monge Formulation

$$W_c(\mu, \nu) \coloneqq \inf_{T_\sharp \mu = \nu} \int_\Omega \ell(\mathbf{x} - T(\mathbf{x}))\, \mathrm{d}\mu(\mathbf{x}) . \tag{8}$$

Benamou-Brenier fluid dynamical formulation

$$\inf_{v} \mathbb{E}_\mu \left[\int_0^{t_f} \ell\left(v\left(\mathbf{x}(t), t\right)\right) \mathrm{d}t \right] \tag{9}$$

$$\text{s.t. } \dot{\mathbf{x}} = v \tag{10}$$

$$\mathbf{x}(0) \sim \mu,\ \mathbf{x}(t_f) \sim \nu, \tag{11}$$

HJ equation

$$\begin{cases} \frac{\partial u}{\partial t} - h(\nabla u) = 0 & \text{in } \Omega \times (0, t_f) \\ u = g & \text{on } \Omega \times \{t = 0\}, \end{cases} \tag{12}$$

Method of Characteristics

The viscosity solution is theoretically characterized by the **characteristic ODEs**

$$\begin{cases} \dot{\mathbf{x}} = \nabla h & (13a) \\ \dot{u} = -h + \mathbf{p}^{\mathrm{T}} \nabla h & (13b) \\ \dot{\mathbf{p}} = 0, & (13c) \end{cases}$$

Bidirectional OT Map

A bidirectional formulation of the OT map arises from the forward and backward characteristic flows of the associated HJ equation:

- Forward Map : $T^{\star}(\mathbf{x}) = \mathbf{x} - t_f \nabla h\left(\nabla u\left(\mathbf{x}, 0\right)\right), \quad \mathbf{x} \sim \mu,$ (14)
- Backward Map: $\left(T^{\star}\right)^{-1}(\mathbf{y}) = \mathbf{y} + t_f \nabla h\left(\nabla u\left(\mathbf{y}, t_f\right)\right), \quad \mathbf{y} \sim \nu.$ (15)

Characteristic-based OT Learning

We propose a deep learning framework for OT based on HJ characteristics, consisting of two key steps:

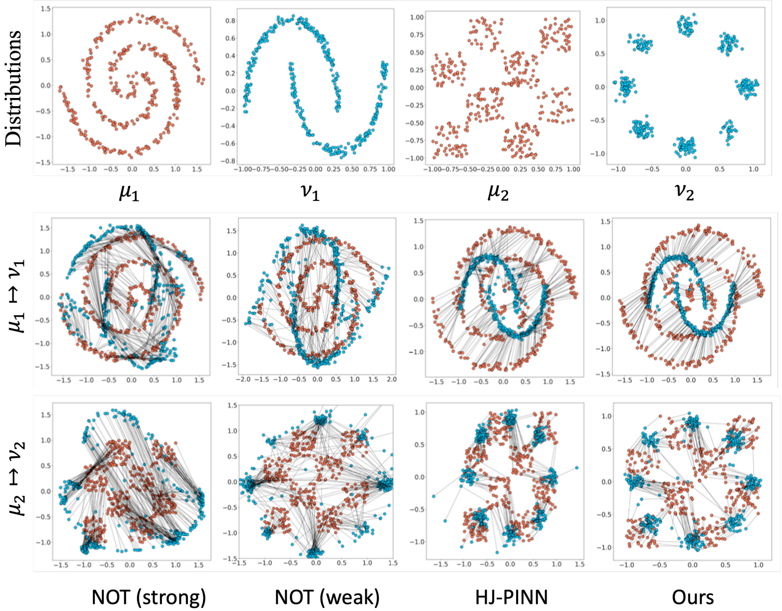
1. Learning the Viscosity Solution: Train a neural network u_θ to approximate the viscosity solution using the implicit solution formula of the HJ equation.
2. Recovering the OT Map: Obtain the bidirectional OT map from the learned solution by the characteristic-based formulation

$$T_\theta(\mathbf{x}) = \mathbf{x} - t_f \nabla h\left(\nabla u_\theta\left(\mathbf{x}, 0\right)\right), \quad \mathbf{x} \sim \mu,$$
$$\left(T_\theta\right)^{-1}(\mathbf{y}) = \mathbf{y} + t_f \nabla h\left(\nabla u_\theta\left(\mathbf{y}, t_f\right)\right), \quad \mathbf{y} \sim \nu.$$

Method	**Optimization**	**# Networks**	**OT direction**	**Sampling**	**Optimality of T**
Dual Formulation	Min-Max	Two	One-way	Direct	No
Dynamical Models	Min	Single	Bidirectional	Iterative	No
HJ-based (Proposed)	Min	Single	Bidirectional	Direct	Yes

Table 3: Comparison of key features across different OT model approaches.

2D Examples


Distributions
μ_1
ν_1
μ_2
ν_2
$\mu_1 \mapsto \nu_1$
$\mu_2 \mapsto \nu_2$
NOT (strong)
NOT (weak)
HJ-PINN
Ours

Accuracy of Learned OT Map

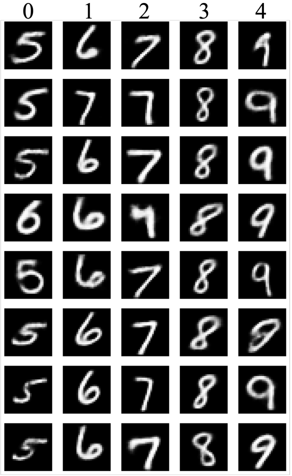
Evaluate the learned transport map in the Gaussian-to-Gaussian setting, $\mu = \mathcal{N}\left(\mathbf{0}, \Sigma_\mu\right)$ and $\nu = \mathcal{N}\left(\mathbf{0}, \Sigma_\nu\right)$, where a closed-form solution to the OT is available.

Table 4: Quantitative comparison of $\mathcal{L}^2$−UVP(↓) across OT methods in increasing dimensions.

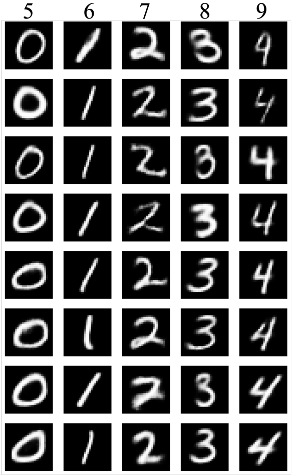
Model	$d = 2$	$d = 4$	$d = 8$	$d = 16$	$d = 32$	$d = 64$
NOT	77.248	125.419	114.056	176.086	182.287	196.831
WGAN-QC	1.596	5.897	31.0367	59.314	113.237	141.407
LS	5.806	9.781	15.963	25.232	41.445	55.360
MM-v1	0.161	0.172	0.173	0.210	**0.374**	**0.415**
HJ-PINN	0.080	0.069	0.163	0.458	0.576	1.683
Ours	**0.010**	**0.021**	**0.086**	**0.146**	0.436	0.858

Class-Conditional OT

Class-wise OT on the MNIST dataset (28×28), transporting digits from $\{0, 1, 2, 3, 4\}$ to its corresponding digit in $\{5, 6, 7, 8, 9\}$ (i.e., $0 \to 5$, $1 \to 6$, ..., $4 \to 9$).



(c) Forward



(d) Backward

Conclusion

- Proposed a novel implicit solution formula for HJ PDEs derived from the characteristics.
- Recovered the classical Hopf formula in convex settings, while simplifying it by eliminating the need for Legendre transforms.
- Developed a simple and effective deep learning-based method for solving high-dimensional HJ PDEs, mitigating the curse of dimensionality.
- Demonstrated the scalability and effectiveness of the proposed method across various high-dimensional and nonconvex benchmark problems.
- Showed that the implicit formula, together with characteristic flows, enables an efficient and principled approach to solving optimal transport problems.

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Thank you!