GeONet: a neural operator for learning the Wasserstein geodesic

DIGIMAT

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Introduction

We present GeONet, a neural operator deep learning framework for learning the Wasserstein geodesic.

GeONet is instantaneous, and allows for real-time predictions in the online setting, unlike traditional optimal transport numerical solvers.

Traditional methods require domain discretization and suffer from curse-of-dimensionality, unlike GeONet.

Finally, GeONet needs initial condition data only.

Background

The optimal transport problem was originally formulated by Monge, which seeks an optimal map such that

$$\min_{T:\mathbb{R}^d\to\mathbb{R}^d}\left\{\int_{\mathbb{R}^d} c(x,T(x))\,\mathrm{d}\mu_0(x) : T_\sharp\mu_0=\mu_1\right\}$$

for general cost function. We will consider quadratic cost $c(x,y)=\frac{1}{2}\|x-y\|_2^2$. The Monge problem induces a distance

$$W_2^2(\mu_0,\mu_1) := \min_\gamma\left\{\int_{\mathbb{R}^d\times\mathbb{R}^d}\|x-y\|_2^2\,\mathrm{d}\gamma(x,y)\right\}.$$

This can be re-expressed in a dual form

$$\frac{1}{2}W_2^2(\mu_0,\mu_1)=\sup\left\{\int_{\mathbb{R}^d}\varphi\,\mathrm{d}\mu_0+\int_{\mathbb{R}^d}\psi\,\mathrm{d}\mu_1 : \varphi(x)+\psi(y)\leqslant\frac{\|x-y\|_2^2}{2},\ \varphi\in L^1(\mu_0),\ \psi\in L^1(\mu_1)\right\}$$

The Benamou-Brenier dynamic formulation expresses the Wasserstein distance as a minimal flow kinetic energy problem

$$\frac{1}{2}W_2^2(\mu_0,\mu_1)=\min_{(\mu,\mathbf{v})}\int_0^1\int_{\mathbb{R}^d}\frac{1}{2}\|\mathbf{v}(x,t)\|_2^2\,\mu(x,t)\,\mathrm{d}x\,\mathrm{d}t$$
$$\text{subject to }\ \partial_t\mu+\mathrm{div}(\mu\mathbf{v})=0,\ \ \mu(\cdot,0)=\mu_0,\ \ \mu(\cdot,1)=\mu_1$$

where the probability density flow satisfies the continuity equation. To solve the above, we apply Lagrange multipliers, which yields a system of PDEs

$$\begin{cases}\partial_t\mu+\mathrm{div}(\mu\nabla u)=0,\ \ \partial_t u+\frac{1}{2}\|\nabla u\|_2^2=0,\\ \mu(\cdot,0)=\mu_0,\ \ \mu(\cdot,1)=\mu_1.\end{cases}$$

A neural operator is effectively a deep learning framework that learns a mapping $\Gamma^\dagger:\mathcal{A}\to\mathcal{U}$ between infinite-dimensional function spaces, typically defined through a PDE or differential operator. We construct a parametric map $\Gamma:\mathcal{A}\times\Theta\to\mathcal{U}$ to approximate the true operator, which can be done via a physics-informed risk

$$\theta^*=\mathrm{argmin}_{\theta\in\Theta}\ \ \mathbb{E}_{(a,u_0,u_T)\sim\mu}\Big[\big\|(\partial_t+\mathcal{D})\Gamma(a,\theta)\big\|_{L^2(\Omega\times(0,T))}^2$$
$$+\lambda_0\big\|\Gamma(a,\theta)(\cdot,0)-u_0\big\|_{L^2(\Omega)}^2+\lambda_T\big\|\Gamma(a,\theta)(\cdot,T)-u_T\big\|_{L^2(\Omega)}^2\Big]$$

Our method

DeepONets are a neural operator framework effective for physics-informed systems. This architecture is set up

$$\Gamma^\dagger(u_0,u_1)(x,t)\approx\sum_{\ell=1}^p\mathcal{B}_\ell(u_0(x_1),\dots,u_0(x_m),u_1(x_1),\dots,u(x_m))\mathcal{T}_\ell(x,t)$$

This architecture acts as a fine equivalence to the universal approximation theorem. It is our aim to learn a nonlinear operator mapping two input probability measures to the connecting geodesic, outlined by

$$\Upsilon^\dagger:\mathcal{P}_2(\Omega)\times\mathcal{P}_2(\Omega)\to\mathrm{AC}(\mathcal{P}_2(\Omega)),$$
$$(\mu_0,\mu_1)\mapsto\{\mu_t\}_{t\in[0,1]},$$

based on training data $\{(\mu_0^{(1)},\mu_1^{(1)}),\dots,(\mu_0^{(n)},\mu_1^{(n)})\}$. We implement 4 neural networks such that

$$\mathcal{C}(x,t,\mu_0,\mu_1,\theta^{\mathrm{cty}},\xi^{\mathrm{cty}})=\sum_\ell\mathcal{B}_\ell^{\mathrm{cty}}\mathcal{T}_\ell^{\mathrm{cty}},$$
$$\mathcal{H}(x,t,\mu_0,\mu_1,\theta^{\mathrm{HJ}},\xi^{\mathrm{HJ}})=\sum_\ell\mathcal{B}_\ell^{\mathrm{HJ}}\mathcal{T}_\ell^{\mathrm{HJ}}\ .$$

i.e., we have branch and trunk neural networks. Our optimization procedure is outlined as minimizing the empirical loss as a sum of continuity, HJ, and boundary losses

$$\phi^*,\psi^*\ \ =\ \ \mathrm{argmin}_{\phi,\psi\in\Theta\times\Xi}\ \ \mathcal{L}_{\mathrm{cty}}+\mathcal{L}_{\mathrm{HJ}}+\mathcal{L}_{\mathrm{BC}},$$

where

$$\mathcal{L}_{\mathrm{cty},i}\ =\ \frac{\alpha_1}{N}\left\|\frac{\partial}{\partial t}\mathcal{C}_{\theta,i}+\mathrm{div}(\mathcal{C}_{\theta,i}\nabla\mathcal{H}_{\xi,i})\right\|_{L^2(\Omega\times(0,1))}^2,$$
$$\mathcal{L}_{\mathrm{HJ},i}\ =\ \frac{\alpha_2}{N}\left\|\frac{\partial}{\partial t}\mathcal{H}_{\xi,i}+\frac{1}{2}\|\nabla\mathcal{H}_{\xi,i}\|_2^2\right\|_{L^2(\Omega\times(0,1))}^2,$$
$$\mathcal{L}_{\mathrm{BC},i}\ =\ \frac{\beta_0}{N}\left\|\mathcal{C}_{\theta,0,i}-\mu_0^{(i)}\right\|_{L^2(\Omega)}^2+\frac{\beta_1}{N}\left\|\mathcal{C}_{\theta,1,i}-\mu_1^{(i)}\right\|_{L^2(\Omega)}^2.$$

Training Algorithm

Algorithm 1 Train GeONet

Input: data pairs $(\mu_0^{(1)},\mu_1^{(1)}),\dots,(\mu_0^{(n)},\mu_1^{(n)})$; discretization size N; initialization of the neural network parameters $\phi\in\Theta\times\Xi,\psi\in\Theta\times\Xi$; weight parameters $\alpha_1,\alpha_2,\beta_0,\beta_1$.

1: **while** $\mathcal{L}_{\mathrm{total}}$ has not converged **do**
2: Independently draw N sample points $\{(x_\ell^i,t_\ell^i)\}_{\ell=1}^N$ from $U(\Omega)\times U(0,1)$
3: Compute $\Phi_i=\partial_t\mathcal{C}_{\phi,i}+\mathrm{div}(\mathcal{C}_{\phi,i}\nabla\mathcal{H}_\psi)$. ▷ `continuity residual`
4: Compute $\Psi_i=\partial_t\mathcal{H}_\psi+\frac{1}{2}\|\mathcal{H}_\psi\|_2^2$. ▷ `Hamilton-Jacobi residual`
5: Compute $B_{0,i}=\mathcal{C}_{\phi,0,i}-\mu_0^{(i)}(x_\ell^i),\ B_{1,i}=\mathcal{C}_{\phi,1,i}-\mu_1^{(i)}(x_\ell^i)$. ▷ `boundary residual`
6: Compute

$$\mathcal{L}_{\mathrm{cty}}=\frac{\alpha_1}{N}\sum_{i=1}^n\|\Phi_i\|_{L^2(\Omega\times(0,1))}^2,\quad\mathcal{L}_{\mathrm{HJ}}=\frac{\alpha_2}{N}\sum_{i=1}^n\|\Psi_i\|_{L^2(\Omega\times(0,1))}^2,$$
$$\mathcal{L}_{\mathrm{BC}}=\frac{1}{N}\sum_{i=1}^n\beta_0\|B_{0,i}\|_{L^2(\Omega)}^2+\beta_1\|B_{1,i}\|_{L^2(\Omega)}^2,$$

where $\|f\|_{L^2(\Omega\times(0,1))}^2:=\sum_{\ell=1}^N f^2(x_\ell,t_\ell)$ and $\|f\|_{L^2(\Omega)}^2:=\sum_{\ell=1}^N f^2(x_\ell)$.
7: Compute $\mathcal{L}_{\mathrm{total}}(\phi,\psi)=\mathcal{L}_{\mathrm{cty}}+\mathcal{L}_{\mathrm{HJ}}+\mathcal{L}_{\mathrm{BC}}$.
8: Minimize $\mathcal{L}_{\mathrm{total}}(\phi,\psi)$ to update ϕ and ψ. ▷ `minimize the loss function`
9: **end while**

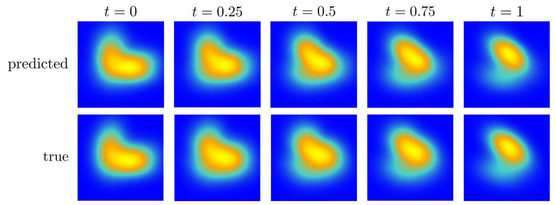
Experiments

We provide experimental results. We employ GeONet on Gaussian mixtures, which serve as continuous density estimators. Furthermore, we employ GeONet on real 32x32 CIFAR-10 images.

We begin by considering mixtures of the form

$$\mu_j(x)=\sum_{i=1}^{k_j}\pi_i\mathcal{N}(x|u_i,\Sigma_i)\qquad\text{subject to}\qquad\sum_{i=1}^{k_j}\pi_i=1$$

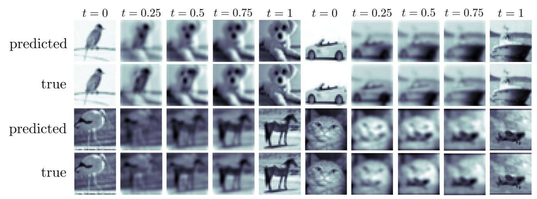
concentrated in a compact hypercube domain.



GeONet error for Gaussian mixtures

number of Gaussians	$t=0$	$t=0.25$	$t=0.5$	$t=0.75$	$t=1$
$k_0=3,k_1=2$	0.39 ± 0.33	2.6 ± 2.8	4.4 ± 5.1	2.9 ± 2.9	0.57 ± 0.61
$k_0=4,k_1=2$	0.73 ± 1.4	4.4 ± 8.1	7.1 ± 13	4.3 ± 6.3	0.58 ± 0.48
$k_0=5,k_1=2$	0.46 ± 0.39	3.3 ± 3.8	5.3 ± 5.9	3.6 ± 4.5	0.85 ± 2.2

Next, we employ GeONet on CIFAR-10 images.



MSE on CIFAR-10 data

Method	$t=0$	$t=0.25$	$t=0.5$	$t=0.75$	$t=1$
ER-GeONet	0.099 ± 0.14	12 ± 19	19 ± 27	11 ± 15	0.11 ± 0.32
GE-GeONet	0.76 ± 1.2	11 ± 19	18 ± 26	10 ± 15	0.47 ± 0.93

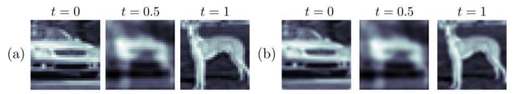
The above results were collected using a simple neural network architecture. We propose to implement a superior DeepONet architecture, which should be able to handle more sophisticated density geodesics.

We also intend to include baseline cases in our error analysis.

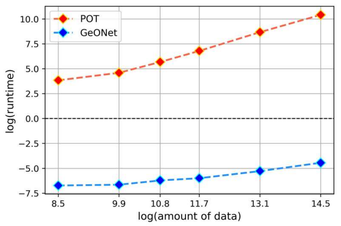
Method characteristics

GeONet is mesh-invariant, and is strong for super-resolution examples.

We may feed data along a low-dimensional discretization, and a geodesic along a high-dimensional domain can be produced.



GeONet requires a training procedure, but inference is instantaneous unlike traditional numerical solvers, which are particularly encumbered with a low regularization parameter and a high-dimensional domain discretization.



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