Neural Optimal Transport with Lagrangian Costs

paper code

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Optimal transport (OT) with Lagrangian costs

Optimal Transport: Old and New. Cedric Villani, 2008; *Computational Optimal Transport*. Gabriel Peyré and Marco Cuturi, 2018.

For a cost function $c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, the (dual) **transport problem** is given by

$$\mathrm{OT}_c(\mu, \nu) \coloneqq \sup_{g \in L^1(\nu)} \int g^c(x)\,\mathrm{d}\mu(x) + \int g(y)\,\mathrm{d}\nu(y)$$

c-transform: $g^c(x) \coloneqq \inf_{y \in \mathcal{Y}} J(y; x)$ where $J(y;x) \coloneqq c(x,y) - g(y)$

Lagrangian costs: general-purpose cost function given by an **optimization sub-routine** over curves

$$c(x,y) \coloneqq \inf_{\gamma \in \mathcal{C}(x,y)} E(\gamma; x, y) \quad E(\gamma; x, y) \coloneqq \left\{ \int_0^1 \mathcal{L}(\gamma_t, \dot{\gamma}_t, t)\,\mathrm{d}t \right\}$$

encompasses ℓ_p norms, barrier functions, non-Euclidean metrics (geodesics), and more

Examples

1) Euclidean kinetic
$\mathcal{L}(\gamma_t, \dot{\gamma}_t, t) \coloneqq \frac{1}{2}\|\dot{\gamma}_t\|^2$,
c becomes the squared Euclidean distance

2) Euclidean kinetic and potential
$\mathcal{L}(\gamma_t, \dot{\gamma}_t, t) \coloneqq \frac{1}{2}\|\dot{\gamma}_t\|^2 - U(\gamma_t)$,

3) Riemannian kinetic
$\mathcal{L}(\gamma_t, \dot{\gamma}_t, t; A) = \frac{1}{2}\|\dot{\gamma}_t\|^2_{A(\gamma_t)}$.
c becomes the squared geodesic distance

OT map for general costs: Our goal is to learn $\hat{y}(x; c, g) \coloneqq \operatorname{argmin}_{y \in \mathcal{Y}} \{c(x,y) - g(y)\}$.

❗**Challenges:** computing (1) the cost c, (2) the c-transform, (3) the optimal potential g
Our approach: approximate (1), (2), (3) with neural networks (obviously!)

Neural OT with Lagrangian Costs

Deep generalized Schrödinger bridge. Liu et al., NeurIPS 2023; *Neural Lagrangian Schrödinger bridge*. Koshizuka and Sato, ICLR 2023; *Optimal transport mapping via input convex neural networks* Makkuva et al., ICML 2020; *Wasserstein-2 Generative Networks*, Korotin et al., ICLR 2021; *On amortizing convex conjugates for optimal transport*. Amos, ICLR 2023; *Tutorial on amortized optimization*. Amos, FnT in ML, 2023.

Parametrization with neural networks: Optimize

(1) Lagrangian path φ_η

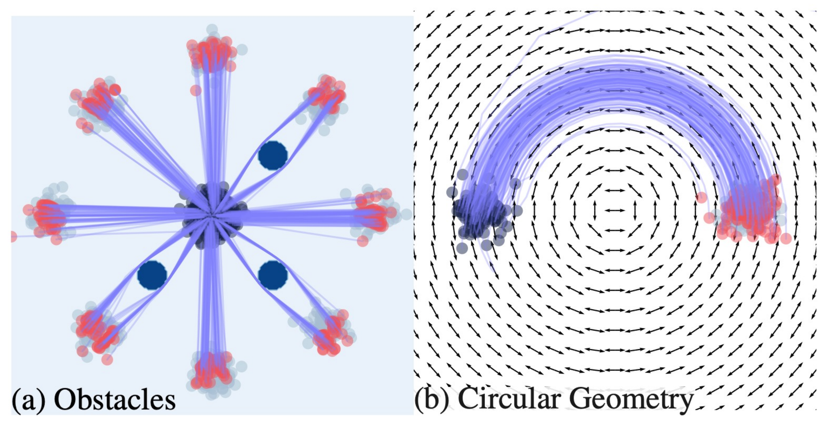
$$\min_\eta \int E(\varphi_\eta; x, \hat{y}(x))\,\mathrm{d}\mu(x).$$

(2) OT map y_ϕ

$$\min_\phi \int \|\hat{y}(x) - y_\phi(x)\|\,\mathrm{d}\mu(x).$$

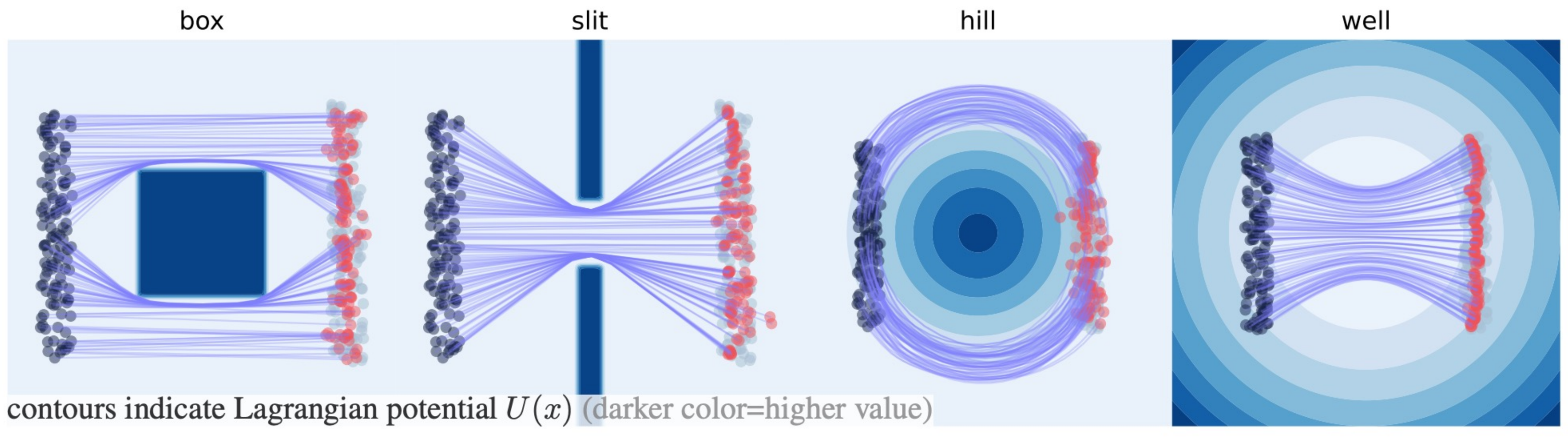
(3) potential g_θ

$$\ell_{\mathrm{dual}}(\theta) \coloneqq \int g_\theta^c(x)\,\mathrm{d}\mu(x) + \int g_\theta(y)\,\mathrm{d}\nu(y)$$



Algorithm 1 Neural Lagrangian Optimal Transport

```
inputs: measures μ and ν, Kantorovich potential g_θ, c-transform predictor y_φ, and spline predictor φ_η
while unconverged do
    sample batches {x_i}_{i=1}^N ~ μ and {y_i}_{i=1}^N ~ ν
    obtain the amortized c-transform predictor y_φ(x_i) for i ∈ [N]
    fine-tune the c-transform by numerically solving Eq. (9), warm-starting with y_φ(x_i)
    update the potential with gradient estimate of ∇_θ ℓ_dual (Eq. (18))
    update the c-transform predictor y_φ using a gradient estimate of Eq. (20)
    update the spline predictor φ_η using a gradient estimate of Eq. (23)
end while
return optimal parameters θ, φ, η
```



Metric learning with Lagrangian OT

Riemannian Metric Learning via Optimal Transport. Scarvelis and Solomon, ICLR 2023.

Task: learn the underlying metric with pairs of probability measures

Table 1. Alignment scores ℓ_{align} for metric recovery in Fig. 4. (higher is better)

	Circle	Mass Splitting	X Paths
Scarvelis and Solomon (2023)	0.995	0.839	0.916
Our approach	**0.997 ± 0.002**	**0.986 ± 0.001**	**0.957 ± 0.001**

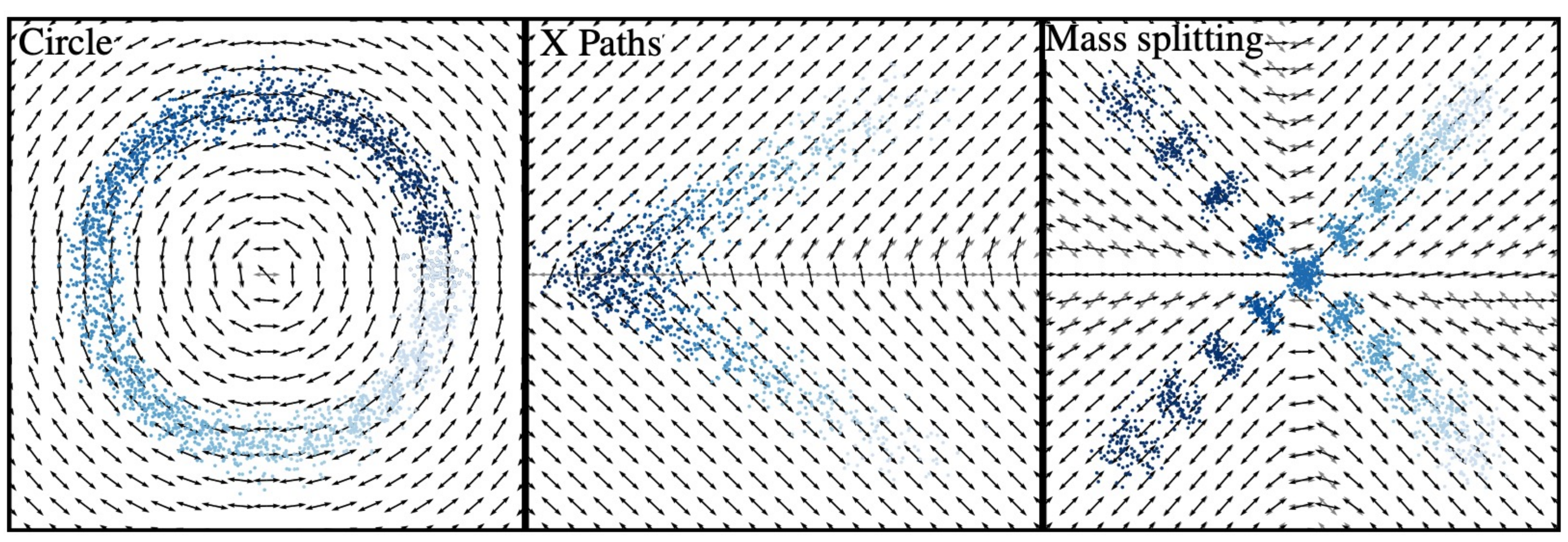


Figure 3. We successfully recover the metrics on the settings from Scarvelis and Solomon (2023).

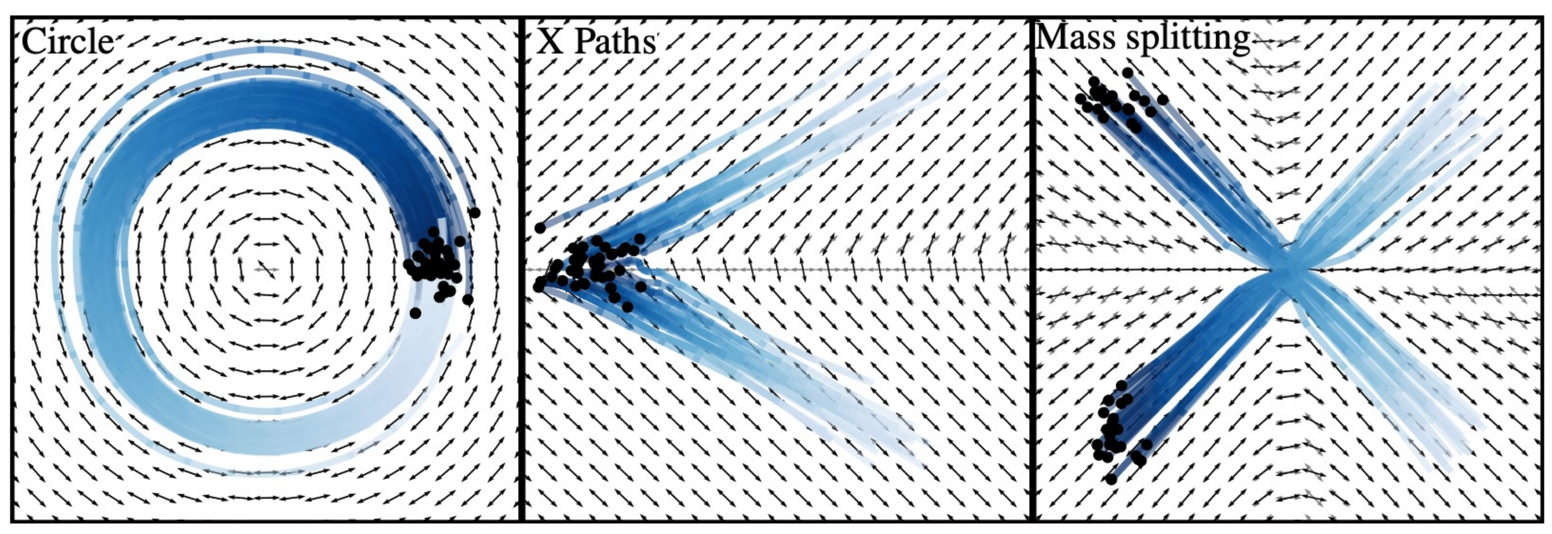


Figure 4. Our transport geodesics are able to reconstruct continuous versions of the original data that can predict the movement of individual particles given only samples from the first measure.