#### Optimal Transport Justin Solomon

6.838: Shape Analysis Spring 2021



### Motivation



Practice



### What is Optimal Transport?

#### A geometric way

# to compare probability measures.



### **Plan For Today**

#### **1.** Introduction to optimal transport

- Construction
- Many formulas
- 2. Applications
- 3. Discrete/discretized transport
  - Entropic regularization
  - Eulerian transport
  - Semidiscrete transport

#### 4. Extensions & frontiers

#### **Useful References**



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#### **Probability as Geometry**



#### "Somewhere over here."

### **Probability as Geometry**



### "Exactly here."

### **Probability as Geometry**



#### "One of these two places."

#### **How We Compute Distances**



#### **Equidistant!**



### What's Wrong?



Measured overlap, not displacement.

#### **Alternative Idea**



#### Match mass from the distributions

#### Observation

# Even the laziest shoveler must do some work.

Property of the distributions themselves!



My house!

## **Measure Coupling**

$$\pi(x,y) :=$$
 Amount moved from  $x$  to  $y$ 

$$\begin{aligned} \pi(x,y) &\geq 0 \; \forall x \in X, y \in Y \text{ mass is positive} \\ \int_Y \pi(x,y) \, dy &= \rho_0(x) \; \forall x \in X & \text{ must scoop} \\ \int_X \pi(x,y) \, dx &= \rho_1(y) \; \forall y \in Y & \text{ must cover} \\ \int_X \pi(x,y) \, dx &= \rho_1(y) \; \forall y \in Y & \text{ must cover the target} \end{aligned}$$

#### **Kantorovich Problem**

$$OT(\mu,\nu;c) := \min_{\pi \in \Pi(\mu,\nu)} \iint_{X \times Y} c(x,y) \, d\pi(x,y)$$

#### **General transport problem**

# *p*-Wasserstein Distance

$$\mathcal{W}_{p}(\mu,\nu) \equiv \min_{\pi \in \Pi(\mu,\nu)} \left( \iint_{X \times X} d(x,y)^{p} d\pi(x,y) \right)^{1/p}$$
  
Shortest path distance Expectation



http://www.sciencedirect.com/science/article/pii/S152407031200029X#

#### 1-Wasserstein in 1D

$$\mathcal{W}_{1}(\rho_{0},\rho_{1}) := \begin{cases} \min_{\pi} & \iint_{\mathbb{R}\times\mathbb{R}} \pi(x,y) | x - y | \, dx \, dy & \text{Minimize total work} \\ \text{s.t.} & \pi \ge 0 \, \forall x, y \in \mathbb{R} & \text{Nonnegative mass} \\ & \int_{\mathbb{R}} \pi(x,y) \, dy = \rho_{0}(x) \, \forall x \in \mathbb{R} & \text{Starts from } \rho_{0} \\ & \int_{\mathbb{R}} \pi(x,y) \, dx = \rho_{1}(y) \, \forall y \in \mathbb{R} & \text{Ends at } \rho_{1} \end{cases}$$



#### In One Dimension: Closed-Form



#### **PDF** ..... ► **CDF**<sup>-1</sup>

$$\mathcal{W}_1(\mu,\nu) = \int_{-\infty}^{\infty} |\mathrm{CDF}(\mu) - \mathrm{CDF}(\nu)| \, d\ell \qquad \begin{array}{l} \text{Doesn't extend} \\ \text{past 1d!} \end{array}$$
$$\mathcal{W}_2^2(\mu,\nu) = \int_{-\infty}^{\infty} \left(\mathrm{CDF}^{-1}(\mu) - \mathrm{CDF}^{-1}(\nu)\right)^2 \, d\ell$$

### **Fully-Discrete Transport**



Linear program: Finite number of variables Algorithms: Simplex, interior point, auction, ...



#### Semidiscrete Transport

$$\mu_0 := \sum_{i=1}^{k_0} a_{0i} \delta_{x_{0i}} \qquad \qquad \mu_1(S) := \int_S \rho_1(x) \, dx$$



### **Monge Formulation**

$$\inf_{\phi_{\sharp}\rho_0=\rho_1}\int_{-\infty}^{\infty}c(x,\phi(x))\rho_0(x)\,dx$$



[Monge 1781]; image courtesy Marco Cuturi

#### Not always well-posed!

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#### **Example: Discrete Transport**

$$X = \{1, 2, \dots, k_1\}, Y = \{1, 2, \dots, k_2\}$$

$$OT(v, w; C) = \begin{cases} \min_{T \in \mathbb{R}^{k_1 \times k_2}} & \sum_{ij} T_{ij} c_{ij} \\ \text{s.t.} & T \ge 0 \\ & \sum_j T_{ij} = v_i \ \forall i \in \{1, \dots, k_1\} \\ & \sum_i T_{ij} = w_j \ \forall j \in \{1, \dots, k_2\}. \end{cases}$$

# Metric when d(x,y) satisfies the triangle inequality.

"The Earth Mover's Distance as a Metric for Image Retrieval" Rubner, Tomasi, and Guibas; IJCV 40.2 (2000): 99—121.

> Revised in: **"Ground Metric Learning"** Cuturi and Avis; JMLR 15 (2014)

### **Kantorovich Duality**

### Flow-Based W<sub>2</sub>

$$\mathcal{W}_{2}^{2}(\rho_{0},\rho_{1}) = \begin{cases} \inf_{\rho,v} \iint_{M \times [0,1]} \frac{1}{2}\rho(x,t) \|v(x,t)\|^{2} \, dx \, dt \\ \text{s.t. } \nabla \cdot (\rho(x,t)v(x,t)) = \frac{\partial \rho(x,t)}{dt} \\ v(x,t) \cdot \hat{n}(x) = 0 \, \forall x \in \partial M \\ \rho(x,0) = \rho_{0}(x) \\ \rho(x,1) = \rho_{1}(x) \end{cases}$$

#### [Benamou & Brenier 2000]



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# Wassersteinization

[wos-ur-stahyn-ahy-sey-sh*uh*-n] noun.

#### Introduction of optimal transport into a computational problem.

cf. least-squarification,  $L_1$  ification, deep-netification, kernelization

### **Key Ingredients**

#### We have tools to

- Solve optimal transport problems numerically
- Differentiate transport distances in terms of their input distributions

#### **Bonus:**

Transport cost from  $\mu$  to  $\nu$  is a **convex** function of  $\mu$  and  $\nu$ .

### **Operations and Logistics**



#### **Minimum-cost flow**

### **Histograms and Descriptors**



[Kusner et al. 2015]

#### Word Mover's Distance (WMD)

### **Registration and Reconstruction**



Fig. 2. First row: Matching of fibres bundles. Second row: Matching of two hand surfaces using a balanced OT fidelity. Target is in purple.

[Feydy, Charlier, Vialard, and Peyré 2017]



# **Engineering Design**



EPFL Computer Graphics and Geometry Laboratory; Rayform SA

# Interpolation



### Blue Noise and Distribution Approximation



$$\min_{x_1,\dots,x_n} \mathcal{W}_2^2\left(\mu, \frac{1}{n}\sum_i \delta_{x_i}\right)$$

Zebra image courtesy F. de Goes; photo by F. Durand; distribution image courtesy S. Claici

#### **Statistical Estimation**



#### **Minimum Kantorovich Estimator**

### **Domain Adaptation**



- 1. Estimate transport map
- 2. Transport labeled samples to new domain
- 3. Train classifier on transported labeled samples

[Courty et al. 2017]

#### **Generative Adversarial Networks (GANs)**



Figure 9: WGAN algorithm: generator and critic are DCGANs.

[Arjovsky et al. 2017]

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Theme in computation: Same in theory, but different in practice

Choose one of each:

Formulation

Discretization

#### **Well-Known Theme**

#### "No Free Lunch"

	Sym	Loc	Lin	Pos	PSD	Con
MEAN VALUE	0	•	•	•	0	0
INTRINSIC DEL	•	0	•	•	•	?
COMBINATORIAL	•	•	0	•	•	0
COTAN	•	•	•	0	•	•

Observe that none of the Laplacians considered in graphics fulfill *all* desired properties. Even more: none of them satisfy the first four properties.

[Wardetzky et al. 2007]

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#### **Entropic Regularization**



Cuturi. "Sinkhorn distances: Lightspeed computation of optimal transport" (NIPS 2013)

### Sinkhorn Algorithm

$$T = \operatorname{diag}(u) K_{\alpha} \operatorname{diag}(v),$$
  
where  $K_{\alpha} := \exp(-C/\alpha)$   
 $u \leftarrow p \oslash (K_{\alpha}v)$   
 $v \leftarrow q \oslash (K_{\alpha}^{\top}u)$ 

Sinkhorn & Knopp. "Concerning nonnegative matrices and doubly stochastic matrices". Pacific J. Math. 21, 343–348 (1967).

# **Alternating projection**

### **Ingredients for Sinkhorn**

Supply vector p
 Demand vector q
 Multiplication by K





Solomon et al. "Convolutional Wasserstein Distances: Efficient Optimal Transportation on Geometric Domains." SIGGRAPH 2015.

### Sinkhorn Divergences

$$\overline{\mathcal{W}}_{c,\varepsilon}(\mu,\nu) := 2\mathcal{W}_{c,\varepsilon}(\mu,\nu) - \mathcal{W}_{c,\varepsilon}(\mu,\mu) - \mathcal{W}_{c,\varepsilon}(\nu,\nu)$$

- Debiases entropy-regularized transport near zero
- Easy to compute: Three calls to Sinkhorn
- Links optimal transport to maximum mean discrepancy (MMD)

$$\overline{\mathcal{W}}_{c,\varepsilon}(\mu,\nu) \xrightarrow[\varepsilon \to \infty]{\varepsilon \to \infty} 2\mathcal{W}_c(\mu,\nu) \overline{\mathcal{W}}_{c,\varepsilon}(\mu,\nu) \xrightarrow[\varepsilon \to \infty]{\varepsilon \to \infty} \mathrm{MMD}_{-c}(\mu,\nu)$$

[Genevay et al. 2016]

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#### Discretization



Images/math from [Lavenant, Claici, Chien, and Solomon 2018]

#### Graph analog: Beckmann Formulation



Better scaling for sparse graphs!

 $\begin{array}{ll} \min_{T} & \sum_{e} c_{e} |J_{e}| \\ \text{s.t.} & D^{\top} J = p_{1} - p_{0} \end{array}$ 

In computer science: Network flow problem

Smooth PDE analog: [Solomon et al. 2014]

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#### **Semidiscrete General Case**



https://www.jasondavies.com/power-diagram/

### **Semidiscrete Algorithm**

$$\begin{split} F(\phi) &:= \sum_{i} \left[ a_{i}\phi_{i} + \int_{\operatorname{Lag}_{\phi}^{c}(x_{i})} \rho(y) [c(x_{i}, y) - \phi_{i}] \, dA(y) \right] \\ \frac{\partial F}{\partial \phi_{i}} &= a_{i} - \int_{\operatorname{Lag}_{\phi}^{c}(x_{i})} \rho(y) \, dA(y) \end{split}$$

- Simple algorithm: Gradient ascent Ingredients: Power diagram
- More complex: Newton's method Converges globally [de Goes et al. 2012; Kitagawa, Mérigot, & Thibert 2016]
- ML setting: Stochastic optimization [Genevay et al. 2016; Staib et al. 2017; Claici et al. 2018]

# Application



#### Redux

Method	Advantages	Disadvantages	
Entropic regularization	<ul> <li>Fast</li> <li>Easy to implement</li> <li>Works on mesh using heat kernel</li> </ul>	• Blurry • Becomes singular as $\alpha \rightarrow 0$	
Eulerian optimization	<ul> <li>Provides displacement interpolation</li> <li>Connection to PDE</li> </ul>	<ul> <li>Hard to optimize</li> <li>Triangle mesh formulation unclear</li> </ul>	
Semidiscrete optimization	<ul> <li>No regularization</li> <li>Connection to "classical" geometry</li> </ul>	<ul> <li>Expensive computational geometry algorithms</li> </ul>	

Many others: Stochastic transport, dual ascent, Monge-Ampère PDE, ...

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### Sinkhorn Autodiff



Figure 1: For a given fixed set of samples  $(z_1, \ldots, z_m)$ , and input data  $(y_1, \ldots, y_n)$ , flow diagram for the computation of Sinkhorn loss function  $\theta \mapsto \hat{E}_{\varepsilon}^{(L)}(\theta)$ . This function is the one on which automatic differentiation is applied to perform parameter learning. The display shows a simple 2-layer neural network  $g_{\theta} : z \mapsto x$ , but this applies to any generative model.

#### [Genevay et al. 2016]

#### **Smoothed Dual Formulations**

**Proposition 19.** The dual of entropy-regularized OT between two probability measures  $\alpha$  and  $\beta$  can be rewritten as the maximization of an expectation over  $\alpha \otimes \beta$ :

$$W^{c}_{\varepsilon}(\alpha,\beta) = \max_{u,v \in \mathcal{C}(\mathcal{X}) \times \mathcal{C}(\mathcal{Y})} \mathbb{E}_{\alpha \otimes \beta}[f^{XY}_{\varepsilon}(u,v)] + \varepsilon,$$

where

$$f_{\varepsilon}^{xy} \stackrel{\text{def.}}{=} u(x) + v(y) - \varepsilon \exp^{\frac{u(x) + v(y) - c(x,y)}{\varepsilon}} \quad \text{for } \varepsilon > 0.$$
(2.2)

and when  $\beta \stackrel{\text{def.}}{=} \sum_{j=1}^{m} \beta_j \delta_{y_j}$  is discrete, the potential v is a m-dimensional vector  $(\mathbf{v}_j)_j$ 



### **New Progress on the Monge Formulation**

#### **Input Convex Neural Networks**

Brandon Amos<sup>1</sup> Lei Xu<sup>2\*</sup> J. Zico Kolter<sup>1</sup>

Fundamentally

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networks.

#### Abstract

This paper presents the input convex neural network architecture. These are scalar-valued (potentially deep) neural networks with constraints on the network parameters such that the output of the network is a convex function of (some of) the inputs. The networks allow for efficient inference via optimization over some inputs to the network given others, and can be applied to settings including structured prediction, data imputation, reinforcement learning, and others. In this paper we lay the basic groundwork for these models, proposing methods for inference, optimization and learning, and analyze their representational power. We show that many existing neural network architectures can be made inputconvex with a minor modification, and develop specialized optimization algorithms tailored to this setting. Finally, we highlight the performance of the methods on multi-label prediction, image completion, and reinforcement learning problems, where we show improvement over the existing state of the art in many cases.

#### 1. Introduction

In this paper, we propose a new neural network architecture that we call the *input convex neural network* (ICNN). These are *scalar-valued* neural networks  $f(x, y; \theta)$  where x and y denotes inputs to the function and  $\theta$  denotes the parameters, built in such a way that the network is convex in (a subset of) *inputs*  $y^3$ . The fundamental benefit to these IC- y) we can globally and efficiently (because the problem is convex) solve the

#### Optimal transport mapping via input convex neural networks

Ashok Vardhan Makkuva<sup>\*1</sup> Amirhossein Taghvaei<sup>\*2</sup> Jason D. Lee<sup>3</sup> Sewoong Oh<sup>4</sup>

#### Abstract

In this paper, we present a novel and principled approach to learn the optimal transport between two distributions, from samples. Guided by the optimal transport theory, we learn the optimal Kantorovich potential which induces the optimal



#### 1. Introduction

Finding a mapping that transports mass from one distribution Q to another distribution P is an important task in various machine learning applications, such as deep generative models (Goodfellow et al., 2014; Kingma & Welling, 2013) and domain adaptation (Gopalan et al., 2011; Ben-



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Extension:

#### **Wasserstein Barycenters**



[Agueh and Carlier 2010]

#### **Barycenters in Bayesian Inference**



Wasserstein Subset Posterior (WASP) [Srivastava et al. 2018] **Quadratic Matching** 



### Variety of Correspondence Tasks





Targets



[Solomon et al. 2016]

#### Extension: Gradient Flows



"Entropic Wasserstein Gradient Flows" [Peyré 2015]

#### Extension: Matrix Fields and Vector Measures



Image from "Quantum Optimal Transport for Tensor Field Processing" [Peyré et al. 2017]

#### **Open problem: Dynamical version? Curved surfaces?**

Extension:

### Sampling Problems



Somewhere between semidiscrete and smooth

#### Wasserstein barycenter

#### Optimal Transport Justin Solomon

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