CS480/680: Introduction to Machine Learning

Lec 18: Optimal Transport

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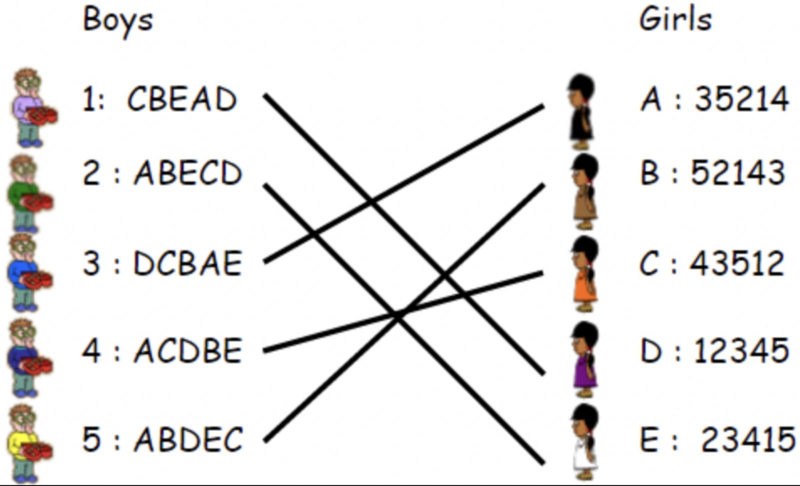
Matching Problem



https://towardsdatascience.com/stable-matching-as-a-game-a68c279d70b

- Matching co-op students/organ donors with companies/patients

Stable Matching

Definition: Blocking pair

A pair (i, j) and (i', j') where both i and j' would prefer to swap.

Example: Blocking pair

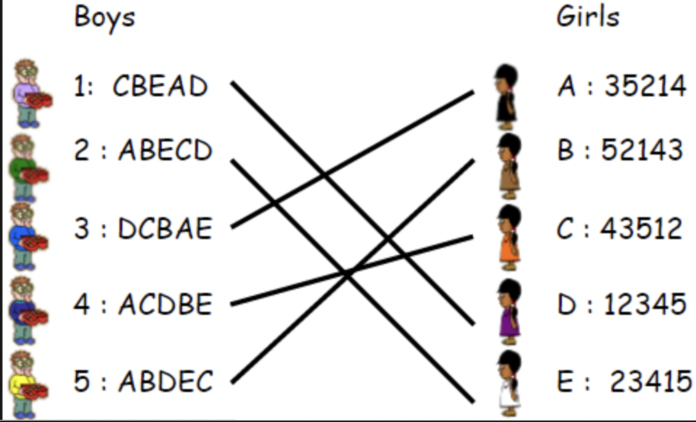
(1, E) and (2, C) —> (1, C) and (2, E)

- A stable matching is one when there is no blocking pair
  - Gale-Shapley algorithm
- More generally, can define a cost $c(i, j)$ for matching i-th boy with j-th girl
- Need $c(i, j) + c(i', j') \leq c(i, j') + c(i', j)$

D. Gale and L. S. Shapley. "College Admissions and the Stability of Marriage". *The American Mathematical Monthly*, vol. 69, no. 1 (1962), pp. 9–15.

Monge's Formulation

$$\min_{\mathbf{T}:[n]\to[n] \text{ bijective}} \sum_{i=1}^{n} c(i, \mathbf{T}(i))$$



H. W. Kuhn. "The Hungarian method for the assignment problem". *Naval Research Logistics Quarterly*, vol. 2, no. 1-2 (1955), pp. 83–97.

From Discrete to Continuous

$$\min_{\mathbf{T}_{\#}p=q} \quad \mathbb{E}[c(\mathsf{X}, \mathbf{T}(\mathsf{X}))]$$

- A distribution p of boys and a distribution q of girls
- Let $\mathsf{X} \sim p$ be a random boy
- $\mathbf{T}(\mathsf{X})$ is the matching for X
- Require $\mathbf{T}_{\#}p = q$ to preserve mass

G. Monge. "Mémoire sur la théorie des déblais et des remblais". In: *Histoire de l'Académie royale des sciences avec les mémoires de mathématique et de physique tirés des registres de cette Académie*. 1781, pp. 666–705.

Kantorovich's Relaxation

$$\min_{\mathbf{T}_{\#}p=q} \mathbb{E}[c(\mathsf{X}, \mathbf{T}(\mathsf{X}))] \geq \min_{\mathsf{X}\sim p, \mathsf{Y}\sim q} \mathbb{E}[c(\mathsf{X}, \mathsf{Y})]$$

Definition: Coupling

$(\mathsf{X}, \mathsf{Y}) \sim \pi$, where the joint coupling π has marginals p and q

- Deterministic pairing: $\mathbf{x}$ is matched with some $\mathbf{y} = \mathbf{Tx}$
- Stochastic pairing: $\mathbf{x}$ is matched to every $\mathbf{y}$ with probability $\pi(\mathbf{y}|\mathbf{x})$
- Surprisingly, at optimality, $\pi(\mathbf{y}|\mathbf{x})$ could be deterministic anyway!

L. V. Kantorovich. "On the Translocation of Masses". *Journal of Mathematical Sciences*, vol. 133, no. 4 (2006). Originally published in Dokl. Akad. Nauk SSSR, vol. 37, No. 7–8, 227–229 (1942)., pp. 1381–1382, L. V. Kantorovich. "On a Problem of Monge". *Journal of Mathematical Sciences*, vol. 133, no. 4 (2006). Originally published in Uspekhi Mat. Nauk, vol. 3, No. 2, 225-226 (1948)., pp. 1383–1383.

Duality

$$\min_{X\sim p, Y\sim q, (X,Y)\sim\pi} \mathbb{E}[c(X,Y)] = \min_{\pi\geq 0} \int c(\mathbf{x},\mathbf{y})\pi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}$$

$$\text{s.t.} \quad \int \pi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{y} = p(\mathbf{x}), \int \pi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{x} = q(\mathbf{y})$$

$$\min_{\pi\geq 0} \max_{u(\cdot),v(\cdot)} \int [c(\mathbf{x},\mathbf{y}) - u(\mathbf{x}) - v(\mathbf{y})]\pi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} + \int u(\mathbf{x})p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int v(\mathbf{y})p(\mathbf{y})\,\mathrm{d}\mathbf{y}$$

$$= \max_{u(\cdot),v(\cdot)} \min_{\pi\geq 0} \int [c(\mathbf{x},\mathbf{y}) - u(\mathbf{x}) - v(\mathbf{y})]\pi(\mathbf{x},\mathbf{y})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} + \int u(\mathbf{x})p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int v(\mathbf{y})p(\mathbf{y})\,\mathrm{d}\mathbf{y}$$

$$= \max_{u(\cdot),v(\cdot)} \int u(\mathbf{x})p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int v(\mathbf{y})p(\mathbf{y})\,\mathrm{d}\mathbf{y}, \quad \text{s.t.} \quad u(\mathbf{x}) + v(\mathbf{y}) \leq c(\mathbf{x},\mathbf{y}), \ \forall \mathbf{x},\mathbf{y}$$

$$\boxed{= \max_{u,v} \mathbb{E}[u(X)] + \mathbb{E}[v(Y)], \quad \text{s.t.} \quad u(\mathbf{x}) + v(\mathbf{y}) \leq c(\mathbf{x},\mathbf{y}), \ \forall \mathbf{x},\mathbf{y}}$$

L. V. Kantorovich and G. S. Rubinshtein. "On a functional space and certain extremum problems". *Dokl. Akad. Nauk SSSR*, vol. 115, no. 6 (1957), pp. 1058–1061.

Conjugacy

$$\boxed{\forall \mathbf{x}, \forall \mathbf{y},\ u(\mathbf{x}) + v(\mathbf{y}) \le c(\mathbf{x}, \mathbf{y})}$$

- $u(\mathbf{x}) \le [\inf_{\mathbf{y}}\ c(\mathbf{x}, \mathbf{y}) - v(\mathbf{y})] =: v^c(\mathbf{x})$
- $v(\mathbf{y}) \le [\inf_{\mathbf{x}}\ c(\mathbf{x}, \mathbf{y}) - u(\mathbf{x})] =: u^c(\mathbf{y})$
- Since we are maximizing $\mathbb{E}[u(\mathsf{X})] + \mathbb{E}[v(\mathsf{Y})]$, at optimality:

$$\boxed{u(\mathbf{x}) = v^c(\mathbf{x}), \qquad v(\mathbf{y}) = u^c(\mathbf{y})}$$

- $u^{cc} \ge u$ and $u^{ccc} = u^c$; similarly for v
- u is called c-concave iff $u = u^{cc}$ (or equivalently $u = v^c$ for some v)

Complementarity

$$\max_{u,v} \min_{\pi \geq 0} \int [c(\mathbf{x},\mathbf{y}) - u(\mathbf{x}) - v(\mathbf{y})]\pi(\mathbf{x},\mathbf{y})\, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{y} + \int u(\mathbf{x})p(\mathbf{x})\, \mathrm{d}\mathbf{x} + \int v(\mathbf{y})p(\mathbf{y})\, \mathrm{d}\mathbf{y}$$

- $\pi(\mathbf{x},\mathbf{y}) > 0 \implies u(\mathbf{x}) + v(\mathbf{y}) = c(\mathbf{x},\mathbf{y})$
- Recall that $u^c = v$, we define the subdifferential:

$$\boxed{\partial u(\mathbf{x}) := \operatorname*{argmin}_{\mathbf{y}} \, [c(\mathbf{x},\mathbf{y}) - u^c(\mathbf{y})] = \{\mathbf{y} : u(\mathbf{x}) + u^c(\mathbf{y}) = c(\mathbf{x},\mathbf{y})\}}$$

  – for a c-concave u, $\boxed{\mathbf{y} \in \partial u(\mathbf{x}) \iff \mathbf{x} \in \partial u^c(\mathbf{y})}$

- Thus, $\boxed{\operatorname{supp} \pi \subseteq \operatorname{gph} \partial u}$

  – in particular, if u is differentiable, π is deterministic and the Kantorovich relaxation is tight!

Cyclic Monotonicity

Definition: Cyclic monotonicity

We call a set $\Gamma \subseteq \mathbb{X} \times \mathbb{Y}$ c-cyclically monotone if for any n and $(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n) \in \Gamma$, any (cyclic) permutation $\sigma : [n] \to [n]$, we always have

$$\sum_{i=1}^{n} c(\mathbf{x}_i, \mathbf{y}_i) \leq \sum_{i=1}^{n} c(\mathbf{x}_i, \mathbf{y}_{\sigma(i)})$$

Theorem: Optimal coupling

Suppose $\mathbb{X} = \mathbb{R}^{d_x}$ and $\mathbb{Y} = \mathbb{R}^{d_y}$, $c : \mathbb{X} \times \mathbb{Y} \to \mathbb{R}$ is continuous, and p and q are probability densities. There exists an optimal coupling π whose support is c-cyclically monotone. Moreover, there exists a c-concave function u such that $\operatorname{supp} \pi \subseteq \operatorname{gph} \partial u$.

L18 L. Rüschendorf. "On c-optimal random variables". *Statistics & Probability Letters*, vol. 27, no. 3 (1996), pp. 267–270.

1-Wasserstein Distance

- $c(\mathbf{x}, \mathbf{y}) = d(\mathbf{x}, \mathbf{y})$ for some distance metric d:

$$\mathbb{W}_1(p, q) := \min_{(\mathsf{X},\mathsf{Y})\sim\pi, \mathsf{X}\sim p, \mathsf{Y}\sim q} \mathbb{E}[d(\mathsf{X}, \mathsf{Y})]$$
$$= \max_{u,v} \ \mathbb{E}[u(\mathsf{X})] + \mathbb{E}[v(\mathsf{Y})], \quad \text{s.t.} \quad \forall \mathbf{x}, \mathbf{y}, \ u(\mathbf{x}) + v(\mathbf{y}) \leq d(\mathbf{x}, \mathbf{y})$$

- Lipschitz envelope: $v^c(\mathbf{x}) := [\inf_{\mathbf{y}} d(\mathbf{x}, \mathbf{y}) - v(\mathbf{y})]$
  - v^c is Lipschitz continuous: $|v^c(\mathbf{x}) - v^c(\mathbf{z})| \leq d(\mathbf{x}, \mathbf{z})$
  - v^c is the largest Lipschitz continuous function majorized by $-v$
- Thus, $u = v^c = -v$ and hence

$$\boxed{\mathbb{W}_1(p, q) = \max_{u} \ \mathbb{E}[u(\mathsf{X})] - \mathbb{E}[u(\mathsf{Y})], \quad \text{s.t.} \quad \forall \mathbf{x}, \mathbf{y}, \ u(\mathbf{x}) - u(\mathbf{y}) \leq d(\mathbf{x}, \mathbf{y})}$$

Wasserstein GAN

$$\min_{\mathbf{T}} \mathrm{W}_1(q, \mathbf{T}_{\#}r) = \min_{\mathbf{T}} \max_{u} \ \mathbb{E}_{\mathsf{X}\sim q}[u(\mathsf{X})] - \mathbb{E}_{\mathsf{Z}\sim r}[u(\mathbf{T}(\mathsf{Z}))], \quad \text{s.t.} \quad u \text{ is Lipschitz}$$
$$\approx \min_{\mathbf{T}} \max_{u} \ \hat{\mathbb{E}}_{\mathsf{X}\sim q}[u(\mathsf{X})] - \hat{\mathbb{E}}_{\mathsf{Z}\sim r}[u(\mathbf{T}(\mathsf{Z}))], \quad \text{s.t.} \quad u \text{ is Lipschitz}$$

- r is the noise density, e.g., standard normal
- q is the data density: only a training sample is available
- $\mathbf{T}$ is the generator network: maps noise to data
- u is the discriminator network: maps data to a real scalar

M. Arjovsky, S. Chintala, and L. Bottou. "Wasserstein Generative Adversarial Networks". In: *Proceedings of the 34th International Conference on Machine Learning*. 2017.

2-Wasserstein Distance

- $c(\mathbf{x},\mathbf{y}) = \frac{1}{2}\|\mathbf{x}-\mathbf{y}\|_2^2$ (note the square):

$$\mathbb{W}_2^2(p,q) := \min_{(\mathsf{X},\mathsf{Y})\sim\pi,\mathsf{X}\sim p,\mathsf{Y}\sim q} \mathbb{E}[\tfrac{1}{2}\|\mathsf{X}-\mathsf{Y}\|_2^2]$$

$$= \max_{u,v} \ \mathbb{E}[u(\mathsf{X})] + \mathbb{E}[v(\mathsf{Y})], \quad \text{s.t. } \ \forall \mathbf{x},\mathbf{y}, \ u(\mathbf{x}) + v(\mathbf{y}) \le \tfrac{1}{2}\|\mathbf{x}-\mathbf{y}\|_2^2$$

- Conjugate: $v^c(\mathbf{x}) := [\inf_{\mathbf{y}} \frac{1}{2}\|\mathbf{x}-\mathbf{y}\|_2^2 - v(\mathbf{y})]$
  - $\frac{1}{2}\|\mathbf{x}\|_2^2 - v^c(\mathbf{x}) = \sup_{\mathbf{y}} \langle \mathbf{x},\mathbf{y}\rangle - [\frac{1}{2}\|\mathbf{y}\|_2^2 - v(\mathbf{y})]$: convex conjugate
- Thus, $u = v^c = \frac{1}{2}\|\cdot\|_2^2 - (\frac{1}{2}\|\cdot\|_2^2 - v)^*$ and hence

$$\boxed{\mathbb{W}_2^2(p,q) = \max_f \ \mathbb{E}[\tfrac{1}{2}\|\mathsf{X}\|_2^2 - f(\mathsf{X})] + \mathbb{E}[\tfrac{1}{2}\|\mathsf{Y}\|_2^2 - f^*(\mathsf{Y})], \quad \text{s.t. } \ f \text{ is convex}}$$

$$\boxed{\pi = (\mathrm{Id} \times \partial f)_{\#} p}, \text{ in particular } q = (\partial f)_{\#} p$$

Y. Brenier. "Polar factorization and monotone rearrangement of vector-valued functions". *Communications on Pure and Applied Mathematics*, vol. 44, no. 4 (1991), pp. 375–417, R. J. McCann. "Existence and uniqueness of monotone measure-preserving maps". *Duke Mathematical Journal*, vol. 80, no. 2 (1995), pp. 309–323.

Potential GAN

$$\min_{\mathbf{T}} \mathrm{W}_2^2(q, \mathbf{T}_{\#}r) = \min_{\mathbf{T}} \max_{f} \mathop{\mathbb{E}}_{\mathsf{X}\sim q}[\tfrac{1}{2}\|\mathsf{X}\|_2^2 - f(\mathsf{X})] + \mathop{\mathbb{E}}_{\mathsf{Z}\sim r}[\tfrac{1}{2}\|\mathbf{T}(\mathsf{Z})\|_2^2 - f^*(\mathbf{T}(\mathsf{Z}))],$$

$$\approx \min_{\mathbf{T}} \max_{f} \mathop{\hat{\mathbb{E}}}_{\mathsf{X}\sim q}[-f(\mathsf{X})] + \mathop{\hat{\mathbb{E}}}_{\mathsf{Z}\sim r}[\tfrac{1}{2}\|\mathbf{T}(\mathsf{Z})\|_2^2 - f^*(\mathbf{T}(\mathsf{Z}))], \text{ s.t. } f \text{ is convex}$$

- r is the noise density, e.g., standard normal
- q is the data density: only a training sample is available
- $\mathbf{T}$ is the generator network: maps noise to data
- f is the discriminator network: maps data to a real scalar

T. Salimans, H. Zhang, A. Radford, and D. Metaxas. "Improving GANs Using Optimal Transport". In: *International Conference on Learning Representations*. 2018, H. Liu, X. Gu, and D. Samaras. "Wasserstein GAN With Quadratic Transport Cost". In: *IEEE/CVF International Conference on Computer Vision (ICCV)*. 2019, pp. 4831–4840.

Potential Flow

$$\min_f \ \mathbb{D}\big(q, (\nabla f)_{\#} r\big), \quad \text{s.t.} \quad f \text{ is convex}$$

- r is the noise density, e.g., standard normal
- q is the data density: only a training sample is available
- ∇f is the generator network: maps noise to data
  - e.g., f is a Relu network with nonnegative weights
- $\mathbb{D}$ is some "distance" function, e.g., the KL divergence

C.-W. Huang, R. T. Q. Chen, C. Tsirigotis, and A. Courville. "Convex Potential Flows: Universal Probability Distributions with Optimal Transport and Convex Optimization". In: *International Conference on Learning Representations*. 2021.

Triangular vs. Potential

- $\mathbf{T} : \mathbb{R}^d \to \mathbb{R}^d$, $\mathbf{T}_{\#}p = q$
- $\mathbf{T}$ is autoregressive
- $\nabla\mathbf{T}$ is always triangular
- composition holds
- no rotational equivariance

- $\mathbf{T} : \mathbb{R}^d \to \mathbb{R}^d$, $\mathbf{T}_{\#}p = q$
- $\mathbf{T} = \nabla f$ for convex $f : \mathbb{R}^d \to \mathbb{R}$
- $\nabla\mathbf{T} = \nabla^2 f$ is symmetric PSD
- composition fails
- rotationally equivariant

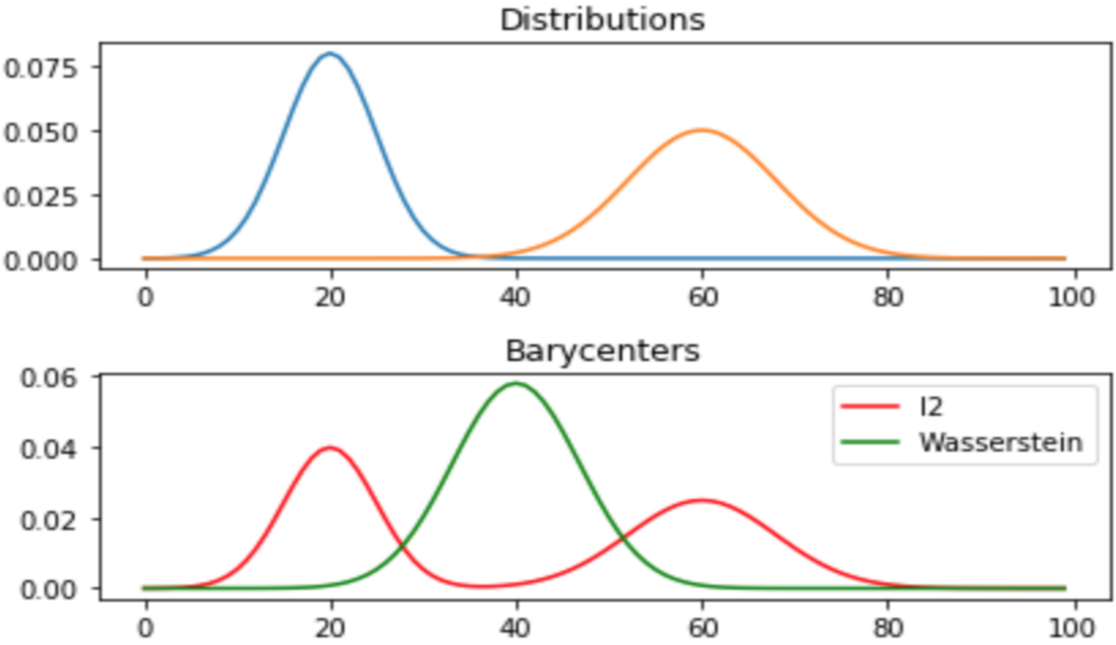
The two are equivalent iff $\mathbf{T}$ is diagonal, in particular, if $d = 1$

Wasserstein Barycenter

- Consider densities p_0 and p_1, say two Gaussians with different mean and variance
- How to interpolate between them?
- Exists convex f such that $p_1 = (\nabla f)_{\#} p_0$
- Obviously $p_0 = (\mathrm{Id})_{\#} p_0$
- Interpolate the push-forward maps!

$$p_t = [(1-t)\mathrm{Id} + t\nabla f]_{\#} p_0 = \underset{p}{\operatorname{argmin}}\ (1-t)\mathbb{W}_2^2(p, p_0) + t\mathbb{W}_2^2(p, p_1)$$

R. J. McCann. "A Convexity Principle for Interacting Gases". *Advances in Mathematics*, vol. 128, no. 1 (1997), pp. 153–179.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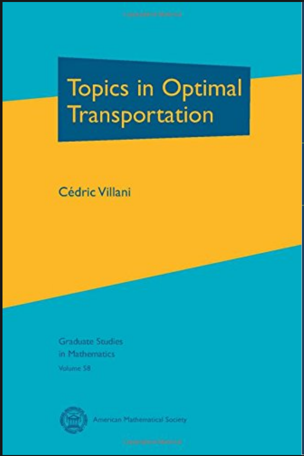
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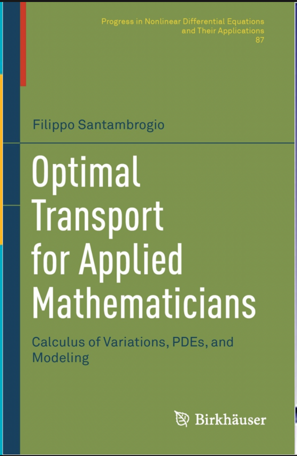
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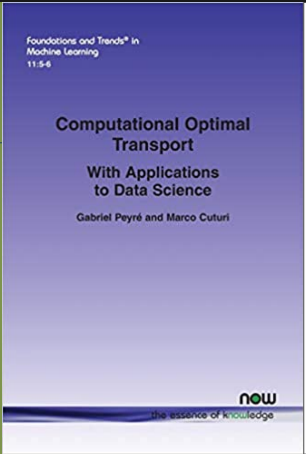
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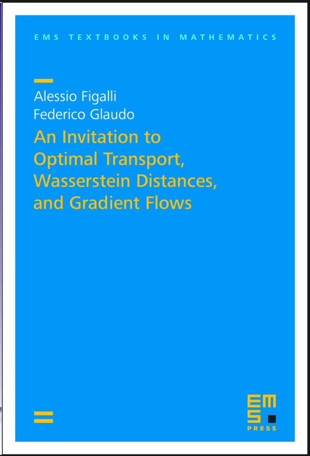
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