Optimal Transport

Theory, Computation and Applications

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Dec. 30th, 2024

Overview

Principal concern: the distance between two probability measures.
First introduced in 1781 by Monge.
Relative subjects: probability theory, geometry, graph theory, machine learning...
Applications:

- Image registration and warping;
- Reflector design;
- Retrieving information from shadowgraphy and proton radiography;
- Seismic tomography and reflection seismology.

Some well-known researchers:

- Gasoard Monge (France);
- Leonid Kantorovich (Russia);
- Yann Brenier (France);
- Xianfeng Gu (顾险峰, China);

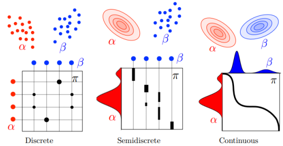

Fig. 1. Three main scenarios for Kantorovich OT

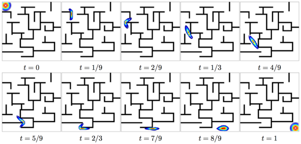

Fig. 2. Solving maze with OT

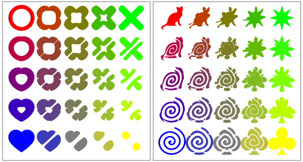

Fig. 3. 2D shape interpolation with OT

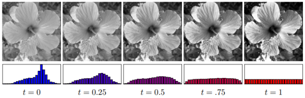

Fig. 4. Histogram equalization with OT

1 Theory

2 Computation

3 Applications

The sand-moving problem

A child wants to make a pile of sand in the shape of a castle.
Cost: 1 kcal per shovel and per meter horizontally.
Target: Minimize the total cost.

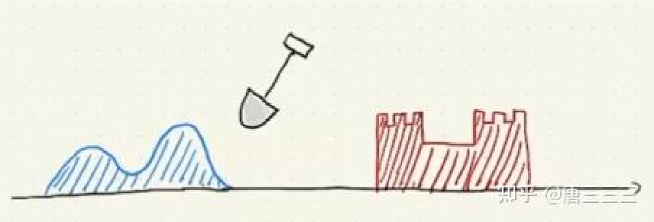

Fig. 5. The sand-moving problem.

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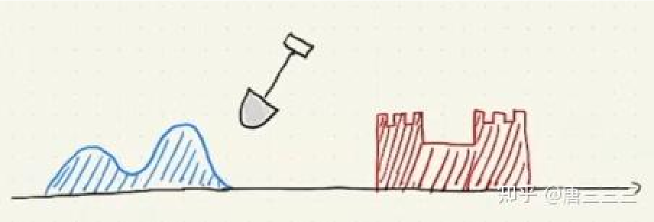

Fig. 5. The sand-moving problem.

Let's denote the source shape by $f(x)$ and the target by $g(x)$. The sand-moving problem cound be formulated as: find a **transport mapping** $T : \mathbb{R} \to \mathbb{R}$ to minimize

$$\int_{\mathbb{R}} |T(x) - x| f(x)\ dx, \tag{1}$$

which satisfies

$$\int_{T(U)} g(x)\ dx = \int_{U} f(x)\ dx \text{ for all open interval } U \subset \mathbb{R}. \tag{2}$$

The allocation problem

There are some steel coils to be transported from warehouses to factories. The transport cost is $1 per coil and per kilometer. How to minimize the total cost?

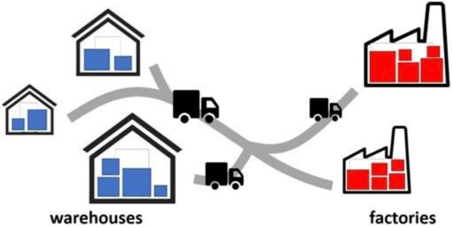

Fig. 6. The allocation problem.

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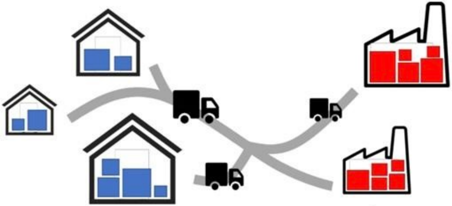

Fig. 6. The allocation problem.

Assume the i-th warehouse has a_i coils and the j-th factory needs b_i coils. And assume the distance between the i-th warehouse and the j-th factory is d_{ij}. The allocation problem could be formulated as: find a **transport matrix** v_{ij} to minimize

$$\sum_{i,j} d_{ij} v_{ij} \tag{3}$$

which satisfies

$$a_i = \sum_j v_{ij}, \quad \forall i, \qquad \text{and} \qquad b_j = \sum_i v_{ij}, \quad \forall j. \tag{4}$$

The Monge formulation

Denote $\mathcal{M}_+^1(\mathcal{X})$ the set of probability measures on $\mathcal{X}$.

Definition (push-forward)

Suppose $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *and a map* $T : \mathcal{X} \to \mathcal{Y}$. *Say* $\nu \in \mathcal{M}_+^1(\mathcal{Y})$ *is the push-forward of* μ *by* T *if*

$$\int_{\mathcal{Y}} h(y)\, d\nu(y) = \int_{\mathcal{X}} h(T(x))\, d\mu(x), \quad \forall h \in \mathcal{C}(\mathcal{Y}). \tag{5}$$

Write $T_{\#}\mu := \nu$.

Example (push-forward of a discrete measure)

Suppose α *is a discrete measure*

$$\alpha = \sum_{i=1}^{n} a_i \delta_{x_i}.$$

Then the push-forward of α *by* T *is*

$$T_{\#}\alpha = \sum_{i=1}^{n} a_i \delta_{T(x_i)}.$$

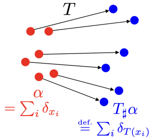

Fig. 7. push-forward of a discrete measure

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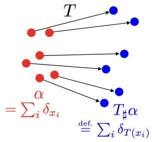


Fig. 7. push-forward of a discrete measure

Given two probability measures μ on $\mathcal{X}$ and ν on $\mathcal{Y}$, and a cost function $c(x, y)$. Optimal transport could be generally formulated as the Monge problem:

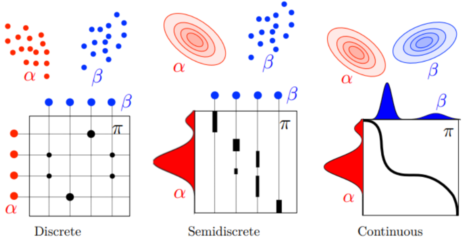
$$\min_{T} \left\{ \int_{\mathcal{X}} c(x, T(x))\ d\mu(x) : T_{\#}\mu = \nu \right\} \tag{6}$$

The Monge problem between discrete measures is introduced by Monge[1].

[1] Gaspard Monge. "Mémoire sur la théorie des déblais et des remblais". In: *Histoire de l'Académie Royale des Sciences* (1781).

The Kantorovich formulation

Here's another general formulation of OT, we first recall the three main scenarios for OT.



2 Leonid Kantorovich. "On the transfer of masses". In: *Doklady Akademii Nauk* 37.2 (1942).

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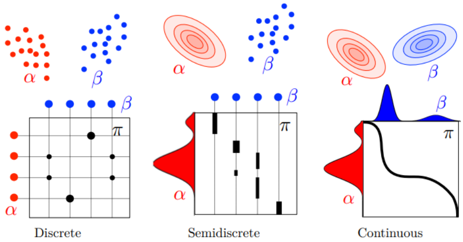

Given two probability measures μ on $\mathcal{X}$ and ν on $\mathcal{Y}$, and a cost function $c(x, y)$. Optimal transport could be generally formulated as the Kantorovich problem[2]:

$$\mathcal{L}_c(\mu, \nu) = \min_{\pi} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\ d\pi(x, y), \tag{7}$$

where π is a measure on $\mathcal{X} \times \mathcal{Y}$, whose marginals are μ and ν, that is,

$$\mu = \int_{\mathcal{Y}} \pi(\cdot, y)\ dy, \qquad \nu = \int_{\mathcal{X}} \pi(x, \cdot)\ dx. \tag{8}$$

[2] Leonid Kantorovich. "On the transfer of masses". In: *Doklady Akademii Nauk* 37.2 (1942).

Wasserstein disrtance

Here we suppose $\mathcal{X} = \mathcal{Y}$ and $c(x, y) = d(x, y)^p$ $(p > 1)$, where d is a distance on $\mathcal{X}$.

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Theorem (Wasserstein distance)

Under the above assumptions, $\mathcal{L}_c(\mu, \nu)^{1/p}$ is a distance on $\mathcal{M}_+^1(\mathcal{X})$.

The distance $\mathcal{W}_p(\mu, \nu) := \mathcal{L}_c(\mu, \nu)^{1/p}$ is called p-Wasserstein distance.

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Definition (weak convergence)

Suppose $\mathcal{X}$ *is compact. Say* $(\mu_k)_{k \geq 1} \subset \mathcal{M}_+^1(\mathcal{X})$ *converges weakly to* $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *if*

$$\int_{\mathcal{X}} g \, d\mu_k \to \int_{\mathcal{X}} g \, d\mu, \quad \forall g \in \mathcal{C}(\mathcal{X}). \tag{9}$$

Theorem (Wasserstein distance and weak convergence[3])

On a compact domain $\mathcal{X}$, $(\mu_k)_{k \geq 1} \subset \mathcal{M}_+^1(\mathcal{X})$ *converges weakly to* $\mu \in \mathcal{M}_+^1(\mathcal{X})$ *if and only if* $\mathcal{W}_p(\mu_k, \nu) \to 0$.

[3] Cédric Villani. *Optimal Transport: Old and New*. Vol. 338. Springer Verlag, 2009.

Equivalence between the Kantorovich and Monge problems

Theorem (Kantorovich dual problem)

The Kantorovich problem can be solved in the dual space by

$$\mathcal{L}_c(\mu,\nu) = \sup_{(f,g)\in\mathcal{R}(c)} \int_{\mathcal{X}} f(x)\ d\mu(x) + \int_{\mathcal{Y}} g(y)\ d\nu(y), \tag{10}$$

where the set of admissible dual potential is

$$\mathcal{R}(c) := \{(f,g) \in \mathcal{C}(\mathcal{X}) \times \mathcal{C}(\mathcal{Y}) : \forall (x,y), f(x) + g(y) \le c(x,y)\}. \tag{11}$$

The pair (f,g) is called Kantorovich potentials.

[4] Yann Brenier. "Polar factorization and monotone rearrangement of vector-valued functions". In: *Communications on Pure and Applied Mathematics* 44.4 (1991).

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Theorem (Brenier[4])

In the case $\mathcal{X} = \mathcal{Y} = \mathbb{R}^d$ and $c(x,y) = \|x-y\|_2^2$, if at least one of the two input measures (denoted μ) has a density ρ_μ with respect to the Lebesgue measure, then the optimal π in the Kantorovich formulation is unique and is supported on the graph $(x, T(x))$ of a Monge map $T : \mathbb{R}^d \to \mathbb{R}^d$. This means that $\pi = (Id, T)_\#\mu$, i.e.

$$\int_{\mathcal{X}\times\mathcal{Y}} h(x,y)\ d\pi(x,y) = \int_{\mathcal{X}} h(x, T(x))\ d\mu(x), \quad \forall h \in \mathcal{C}(\mathcal{X}\times\mathcal{Y}). \tag{12}$$

Furthermore, this map T is uniquely defined as the gradient of a convex function φ, $T(x) = \nabla\varphi(x)$, where φ is the unique (up to an additive constant) convex function such that $(\nabla\varphi)_\#\mu = \nu$. This convex function is related to the dual potential f solving (10) as

$$\varphi(x) = \frac{\|x\|_2^2}{2} - f(x). \tag{13}$$

[4] Yann Brenier. "Polar factorization and monotone rearrangement of vector-valued functions". In: *Communications on Pure and Applied Mathematics* 44.4 (1991).

Dynamic formulation

In the case $\mathcal{X} = \mathcal{Y} = \mathbb{R}^d$, and $c(x, y) = \|x - y\|_2$, the optimal transport distance $\mathcal{W}_2^2(\mu, \nu) = \mathcal{L}_c(\mu, \nu)$ can be defined as

$$\mathcal{W}_2^2(\mu, \nu) = \min_{(\alpha_t, v_t)_t} \int_0^1 \int_{\mathbb{R}^d} \|v_t(x)\|^2 \; d\alpha_t(x) \; dt, \tag{14}$$

where α_t is a scalar-valued measure and v_t a vector-valued measure which satisfy the conservation of mass formula,

$$\frac{\partial \alpha_t}{\partial t} + \nabla \cdot (\alpha_t, v_t) = 0, \tag{15}$$

and the boundary conditions $\alpha_0 = \mu$ and $\alpha_1 = \nu$.

1. Theory
2. Computation
3. Applications

1-D discrete case

Here $\mathcal{X} = \mathcal{Y} = \mathbb{R}$. Suppose $\alpha = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$ and $\beta = \frac{1}{n}\sum_{i=1}^{n} \delta_{y_i}$ where $x_1 \leq \cdots \leq x_n$ and $y_1 \leq \cdots \leq y_n$.

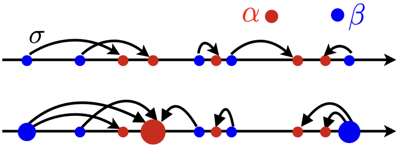


Fig. 8. 1-D optimal transport in discrete case

Then the p-Wasserstein distance can be simply computed by

$$\mathcal{W}_p(\alpha, \beta)^p = \frac{1}{n}\sum_{i=1}^{n} |x_i - y_i|^p. \tag{16}$$

It's in fact a greedy algorithm.

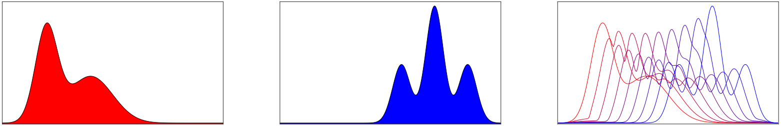
1-D continuous case

If μ, ν are 1-D measures with densities. Suppose their cummulative distribution functions are $\mathcal{C}_\mu$ and $\mathcal{C}_\nu$, respectively. Then the $\mathcal{W}_1$ distance could be computed by

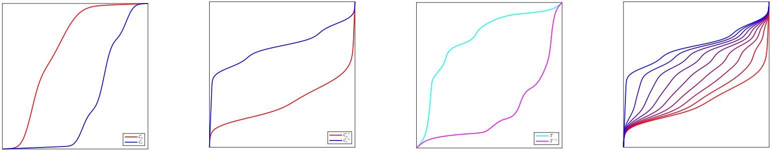
$$\mathcal{W}_1(\mu,\nu) = \int_{\mathbb{R}} \left|\mathcal{C}_\mu(x) - \mathcal{C}_\nu(x)\right| \, dx = \int_{\mathbb{R}} \left| \int_{-\infty}^{x} d(\mu - \nu) \right| \, dx. \tag{17}$$

And the Monge map is then defined by

$$T = \mathcal{C}_\nu^{-1} \circ \mathcal{C}_\mu. \tag{18}$$



μ ν $(tT + (1-t)\mathsf{Id})_{\#}\mu$



$(\mathcal{C}_\mu, \mathcal{C}_\nu)$ $(\mathcal{C}_\mu^{-1}, \mathcal{C}_\nu^{-1})$ (T, T^{-1}) $(1-t)\mathcal{C}_\mu^{-1} + t\mathcal{C}_\nu^{-1}$

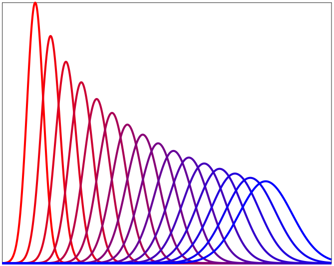
Fig. 9. Computation of OT and displacement interpolation between two 1-D measures.

1-D Gaussian

If $\mu = \mathcal{N}(m_1, \sigma_1^2), \nu = \mathcal{N}(m_2, \sigma_2^2)$ are 1-D Gaussians. Then the $\mathcal{W}_2$ distance can be directly computed by

$$\mathcal{W}_2(\mu, \nu) = \sqrt{|m_1 - m_2|^2 + |\sigma_1 - \sigma_2|^2}, \tag{19}$$

which is thus the Euclidean distance on the 2-D plane plotting the mean and the standard deviation of a Gaussian $\mathcal{N}(m, \sigma)$.



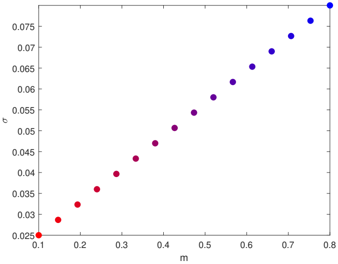


Fig. 10. Computation of displacement interpolation between two 1-D Gaussians.

Learn more in [Takatsu, 2011][5].

[5] Asuka Takatsu. "Wasserstein geometry of Gaussian measures". In: *Osaka Journal of Mathematics* 48.4 (2011).

Discretization

Suppose μ is a measure with density ρ, supported on $[0,1]$. Let

$$\tilde{\mu} = \sum_{i=0}^{N} u_i \delta_{x_i}, \tag{20}$$

where

$$u_i = \frac{\rho(x_i)}{N+1}, \quad x_i = \frac{i}{N}, \quad i = 0, ..., N. \tag{21}$$

We call $\tilde{\mu}$ the *discretization* of μ. This technique can also be used in $\mathbb{R}^d$.

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Let $\tilde{\nu} = \sum_{i=0}^{M} v_i \delta_{y_i}$ and $(\boldsymbol{C})_{ij}$ be the cost matrix. The Kantorovich problem then becomes

$$L_{\boldsymbol{C}}(\mathbf{u}, \mathbf{v}) := \min_{\boldsymbol{P} \in U(\mathbf{u},\mathbf{v})} \langle \boldsymbol{P}, \boldsymbol{C} \rangle := \min_{\boldsymbol{P} \in U(\mathbf{u},\mathbf{v})} \sum_{i,j} \boldsymbol{P}_{ij} \boldsymbol{C}_{ij}, \tag{22}$$

where

$$U(\mathbf{u}, \mathbf{v}) := \left\{ \boldsymbol{P} \,\middle|\, \sum_j \boldsymbol{P}_{ij} = u_i, \forall i, \quad \text{and} \quad \sum_i \boldsymbol{P}_{ij} = v_j, \forall j \right\}. \tag{23}$$

Entropy regularization

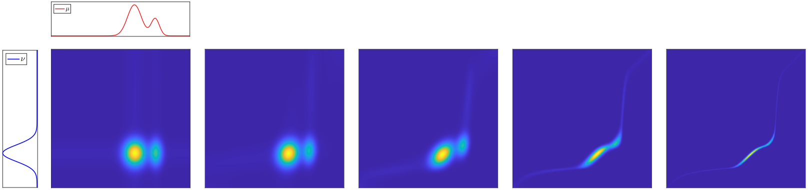
Define the entropy

$$H(\boldsymbol{P}) := -\sum_{i,j} \boldsymbol{P}_{ij}(\log(\boldsymbol{P}_{ij}) - 1). \tag{24}$$

Then the regularized Kantorovich problem[6] is defined by

$$L^{\varepsilon}_{\boldsymbol{C}}(\boldsymbol{u}, \boldsymbol{v}) := \min_{\boldsymbol{P} \in U(\boldsymbol{u}, \boldsymbol{v})} \langle \boldsymbol{P}, \boldsymbol{C} \rangle - \varepsilon H(\boldsymbol{P}). \tag{25}$$

It can be shown that $L^{\varepsilon}_{\boldsymbol{C}}(\boldsymbol{u}, \boldsymbol{v}) = L_{\boldsymbol{C}}(\boldsymbol{u}, \boldsymbol{v}) + O(\varepsilon)$.



$\varepsilon = 1$ $\varepsilon = 5 \times 10^{-2}$ $\varepsilon = 10^{-2}$ $\varepsilon = 10^{-3}$ $\varepsilon = 10^{-4}$

Fig. 11. Graphs of optimal $\boldsymbol{P}$s when choose different ε. Set $\boldsymbol{C}_{ij} = |x_i - x_j|^2$.

[6] Alan G. Wilson. "The use of entropy maximizing models, in the theory of trip distribution, mode split and route split". In: *Journal of Transport Economics and Policy* (1969), pp. 108–126.

Sinkhorn iteration

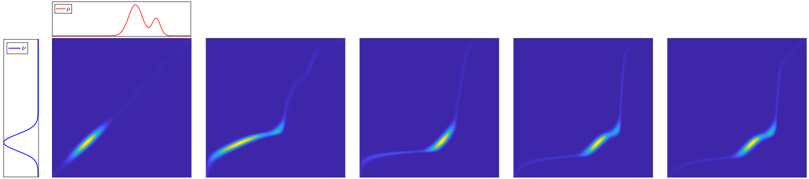
Let $\boldsymbol{K}_{ij} = e^{-\frac{\boldsymbol{C}_{ij}}{\varepsilon}}$. Sinkhorn iteration writes

$$\boldsymbol{a}^{(l+1)} \leftarrow \frac{\boldsymbol{u}}{\boldsymbol{K}\boldsymbol{b}^{(l)}}, \quad \text{and} \quad \boldsymbol{b}^{(l+1)} \leftarrow \frac{\boldsymbol{v}}{\boldsymbol{K}^T\boldsymbol{a}^{(l+1)}}, \quad \text{for } l = 0, 1, \ldots \tag{26}$$

which starts with an arbitary $\boldsymbol{b}^{(0)}$. The transport matrix $\boldsymbol{P}$ can be rebuilt by

$$\boldsymbol{P}^{(l)} = \text{diag}\left(\boldsymbol{b}^{(l)}\right) \cdot \boldsymbol{K} \cdot \text{diag}\left(\boldsymbol{a}^{(l)}\right). \tag{27}$$

The convergence is proved by Sinkhorn[7]. And Altschuler et al[8] give an analysis of the computational complexity.



$l = 1$ $l = 10$ $l = 50$ $l = 100$ $l = 1000$

Fig. 12. Graphs of $\boldsymbol{P}^{(l)}$. Set $\boldsymbol{C}_{ij} = |x_i - x_j|^2$ and $\varepsilon = 10^{-3}$.

[7] Richard Sinkhorn. “A relationship between arbitrary positive matrices and doubly stochastic matrices”. In: *Annals of Mathematical Statistics* 35 (1964).

[8] Jason Altschuler, Jonathan Weed, and Philippe Rigollet. “Near-linear time approximation algorithms for optimal transport via Sinkhorn iteration”. In: *Advances in Neural Information Processing Systems* (2017).

1. Theory
2. Computation
3. **Applications**

2-D shape interpolation

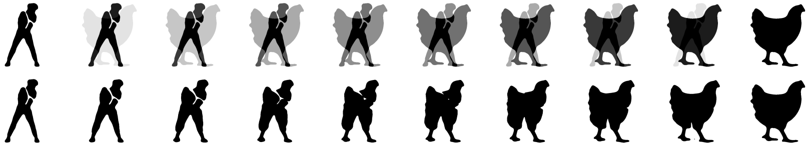


Fig. 13. From Kunkun to chicken. Top: color interpolation. Bottom: shape interpolation.

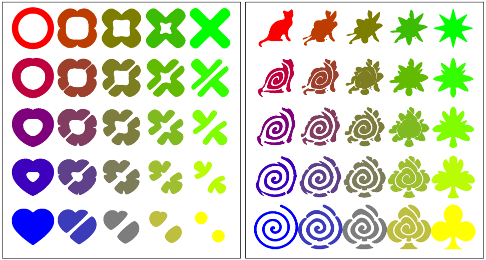


Fig. 14. Barycenter of four shapes[9].

[9] Gabriel Peyré, Marco Cuturi, et al. "Computational optimal transport: With applications to data science". In: *Foundations and Trends® in Machine Learning* 11.5-6 (2019), pp. 355–607.

Color transfer

Compute a transformation T such that

$$I_Z(x) = T(I_X(x)), \quad \text{for all pixel } x, \tag{28}$$

where the new color distribution μ_Z is close or equal to μ_Y.

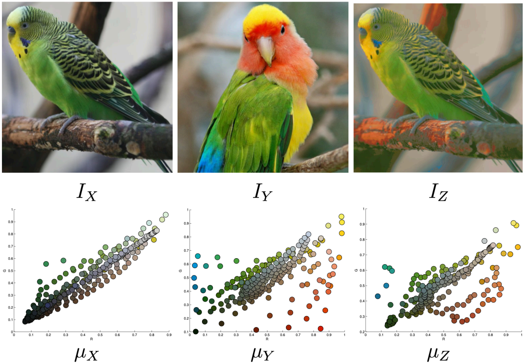


Fig. 15. Example of color transfer[10]. The second row representes RGB color distributions using the 2-D projection of every pixel in the RG plane

[10] Nicolas Papadakis. "Optimal transport for image processing". PhD thesis. Université de Bordeaux; Habilitation thesis, 2015.

Color transfer

Fig. 16. Another example of color transfer[11].

[11] Nicolas Bonneel and Julie Digne. "A survey of optimal transport for computer graphics and computer vision". In: *Computer Graphics Forum*. Vol. 42. 2. Wiley Online Library. 2023, pp. 439–460.

Fluid dynamics

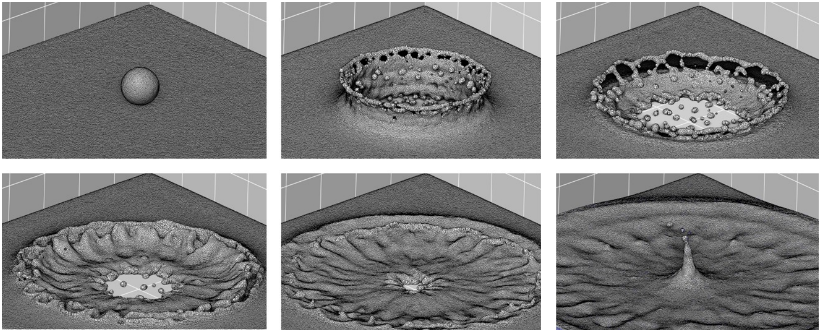


Fig. 17. Simulation of the free boundary problem using partial OT[12].

[12] Bruno Lévy. "Partial optimal transport for a constant-volume Lagrangian mesh with free boundaries". In: *Journal of Computational Physics* 451 (2022), p. 110838.

Area-preservation mapping[13]

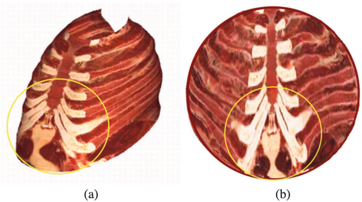


Fig. 18. Surface flattening of a chest model using area-preservation mapping for direct display and accurate measurement. The yellow circles highlight the corresponding ROIs between (a) the 3D surface model and (b) the 2D flattened plane.

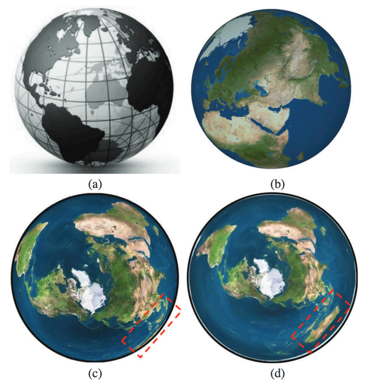


Fig. 19. (a) A 3D earth model. (b) Direct projection mapping with large information loss. (c) Conformal mapping result with large area distortions. (d) Area-preservation mapping result with accurate area preservation and small angle distortion.

[13] Xin Zhao et al. "Area-Preservation Mapping using Optimal Mass Transport". In: *IEEE Transactions on Visualization and Computer Graphics* 19.12 (2013), pp. 2838–2847. DOI: 10.1109/TVCG.2013.135.

Domain adaptation[14]

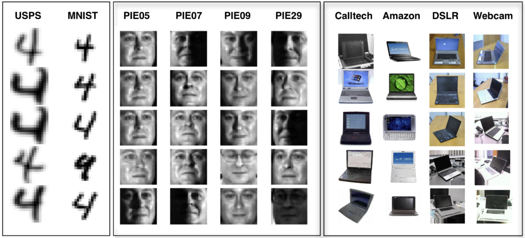
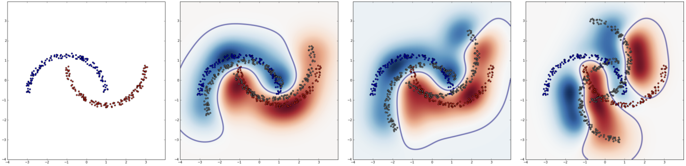


Fig. 20. Examples of domain adaptation.



(a) source domain (b) rotation=20° (c) rotation=40° (d) rotation=90°

Fig. 21. OT-based domain adaptation algorithm tested in a toy example.

[14] Nicolas Courty et al. "Optimal Transport for Domain Adaptation". In: *IEEE Transactions on Pattern Analysis and Machine Intelligence* 39 (2017).

Thank You