Regularizing Optimal Transport Using Regularity Theory

Learning meets Astrophysics

January 17, 2020

François-Pierre Paty
francoispierrepaty.github.io

Based on a joint work with ***Alexandre d'Aspremont*** *and* ***Marco Cuturi*** (AISTATS 2020)

ENSAE

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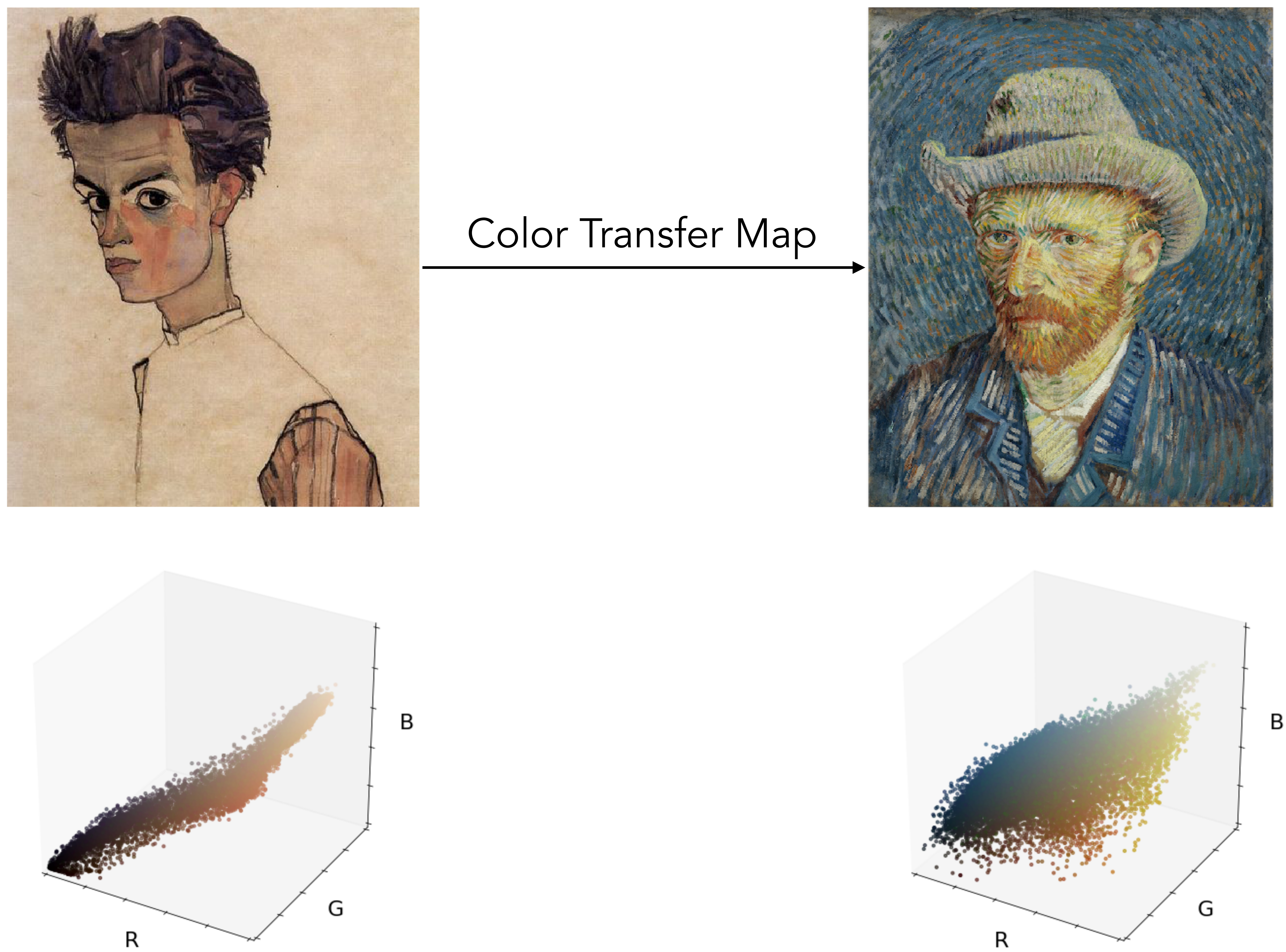
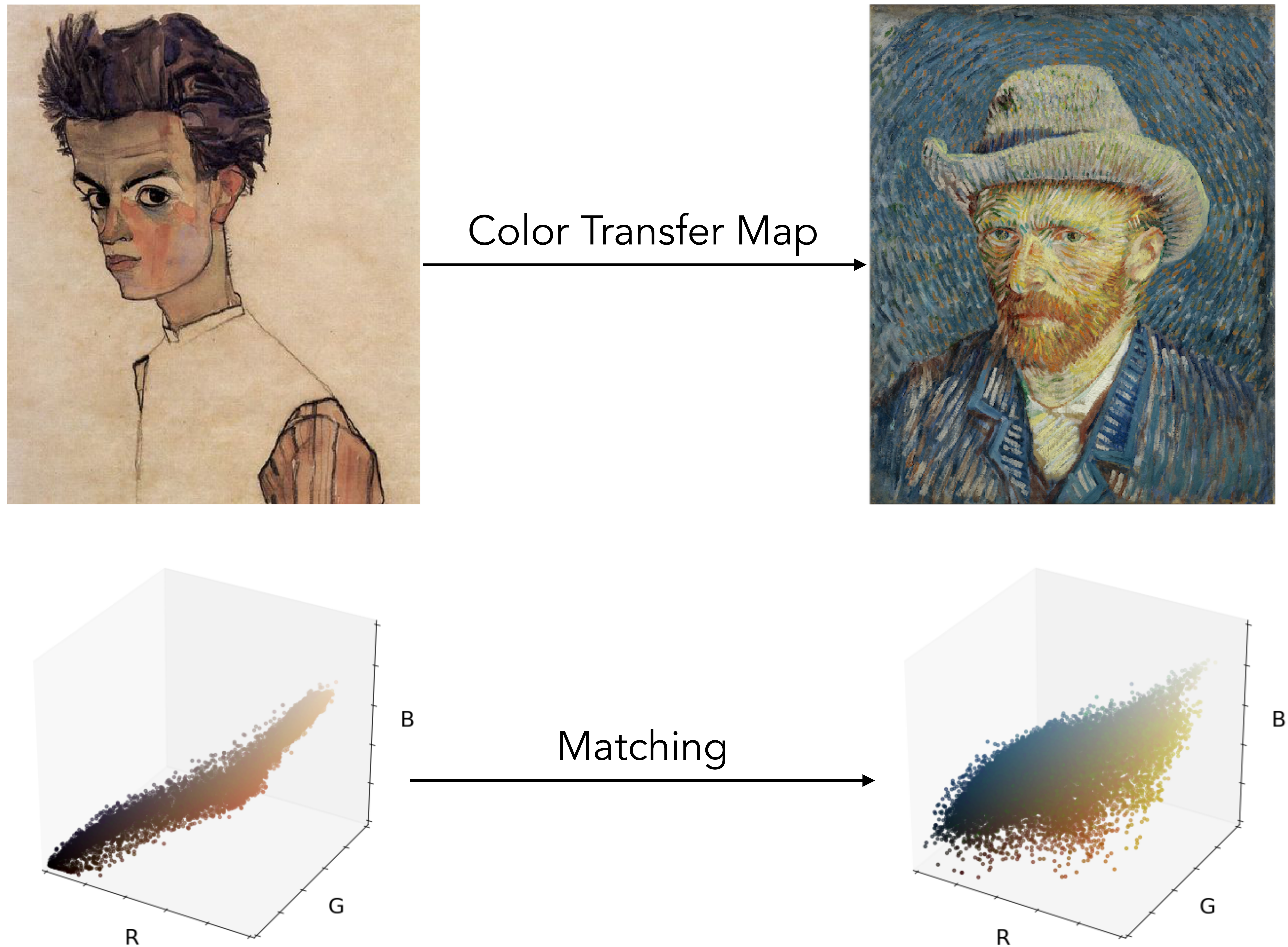
Gaspard Monge

Color Transfer Map


Color Transfer Map
B
G
R
B
G
R


Color Transfer Map
B
Matching
B
G
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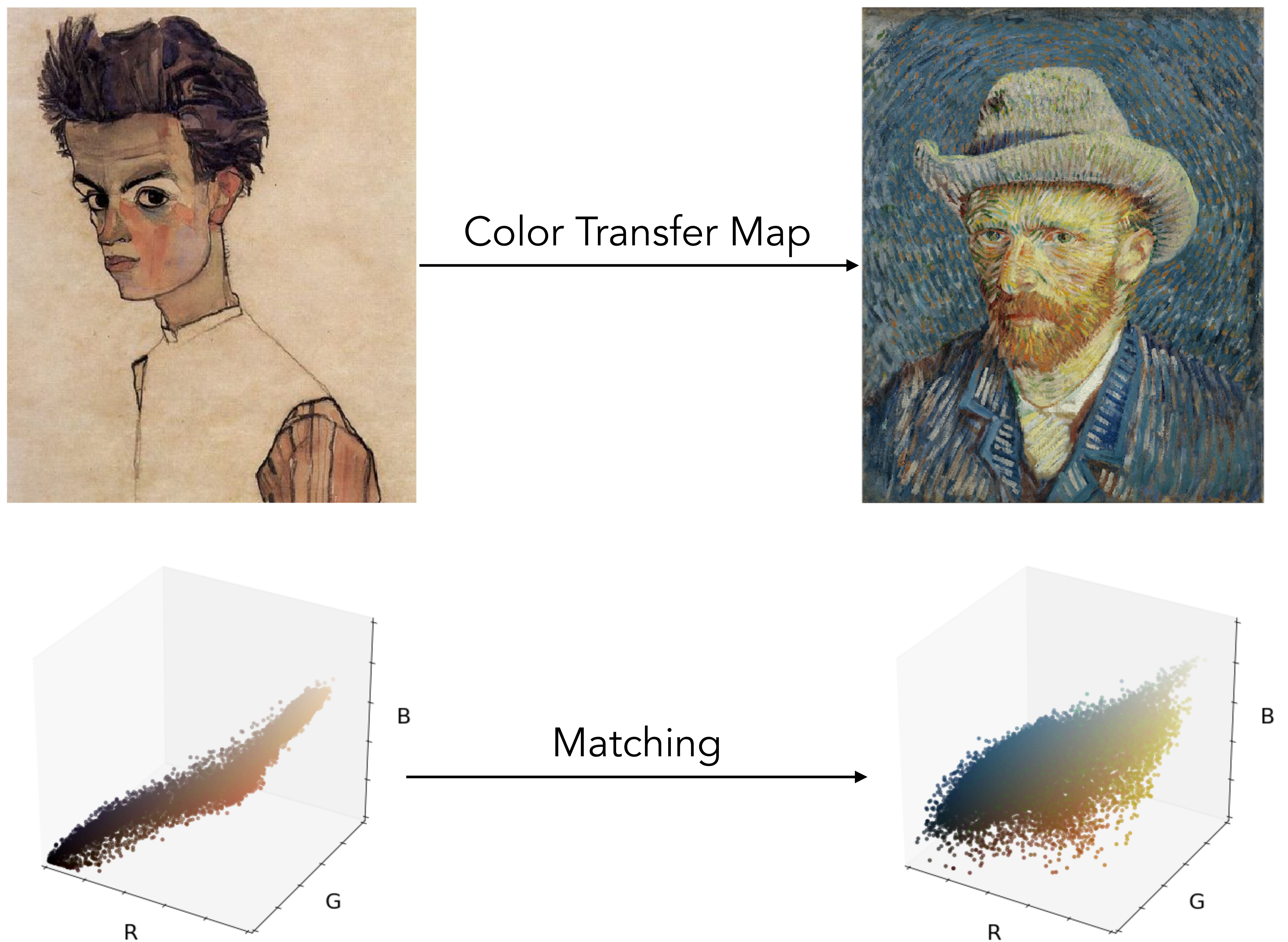
Color Transfer Map
B
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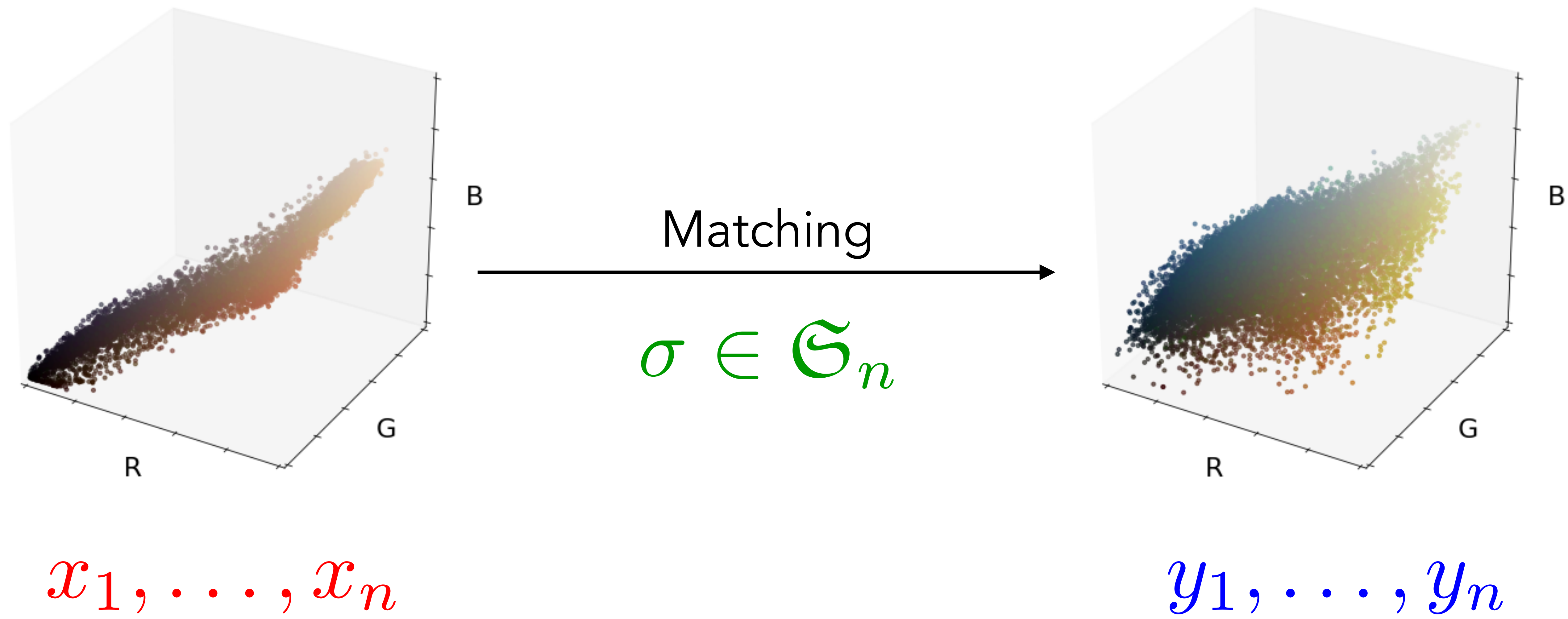
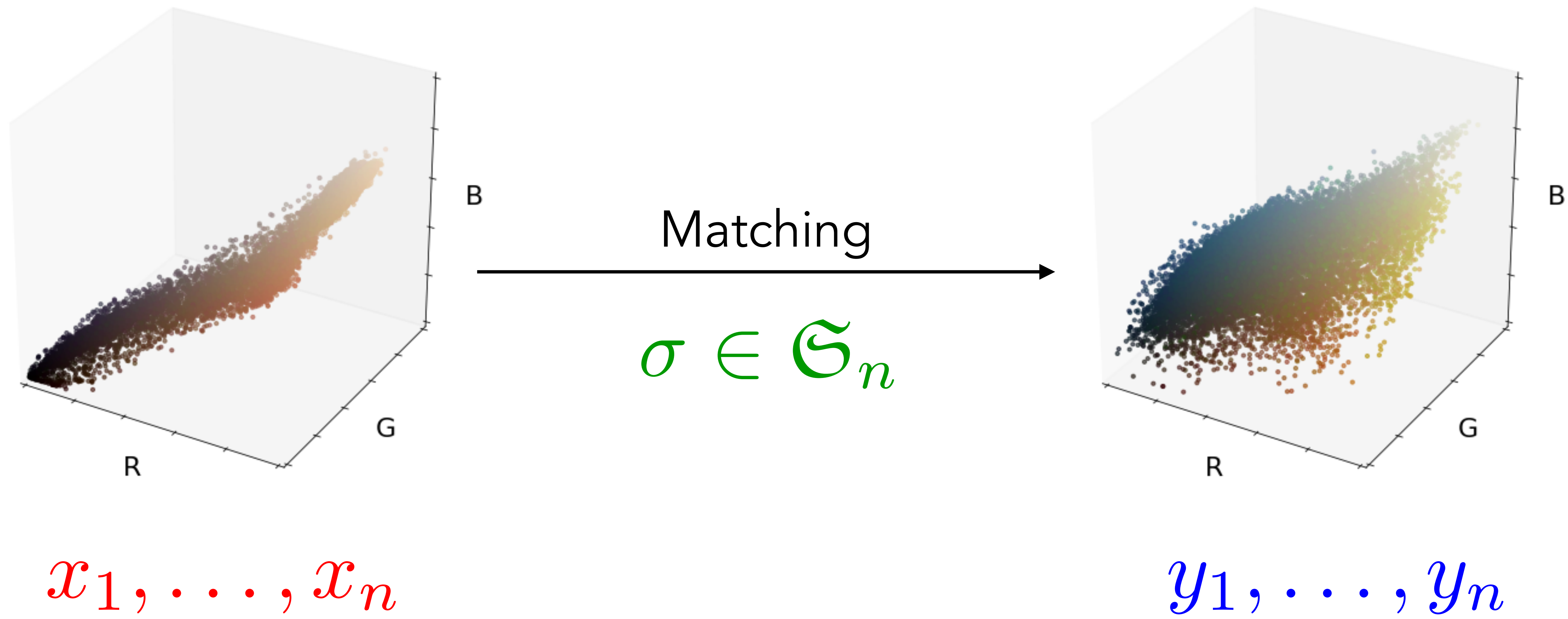


B
G
R
Matching
$\sigma \in \mathfrak{S}_n$
B
G
R
$x_1, \ldots, x_n$
$y_1, \ldots, y_n$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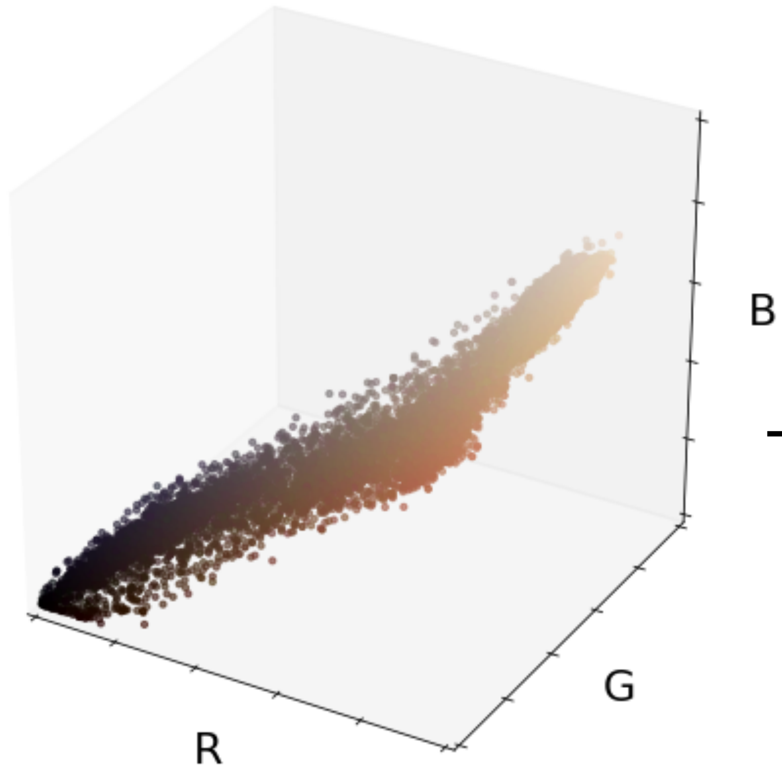

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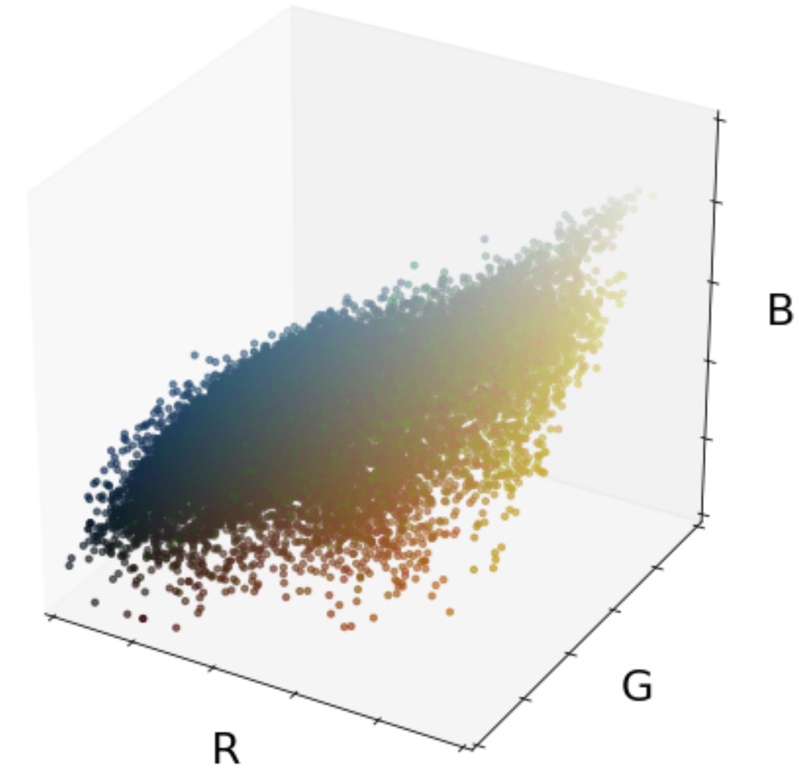
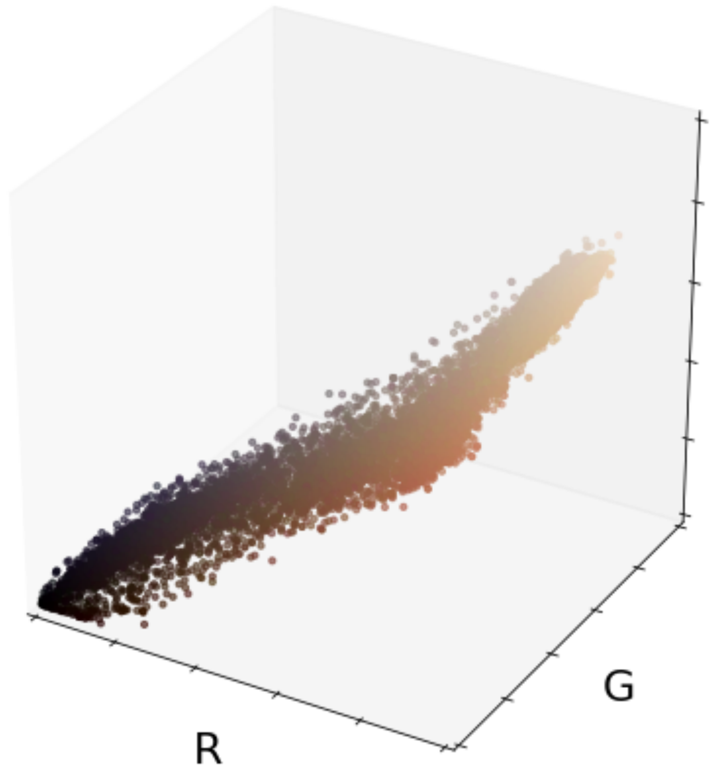


$x_1, \ldots, x_n$ $\qquad$ $y_1, \ldots, y_n$

$$\left\| x_i - y_{\sigma(i)} \right\|^2$$



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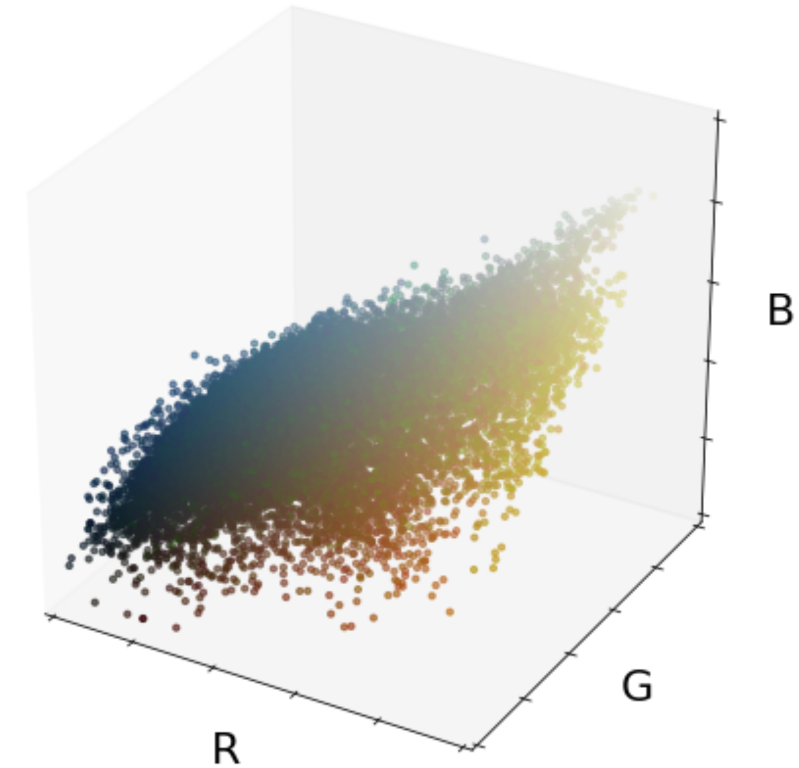

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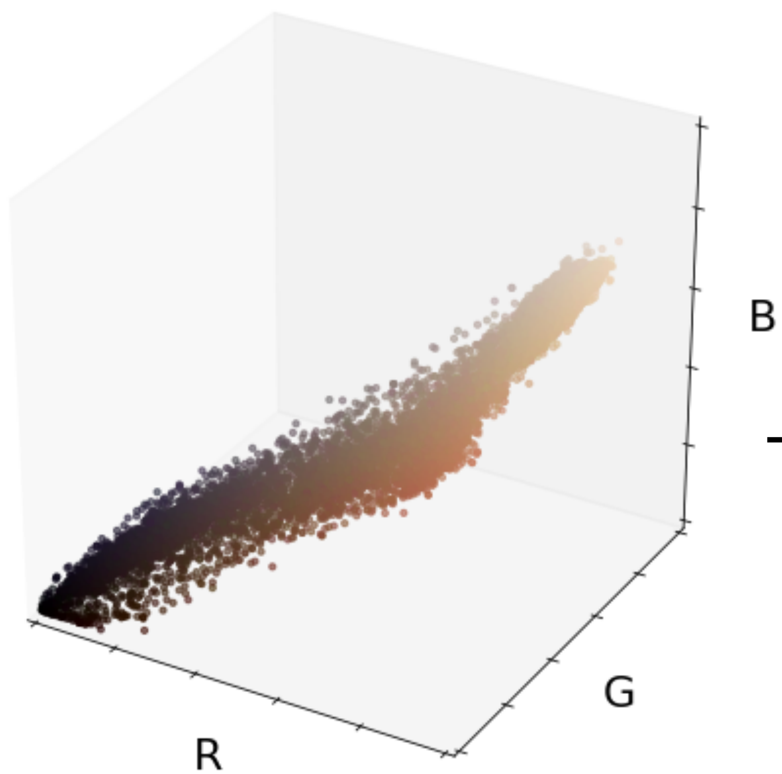
$$\sum_{i=1}^{n} \| x_i - y_{\sigma(i)} \|^2$$



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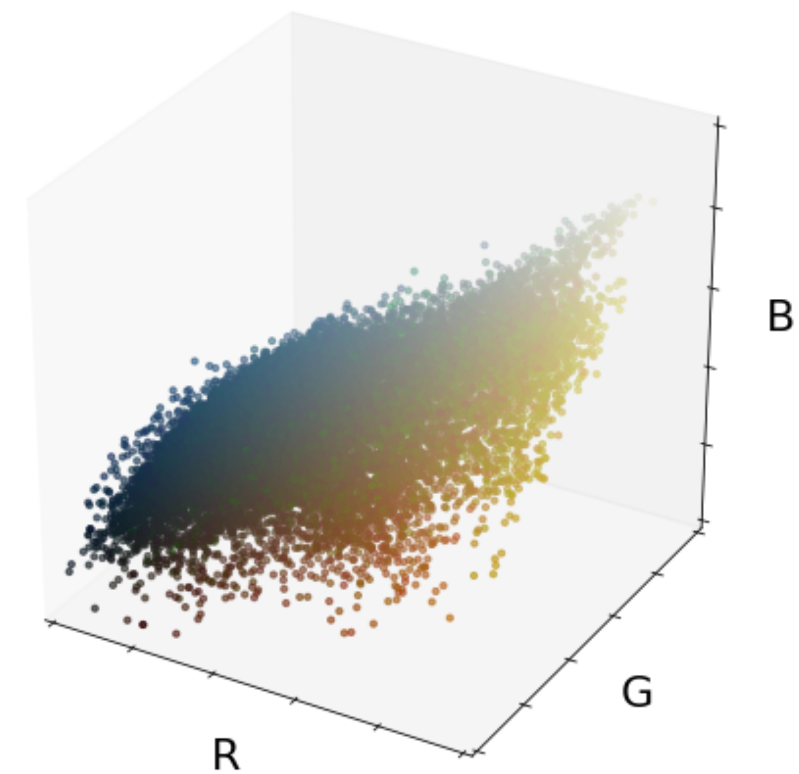

$x_1, \ldots, x_n$

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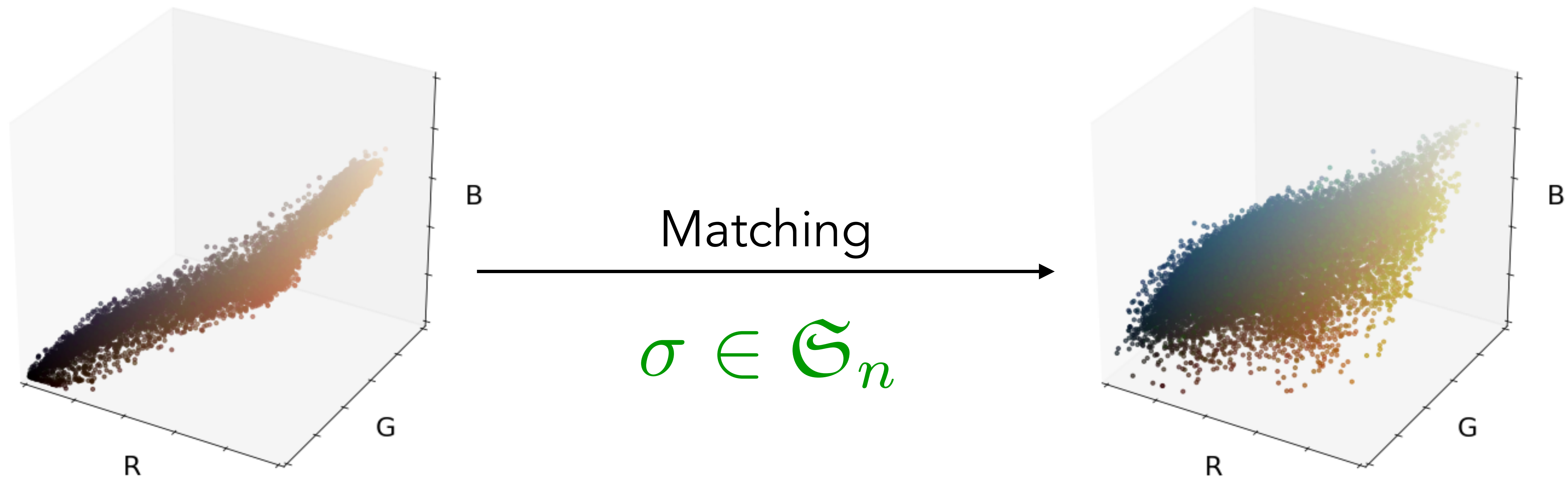
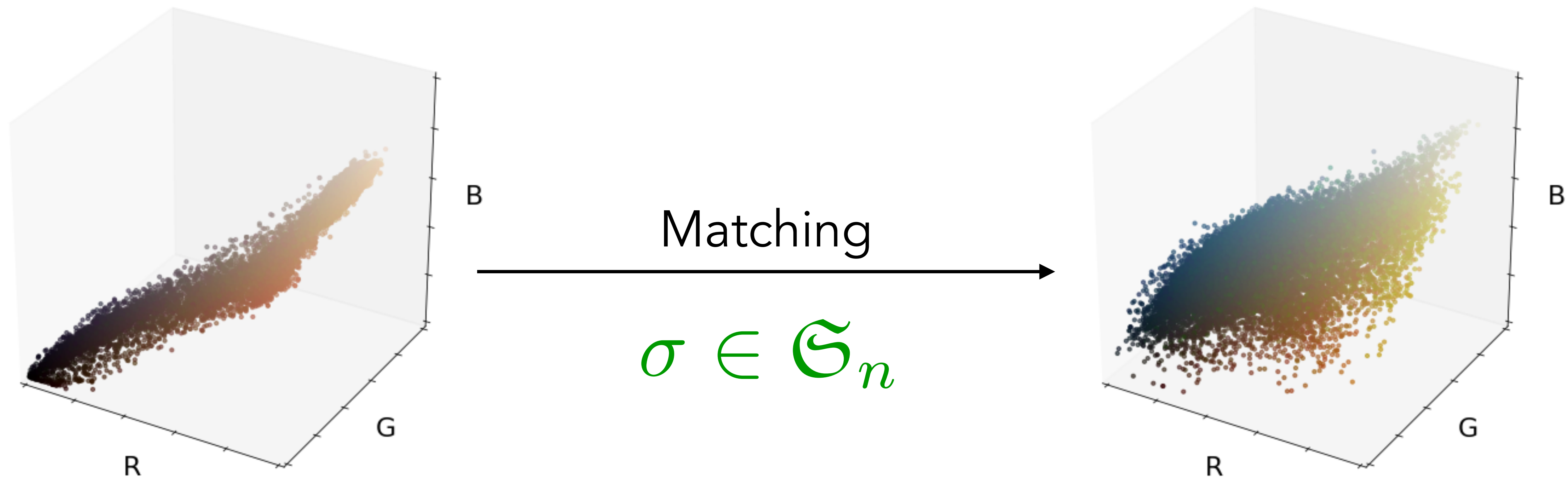
$$\min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} \| x_i - y_{\sigma(i)} \|^2$$



Discrete Monge Problem (1781)

$$\min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} \|x_i - y_{\sigma(i)}\|^2$$



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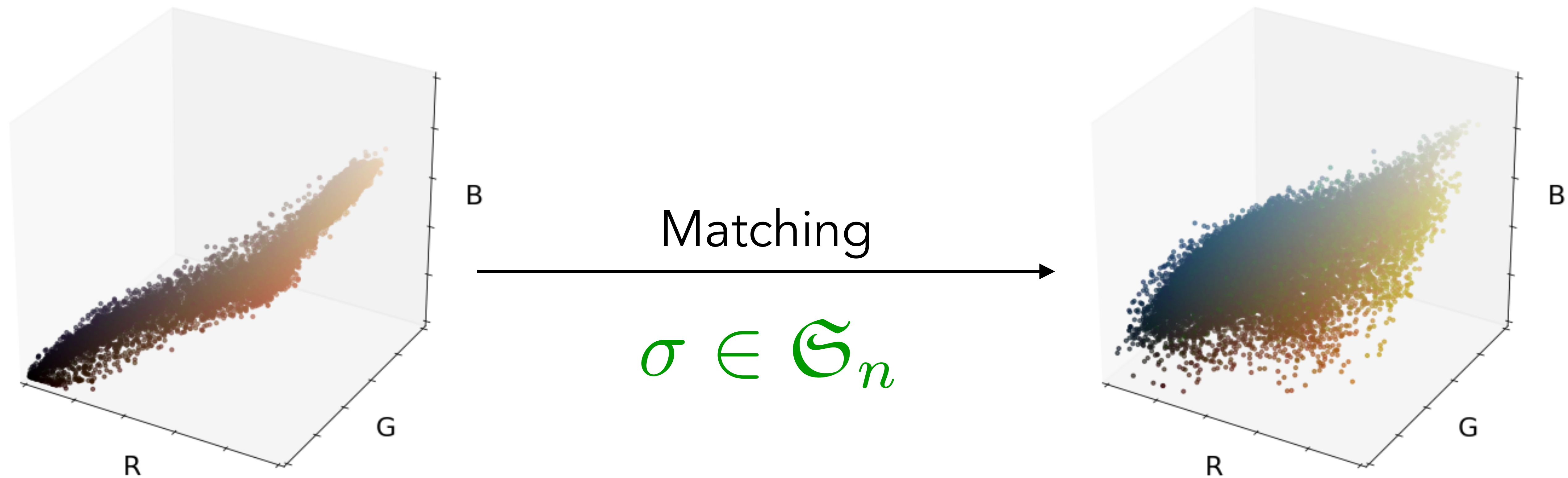

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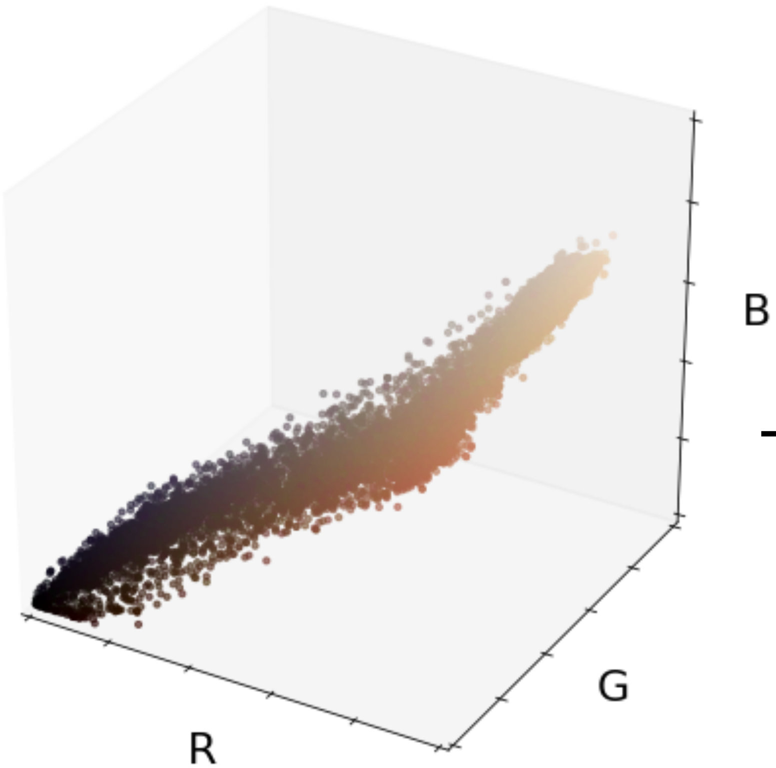

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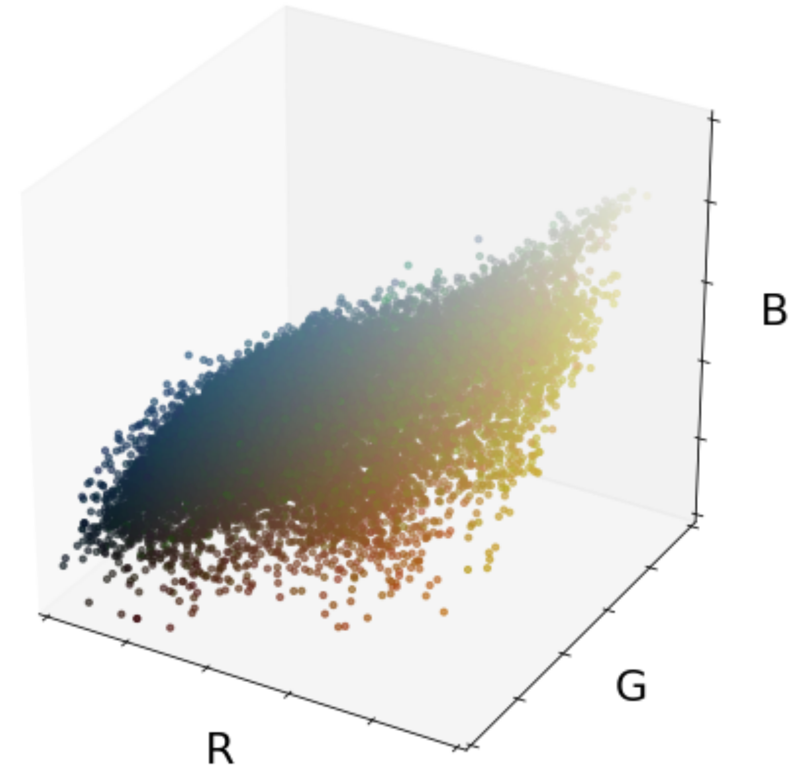

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(i) How to handle repeated points ?
(ii) How to handle different numbers of points ?
(iii) How to compute this combinatorial problem ?

OPTIMAL TRANSPORT

Leonid Kantorovich

$$\min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} \| x_i - y_{\sigma(i)} \|^2$$

$$\min_{\sigma \in \mathfrak{S}_n} \sum_{i=1}^{n} \sum_{j=1}^{n} \|x_i - y_j\|^2 \, \mathbb{1}_{\sigma(i)=j}$$

$$\min_{P \in \mathfrak{P}_n} \sum_{i=1}^{n} \sum_{j=1}^{n} \|x_i - y_j\|^2 P_{ij}$$

$$\mathfrak{P}_n = \{P \in \mathbb{R}^{n \times n} \text{ permutation matrix}\}$$

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If $\mathbf{a} \in \mathbb{R}^n, \mathbf{b} \in \mathbb{R}^m$ are probability weights, we define the associated **transportation polytope**:

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If $\mathbf{a} \in \mathbb{R}^n, \mathbf{b} \in \mathbb{R}^m$ are probability weights, we define the associated **transportation polytope**:

$$\mathfrak{U}(\mathbf{a}, \mathbf{b}) = \{P \in \mathbb{R}_+^{n \times m} \,|\, P\mathbb{1}_m = \mathbf{a}, P^\top \mathbb{1}_n = \mathbf{b}\}$$

Discrete Kantorovitch Problem

$$W_2^2(\mu,\nu) = \min_{P \in \mathfrak{U}(\mathbf{a},\mathbf{b})} \sum_{i=1}^{n} \sum_{j=1}^{m} \|x_i - y_j\|^2 P_{ij}$$

where $\mu = \sum_{i=1}^{n} \mathbf{a}_i \delta_{x_i}$ and $\nu = \sum_{j=1}^{m} \mathbf{b}_j \delta_{y_j}$ are probability measures

2-Wasserstein distance

If $\mathbf{a} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$ are probability weights, we define the associated **transportation polytope**:

$$\mathfrak{U}(\mathbf{a},\mathbf{b}) = \{P \in \mathbb{R}_+^{n \times m} \mid P\mathbb{1}_m = \mathbf{a}, P^\top \mathbb{1}_n = \mathbf{b}\}$$

Why should we care?

Many applications in Machine Learning, some related to Astrophysics:

- Brenier et al., Reconstruction of the early Universe as a convex optimization problem 1999
- Wasserstein Dictionary Learning
- Computer Graphics
- Generative Models
- Model fitting (Minimum Kantorovich Estimators)

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$$T : \mathbb{R}^d \to \mathbb{R}^d$$

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Monge problem

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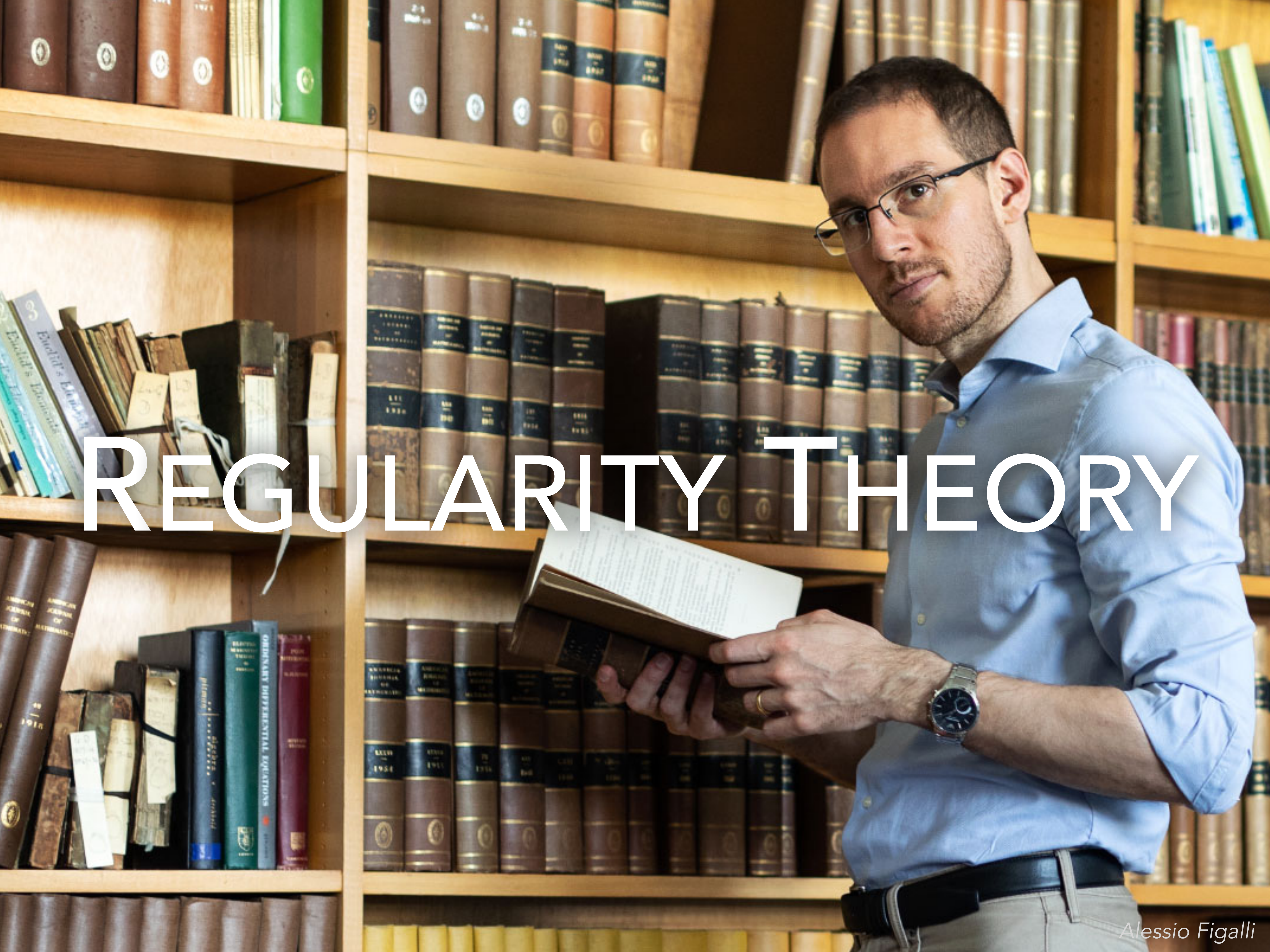
$$X \sim \mu \Longrightarrow T(X) \sim \nu$$


REGULARITY THEORY
Alessio Figalli

Let μ and ν be two probability measures over $\mathbb{R}^d$.

$$\inf_{T_\sharp \mu = \nu} \int \|x - T(x)\|^2 d\mu(x)$$

When does the Monge problem admit a solution ?

What can be said about it ?

Let μ and ν be two probability measures over $\mathbb{R}^d$.

$$\inf_{T_\sharp \mu = \nu} \int \|x - T(x)\|^2 d\mu(x)$$

Brenier Theorem

1. If μ is *absolutely continuous* with respect to the Lebesgue measure, the Monge problem admits a unique solution
2. If the Monge problem admits a solution T, then there exists a convex function f, called a **Brenier potential**, s.t.

$$T = \nabla f$$

When the optimal map exists (*e.g.* when μ has a density), what kind of regularity does it exhibit ?

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Without further assumptions on μ and ν , we cannot even hope for continuity. Many results by *Caffarelli, De Philippis, Kim, Figalli…*

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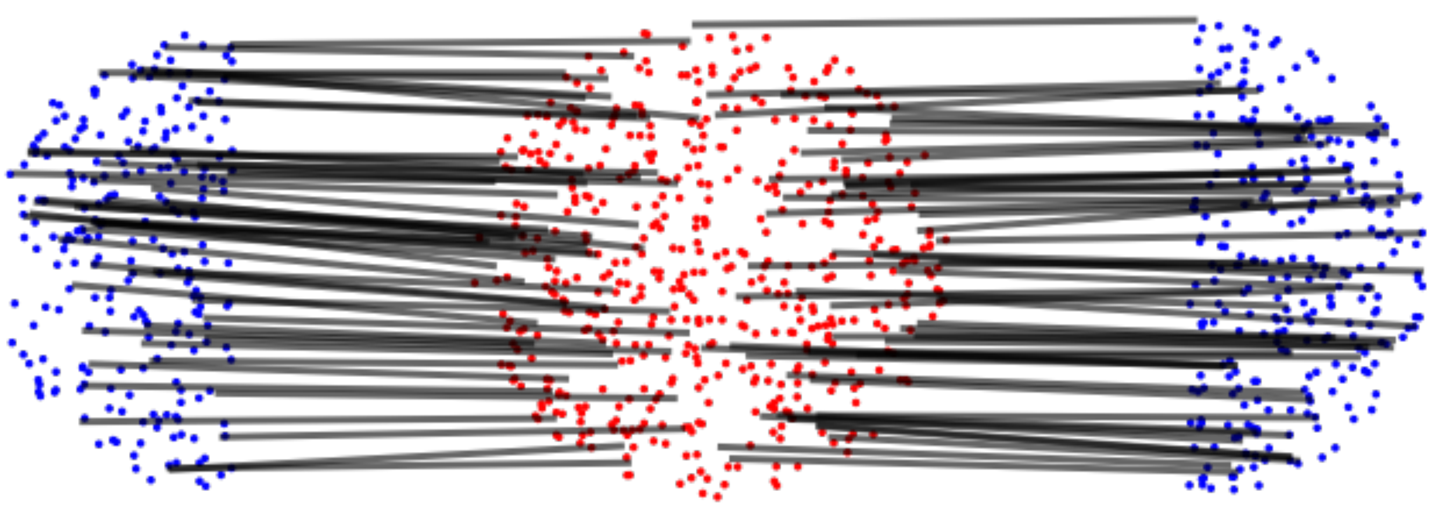
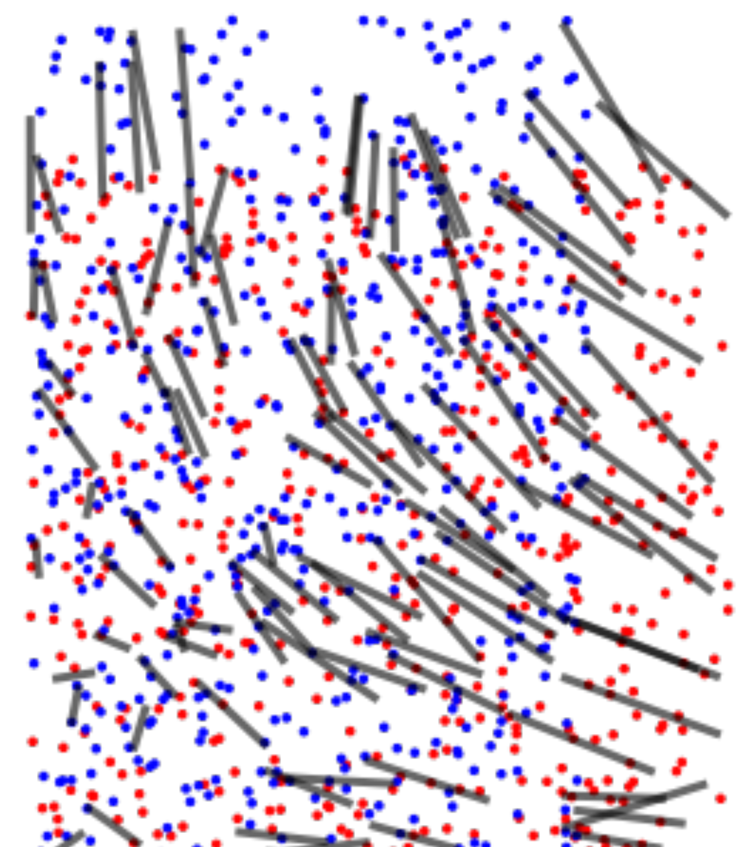
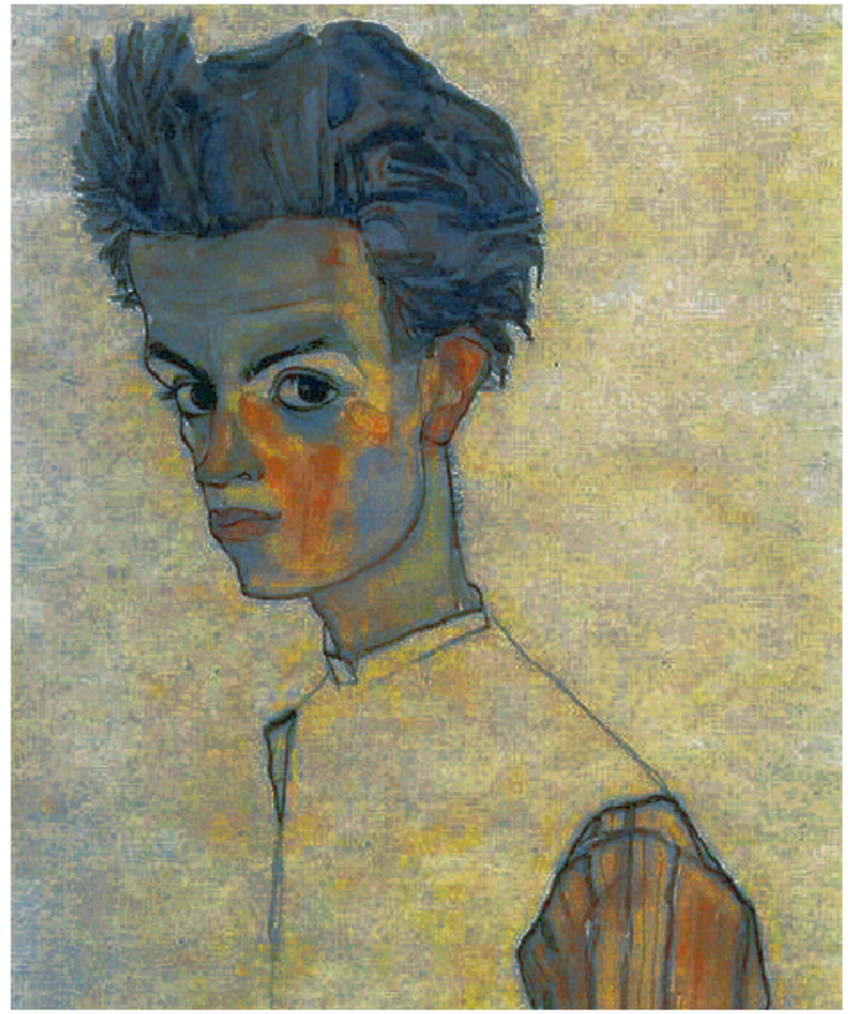
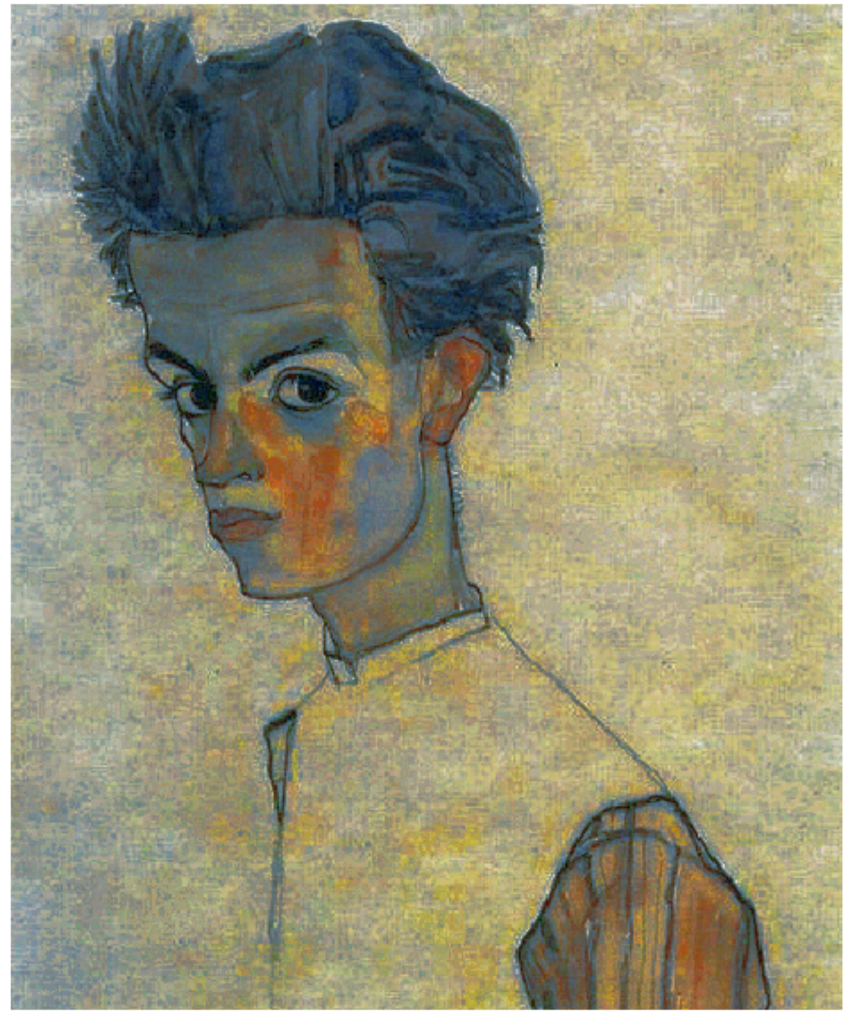




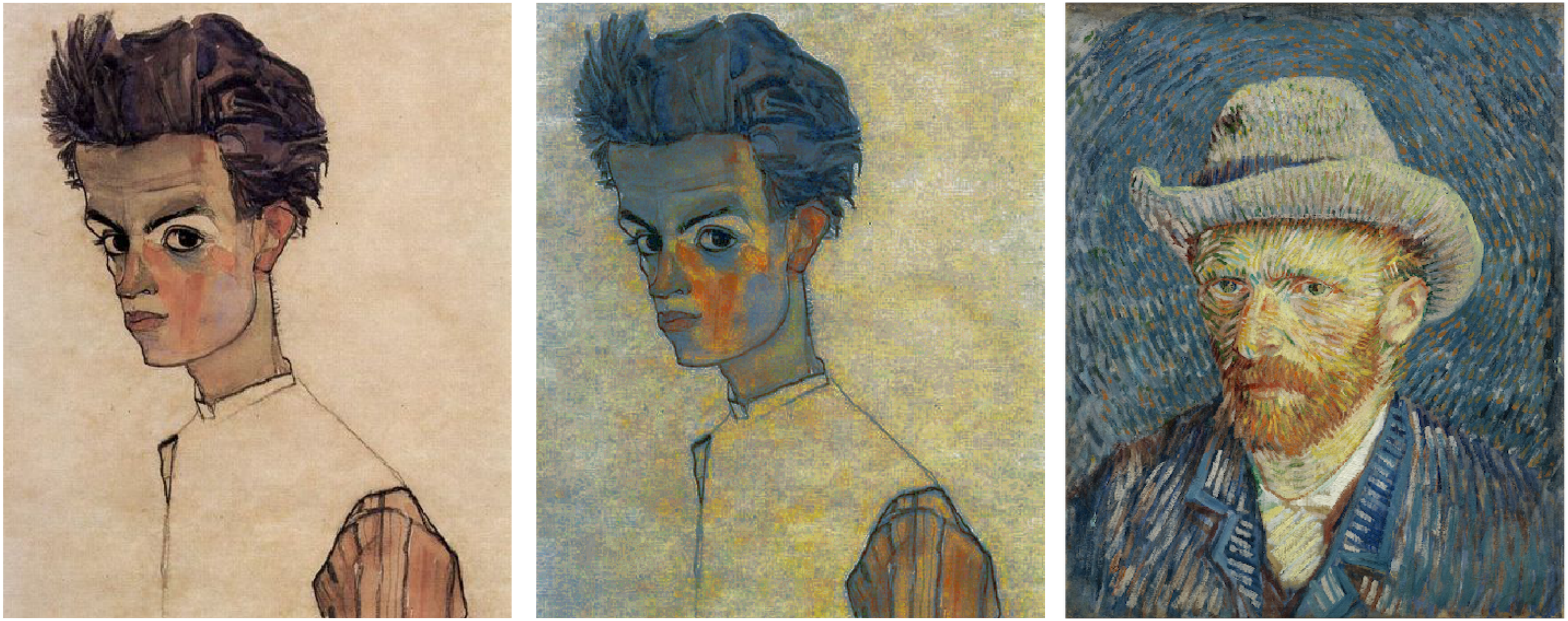



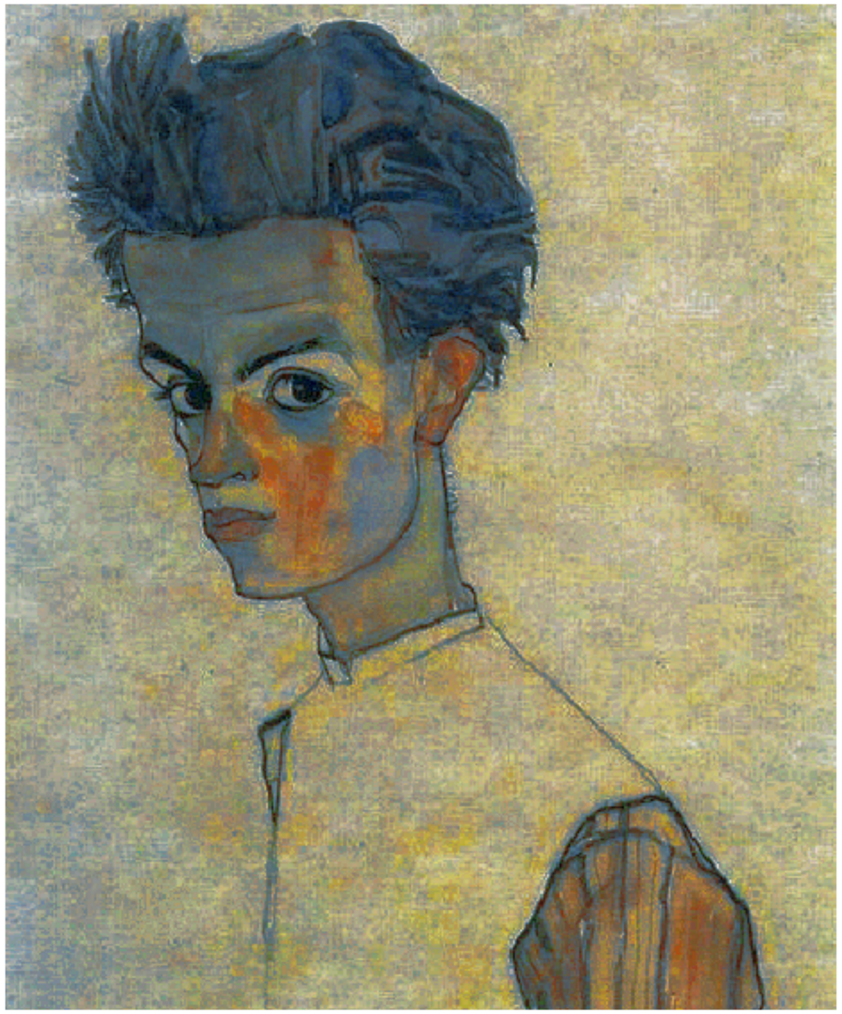

  

Instead of finding assumptions under which the optimal map exists and exhibits some regularity, we will enforce such regularity directly in the OT problem.

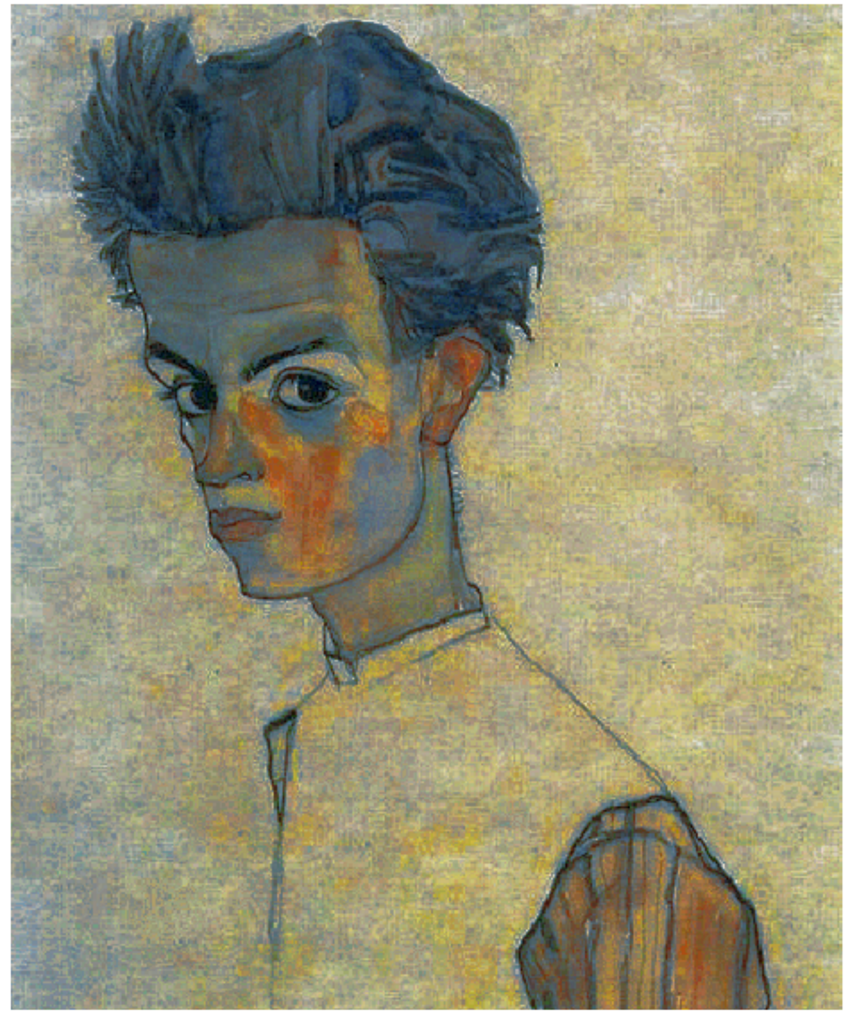
Smooth and Strongly Convex Brenier Potentials

Yann Brenier



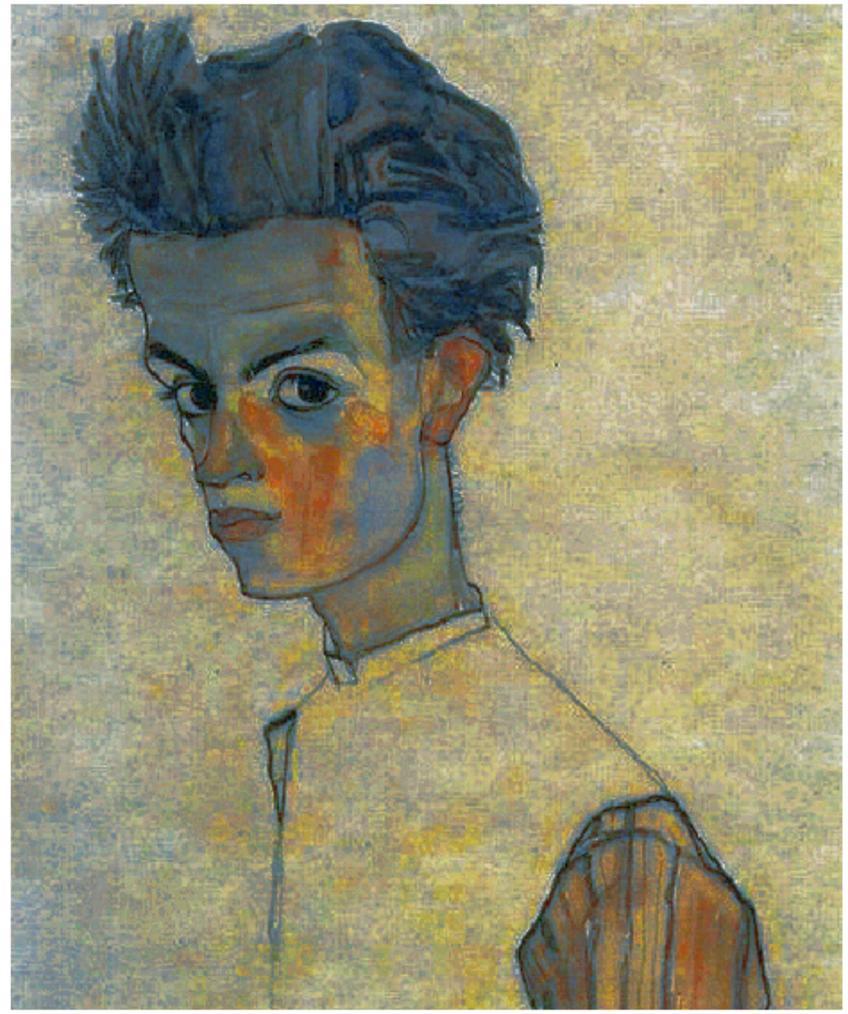
  

$$\ell\|x - y\| \leq \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$


$$\ell\|x-y\| \leq \|\nabla f(x) - \nabla f(y)\| \leq L\|x-y\|$$

We ask that $T = \nabla f$ is a bi-Lipschitz map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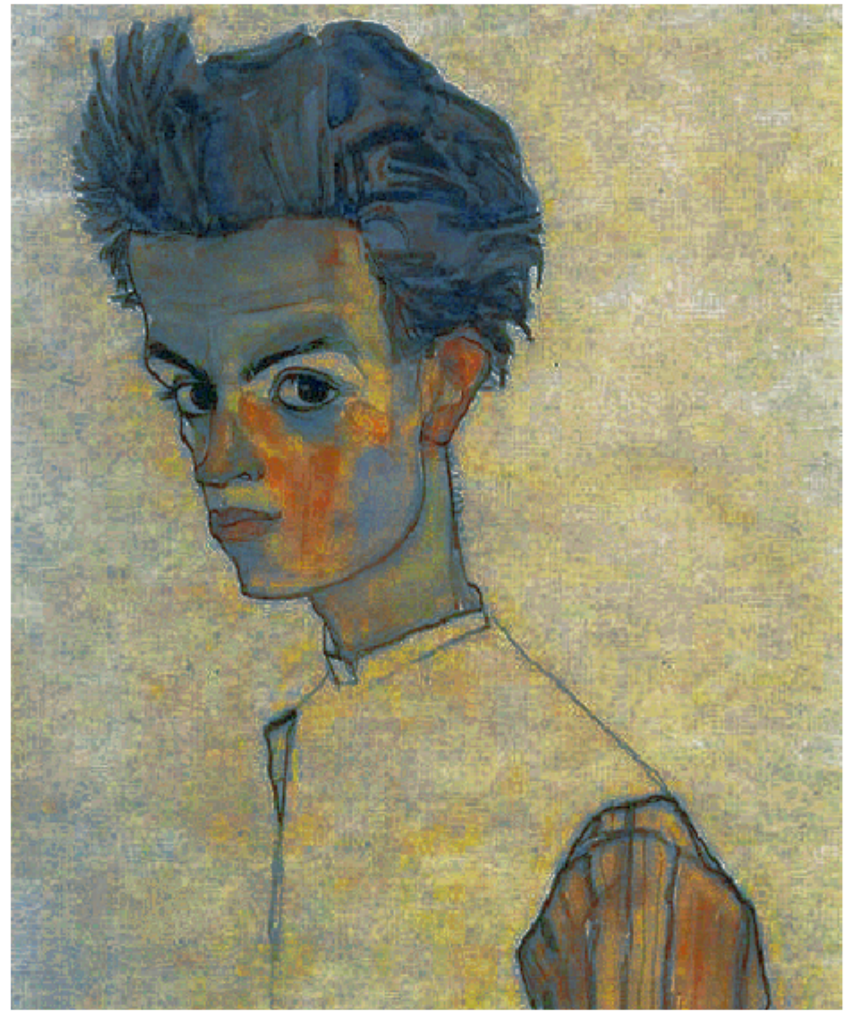
We ask that f is **smooth** and **strongly convex**


$$\ell \|x - y\| \leq \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

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$$\rightarrow f \in \mathcal{F}_{\ell,L}$$

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Instead, we will try to best approximate ν as a push-forward of μ through a regular map:

$$\min_{f \in \mathcal{F}_{\ell, L}} W_2 \left[\nabla f_\sharp \mu, \nu \right]$$

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$$\min_{\substack{z_1,\ldots z_n \in \mathbb{R}^d \\ u \in \mathbb{R}^n}} W_2^2 \left(\sum_{i=1}^{n} a_i \delta_{z_i}, \nu \right)$$

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$$u_i \geq u_j + \langle z_j, x_i - x_j \rangle + \frac{1}{2(1-\ell/L)} \left(\frac{1}{L} \|z_i - z_j\|^2 + \ell \|x_i - x_j\|^2 - 2\frac{\ell}{L} \langle z_j - z_i, x_j - x_i \rangle \right)$$

$$x_1, \ldots, x_n \sim \mu \qquad y_1, \ldots, y_n \sim \nu$$

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \qquad \hat{\nu}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{y_i}$$

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$$f^\star \in \underset{f \in \mathcal{F}_{\ell, L}}{\arg\min}\, W_2 \left[\nabla f_\sharp \hat{\mu}_n, \hat{\nu}_n \right]$$

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We can easily compute the map on any new point x by solving a cheap QCQP

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$$\min_{v \in \mathbb{R},\, g \in \mathbb{R}^d} v$$

$$\text{s.t.}\ \forall i,\ v \geq u_i + \langle z_i^\star, x - x_i \rangle + \frac{1}{2(1-\ell/L)} \left(\frac{1}{L} \|g - z_i^\star\|^2 + \ell \|x - x_i\|^2 - 2\frac{\ell}{L} \langle z_i^\star - g, x_i - x \rangle \right)$$

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We define the *SSNB estimator* as a plug-in:

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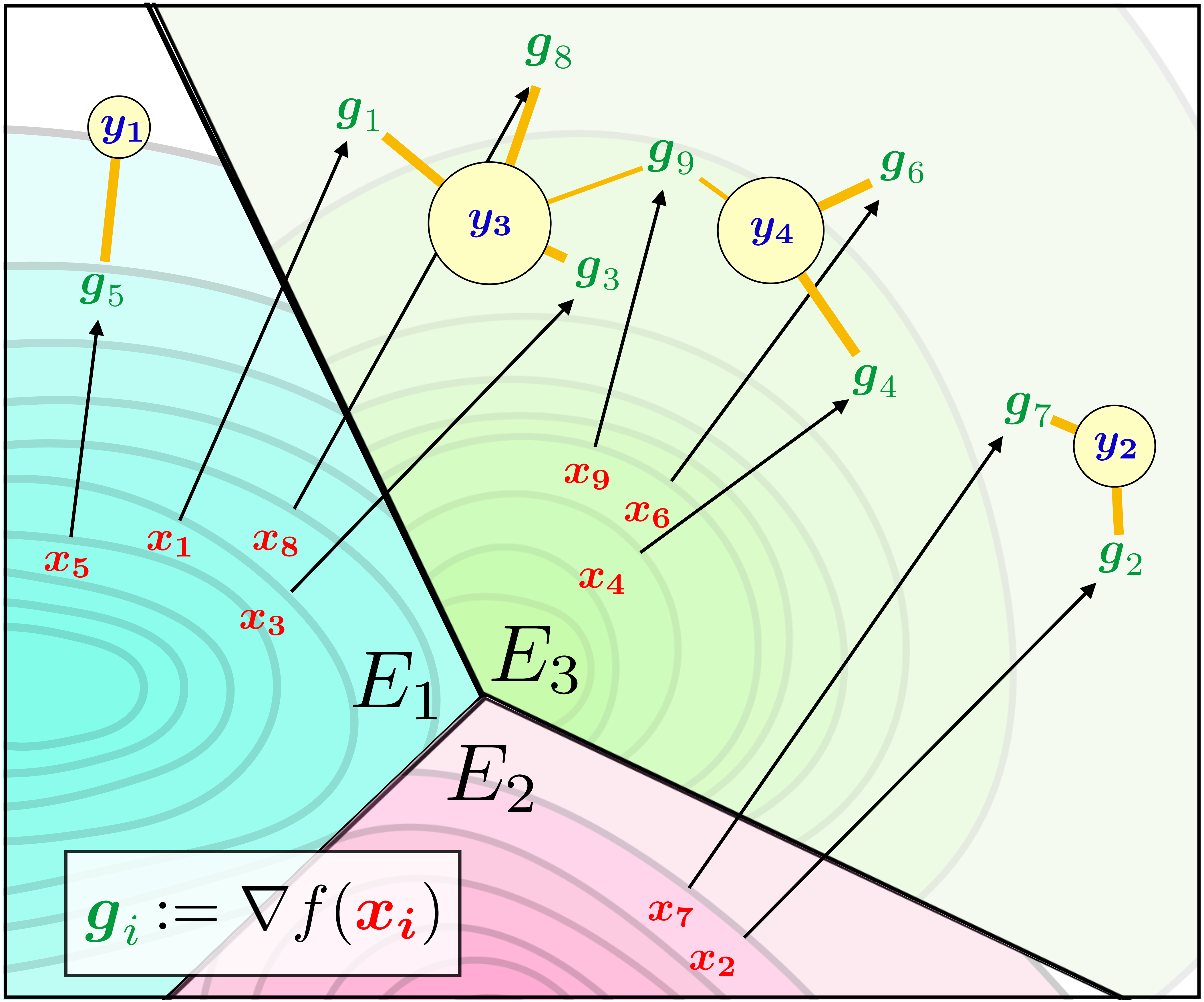
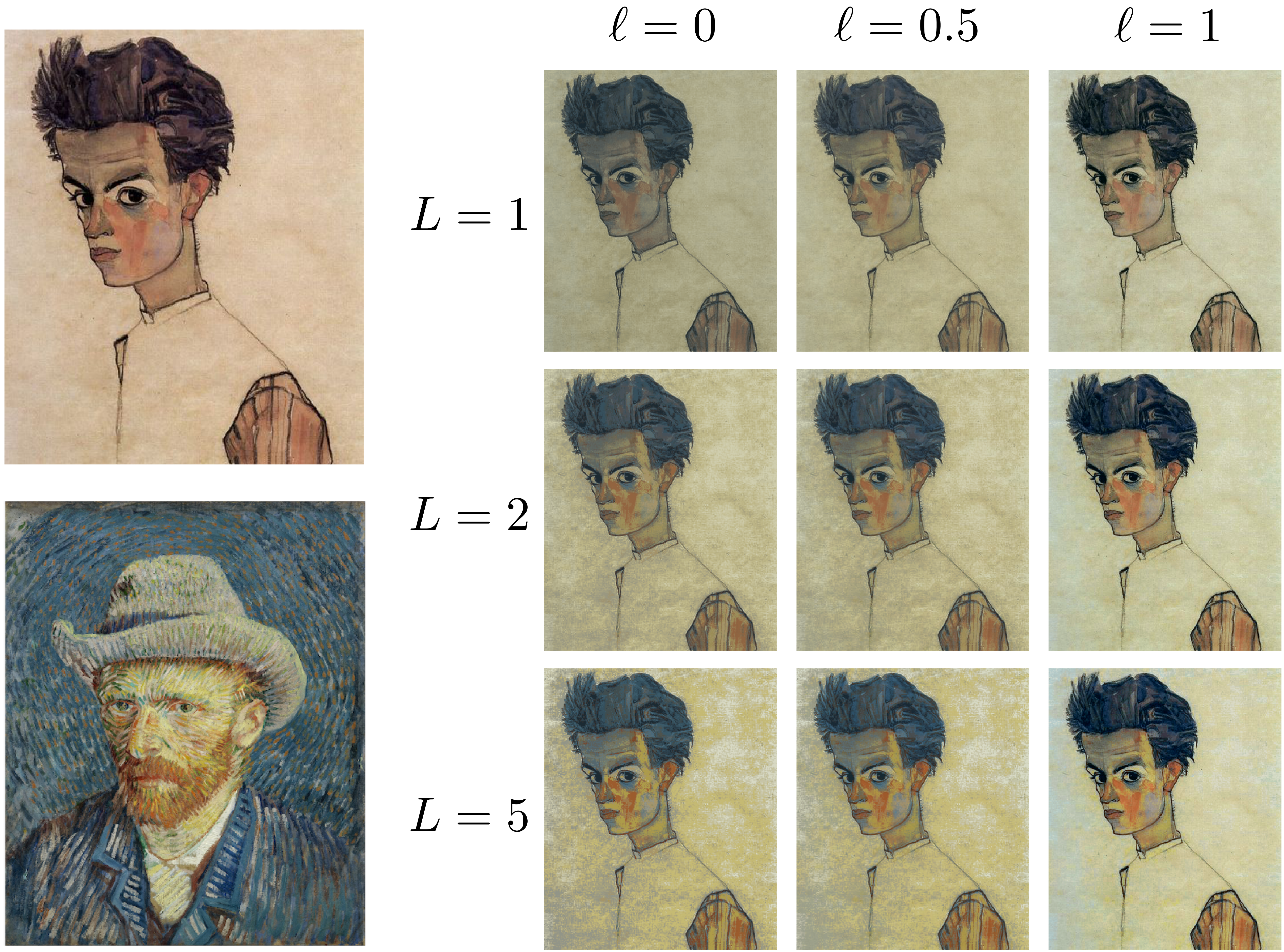
$$\widehat{W}_2^2 = \int \|x - \nabla f^\star(x)\|^2 d\mu(x)$$

Regularity "by part"





$\ell = 0$
$\ell = 0.5$
$\ell = 1$
$L = 1$
$L = 2$
$L = 5$


QUESTIONS ?
Cédric Villani