Regularity as Regularization: Smooth and Strongly Convex Brenier Potentials in Optimal Transport

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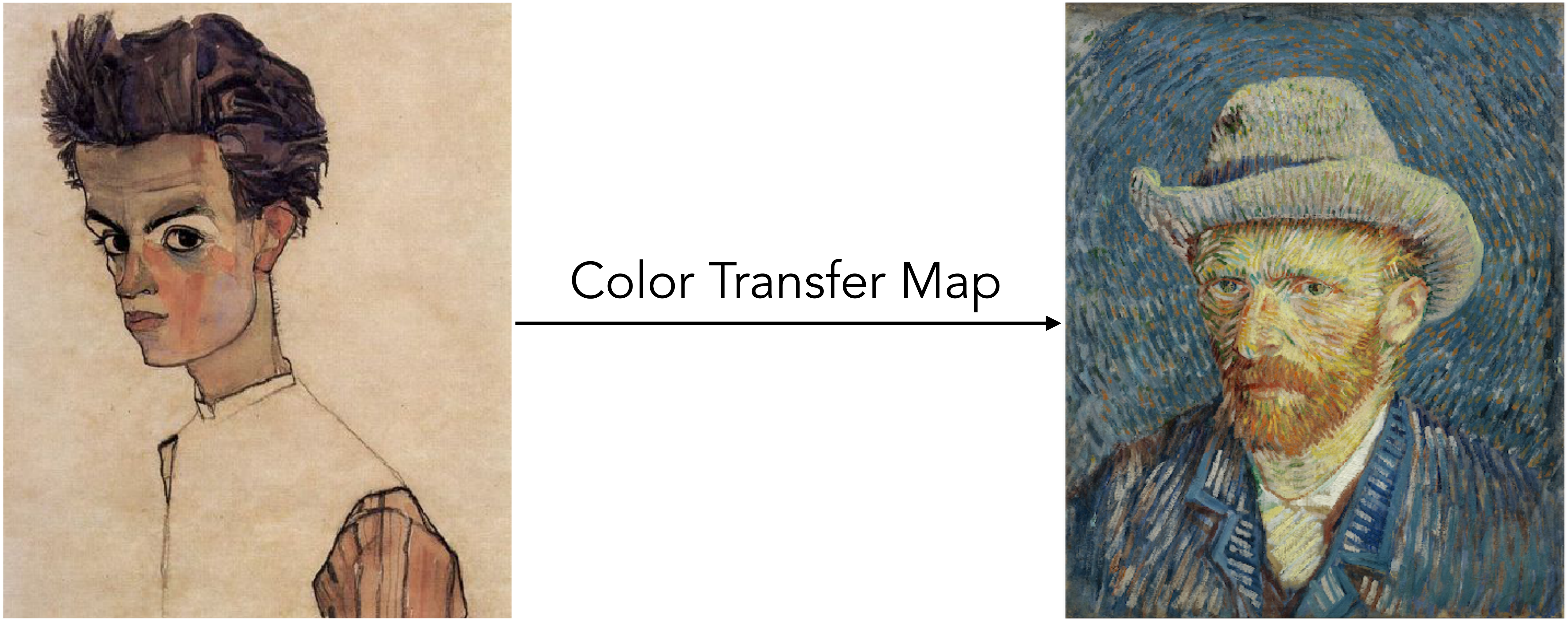
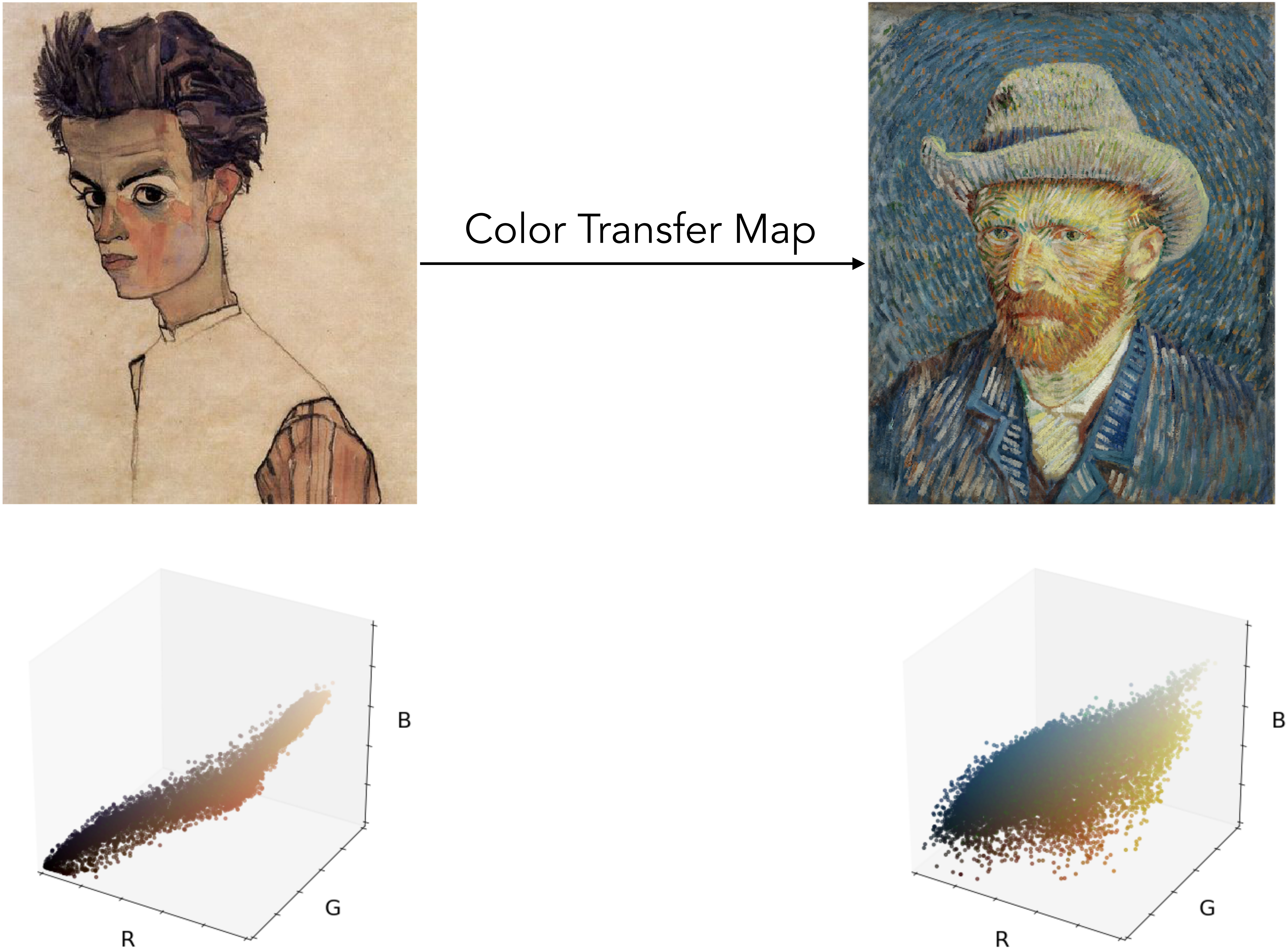
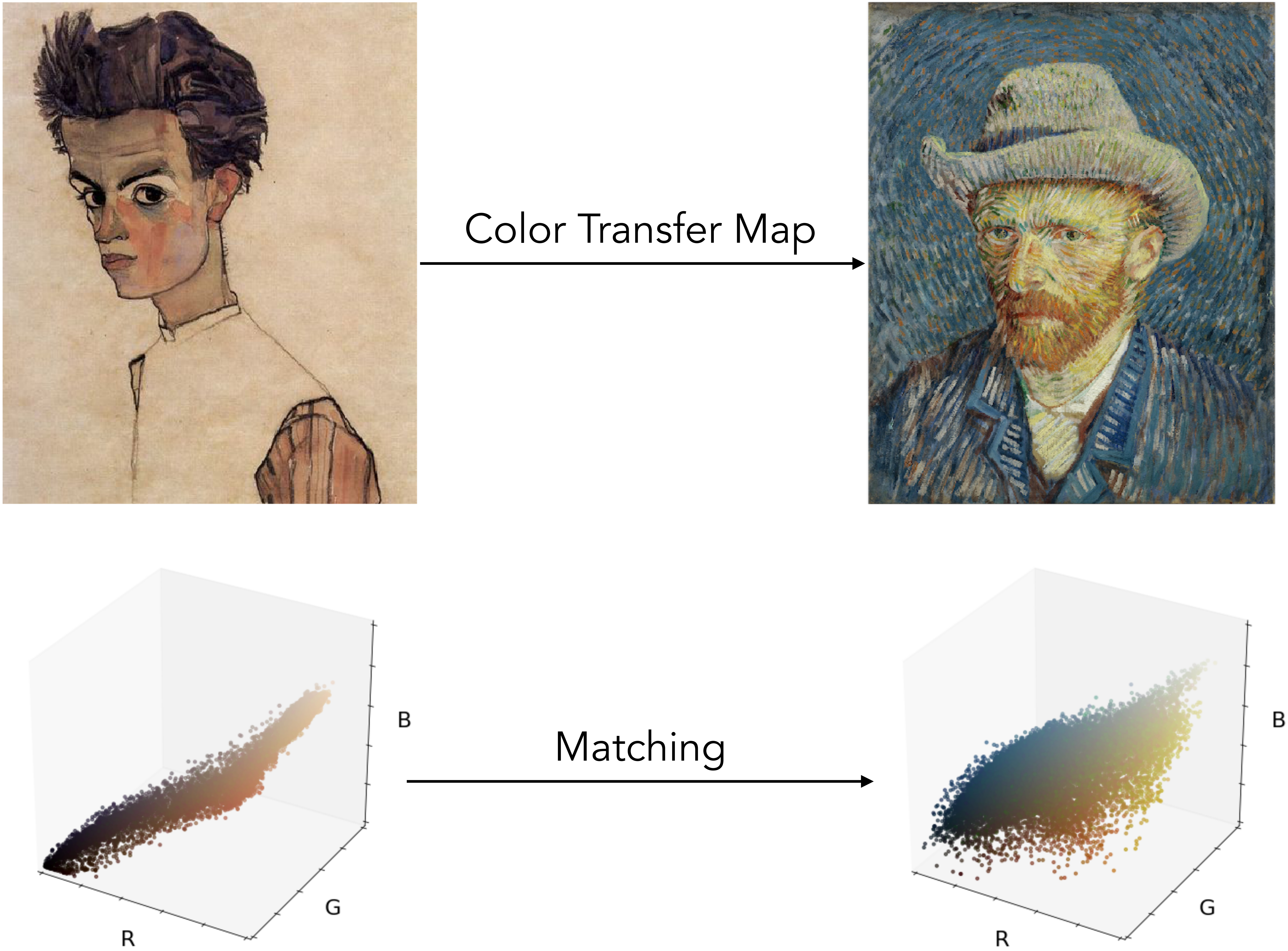
Introduction

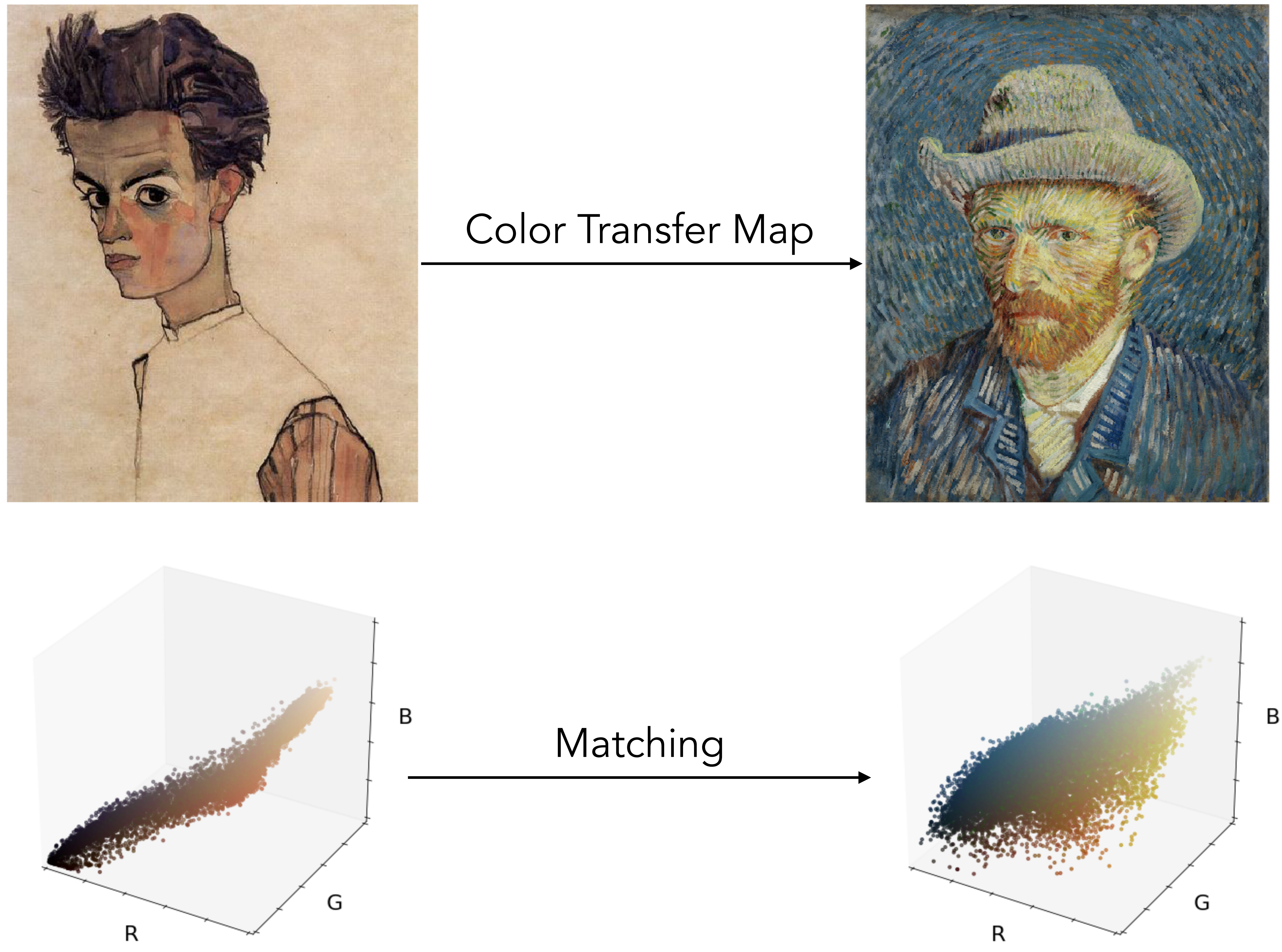
Gaspard Monge


Color Transfer Map


Color Transfer Map
B
G
R
B
G
R



Color Transfer Map
Matching
B
G
R
B
G
R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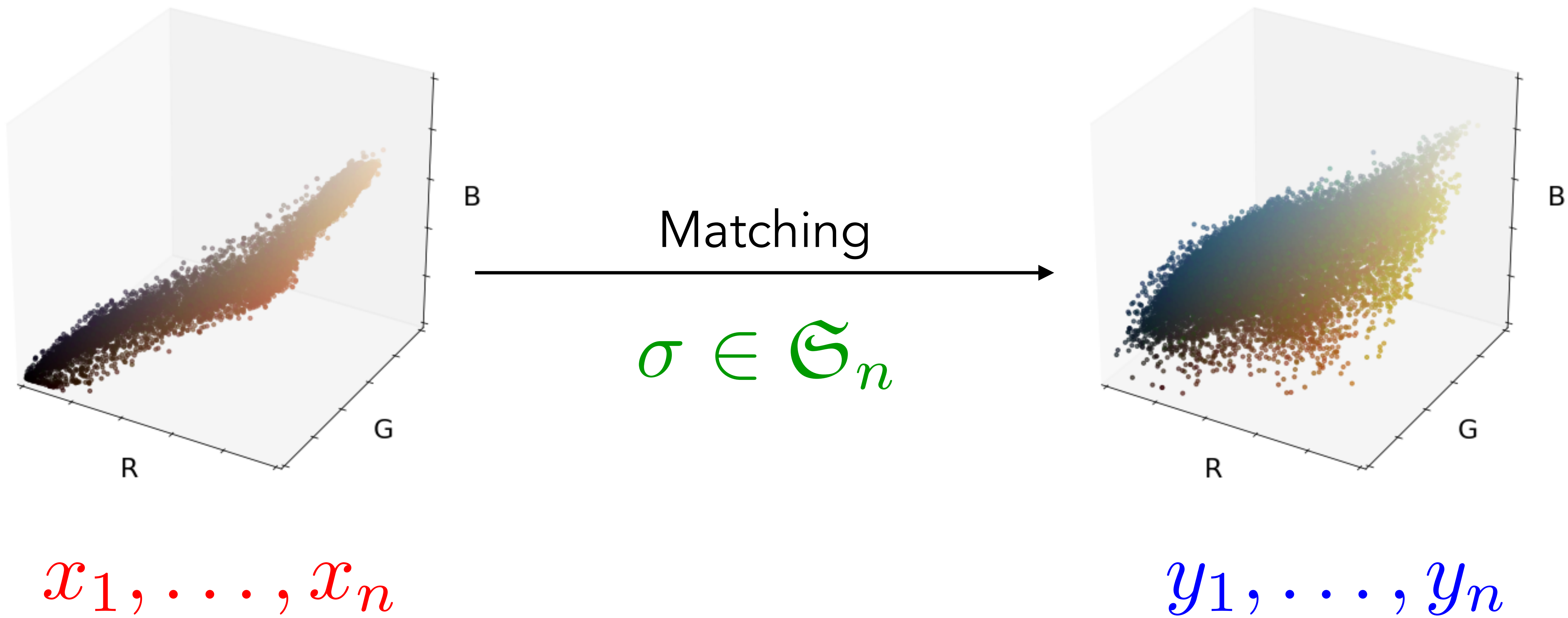
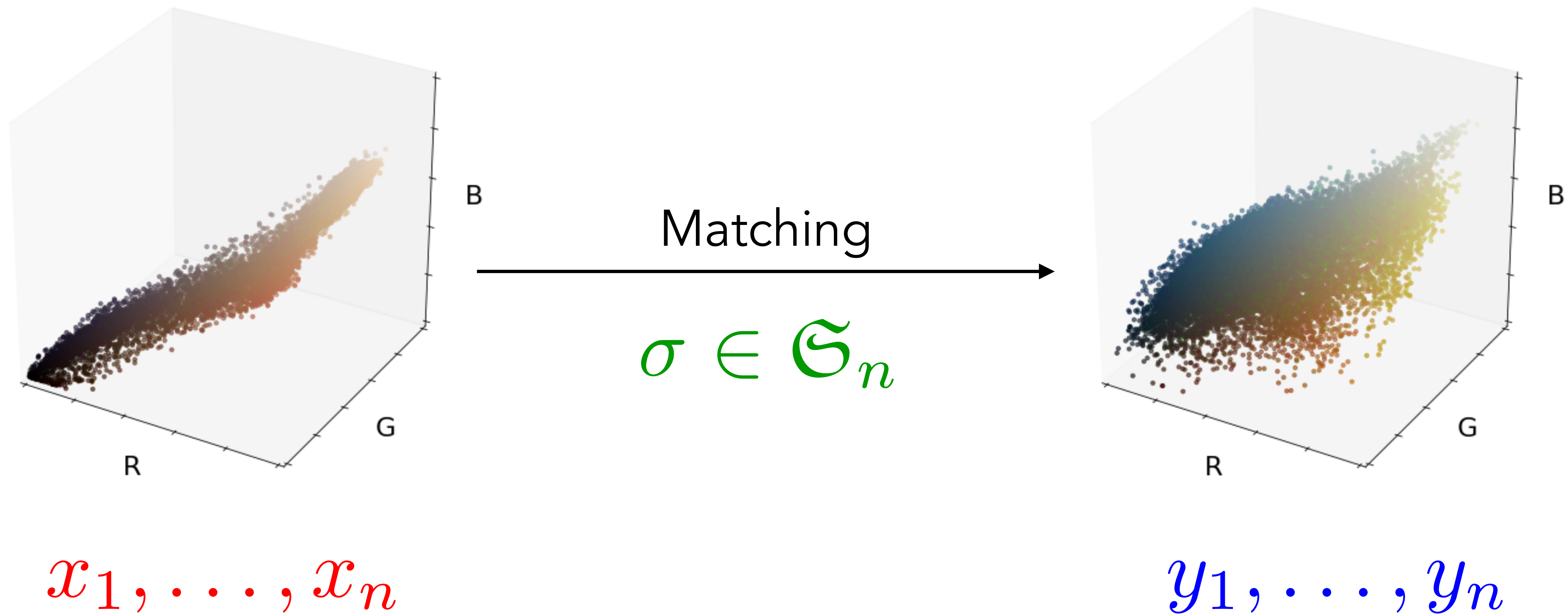


B
R
G
Matching
$\sigma \in \mathfrak{S}_n$
B
R
G
$x_1, \ldots, x_n$
$y_1, \ldots, y_n$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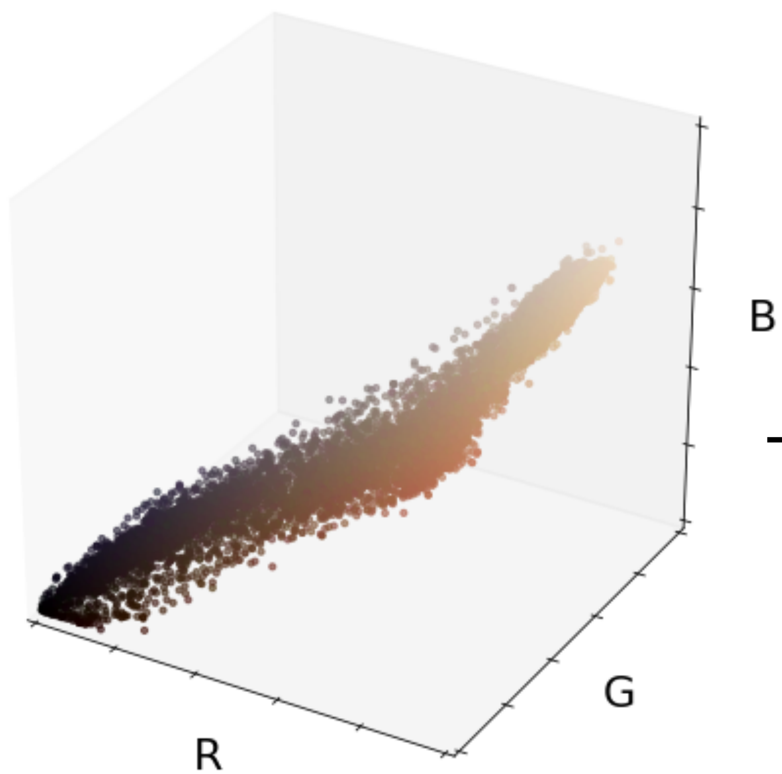
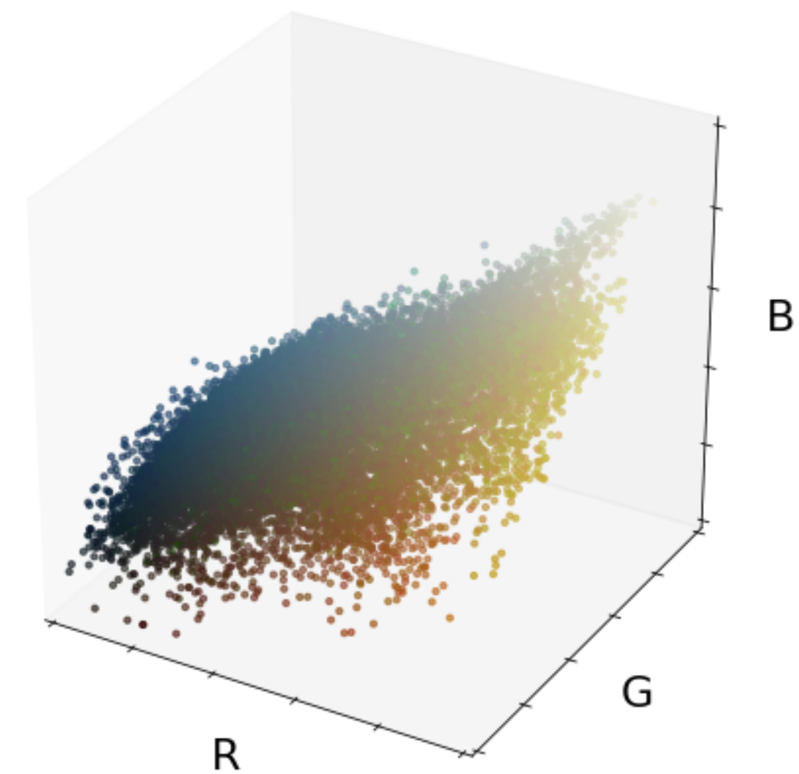


Matching

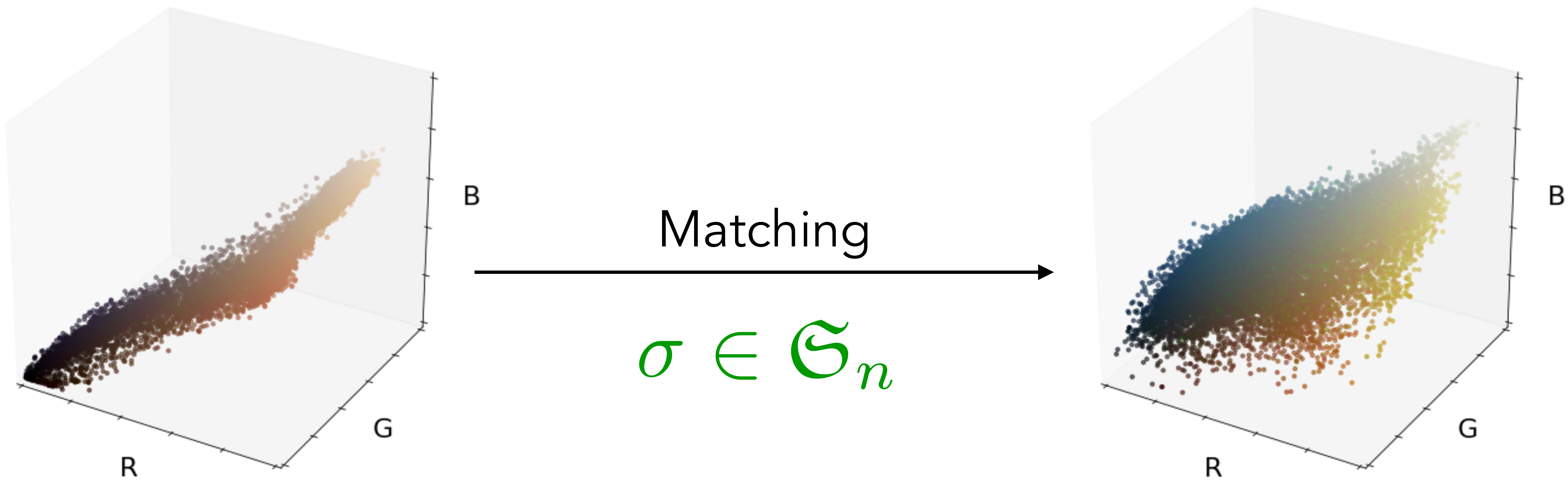
$\sigma \in \mathfrak{S}_n$



$x_1, \ldots, x_n$

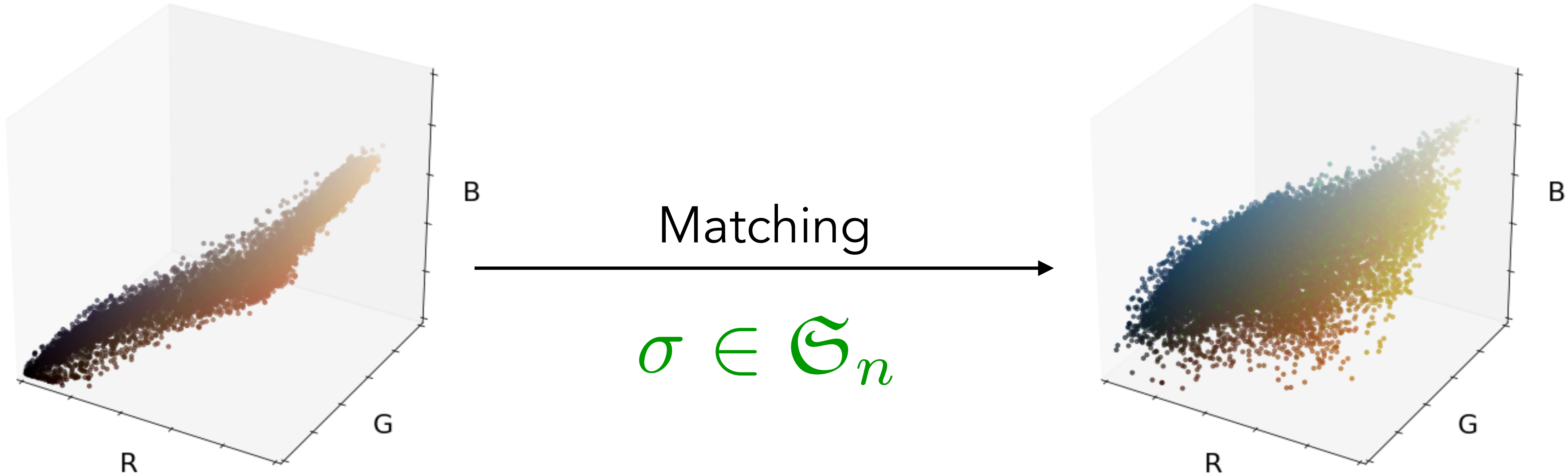
$y_1, \ldots, y_n$

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



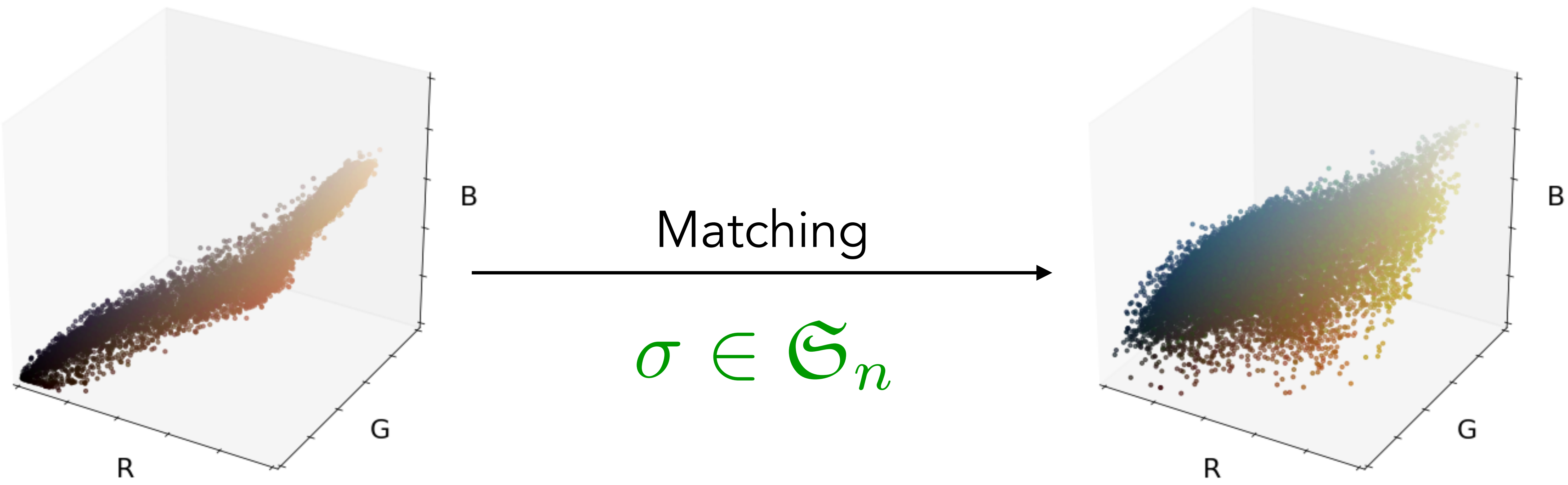
$x_1, \ldots, x_n$ $y_1, \ldots, y_n$

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



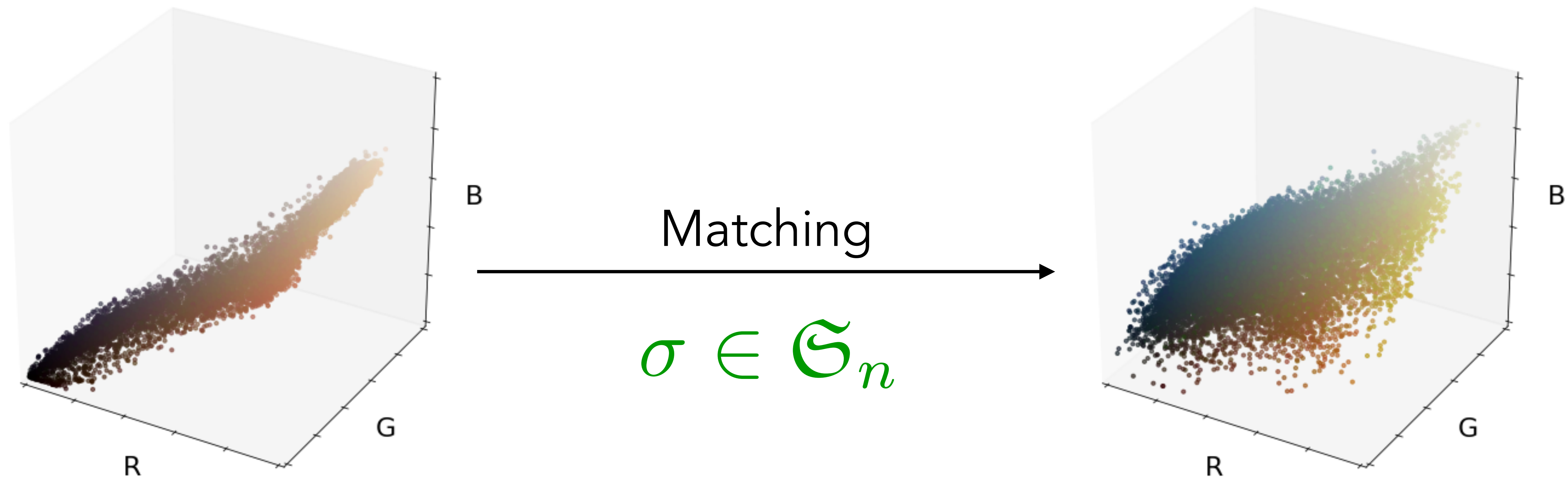
$x_1, \dots, x_n$ $\qquad$ $y_1, \dots, y_n$

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



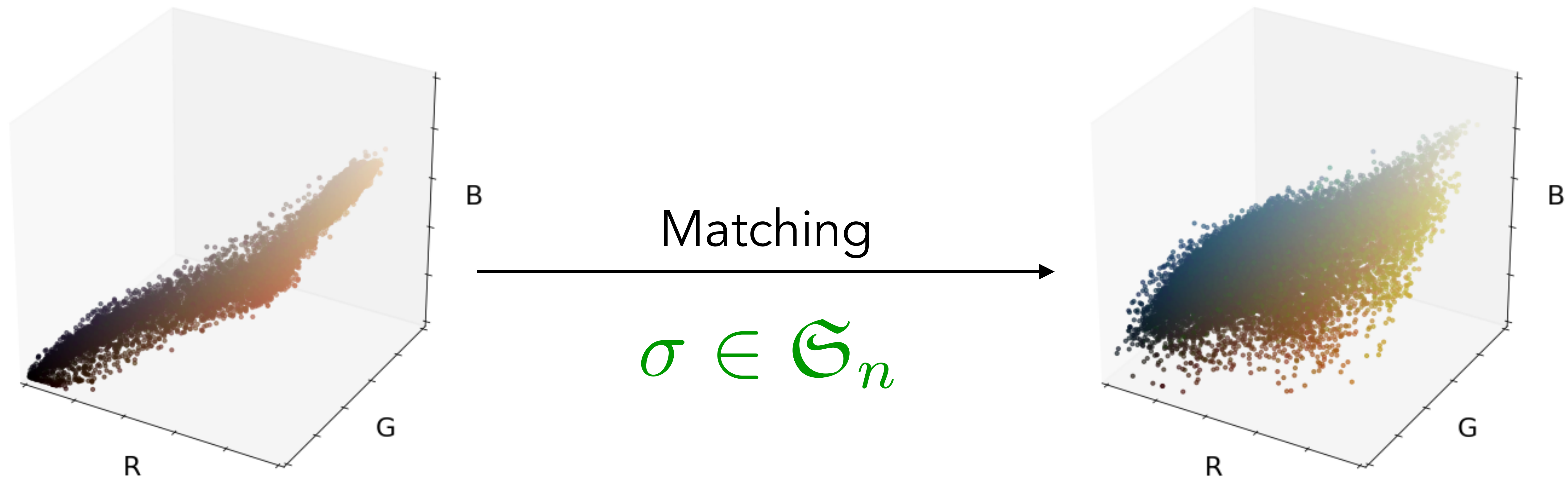
<u>Discrete Monge Problem (1781)</u>

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



Discrete Monge Problem (1781)

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



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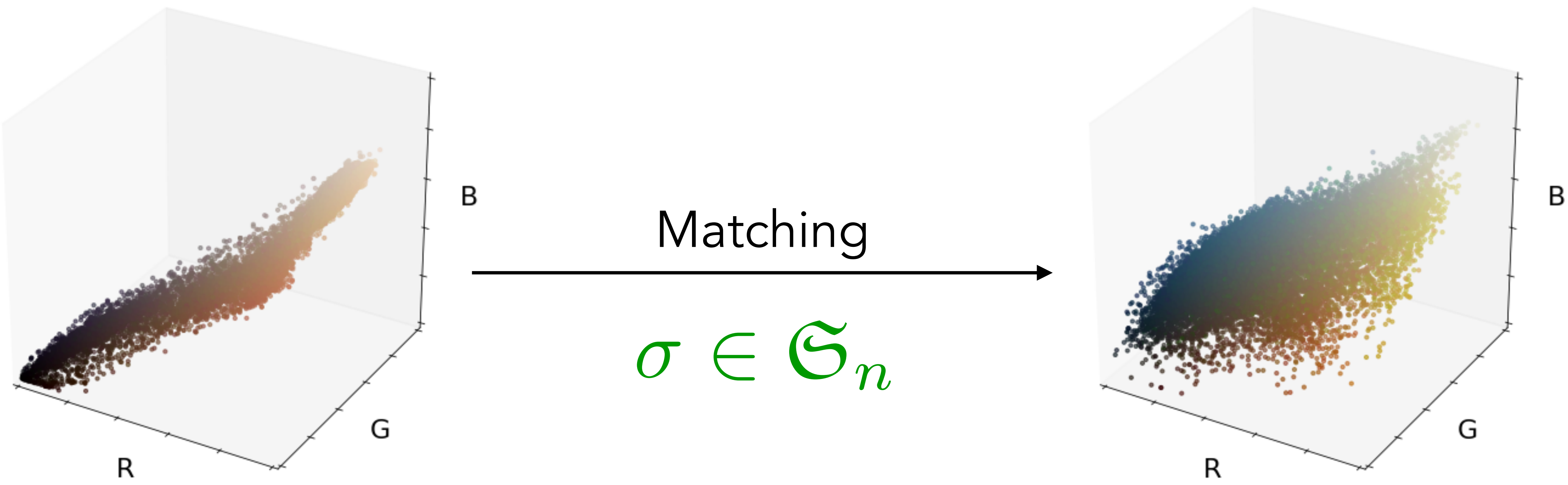

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(i) How to handle repeated points ?

(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 Kantorovich 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**:

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

In practice, one color should be mapped to exactly one color. In other words, we want to find a map

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

that is optimal in some sense.

Monge problem

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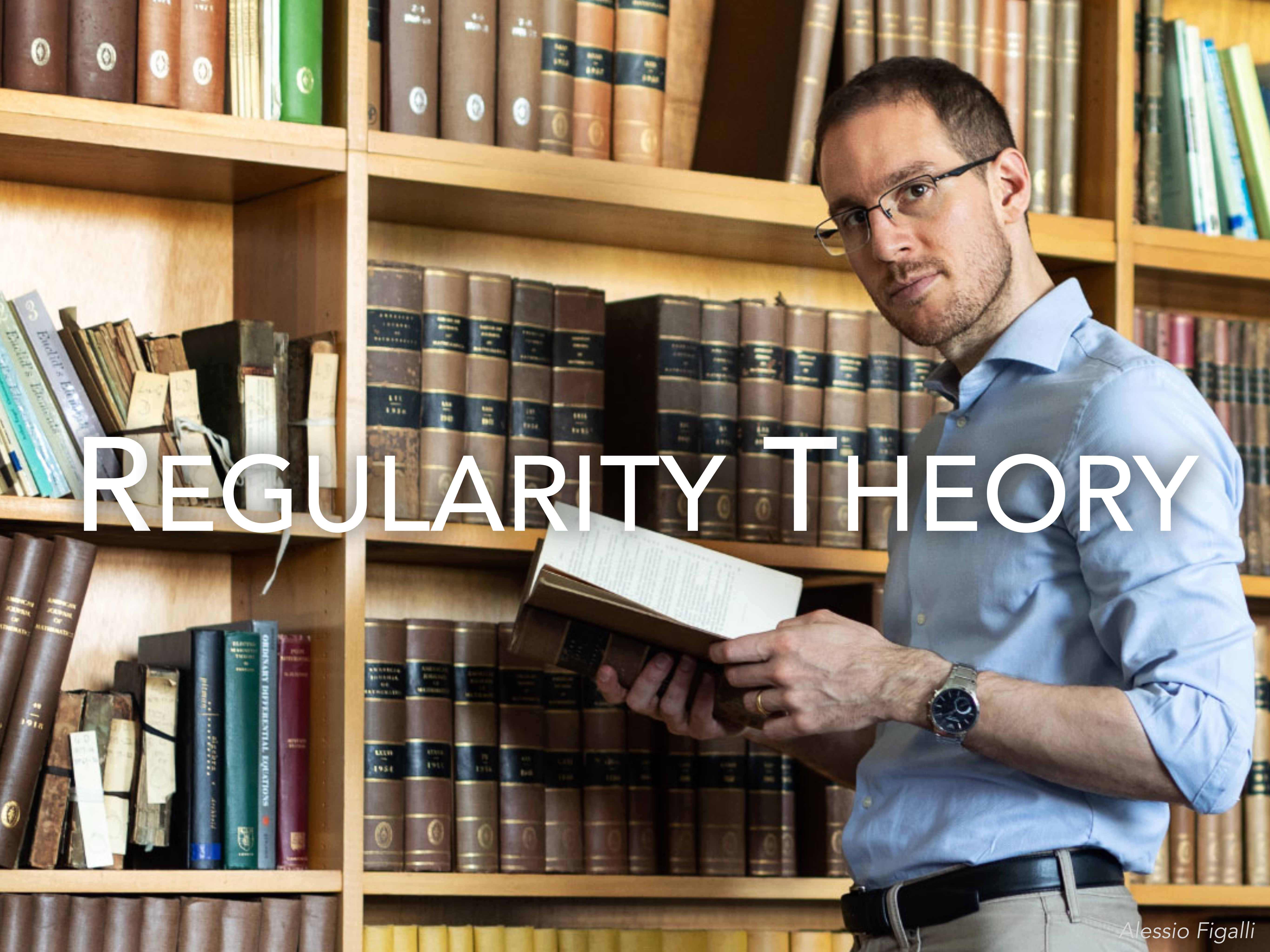
$$X \sim \mu \Longrightarrow T(X) \sim \nu$$


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 ?

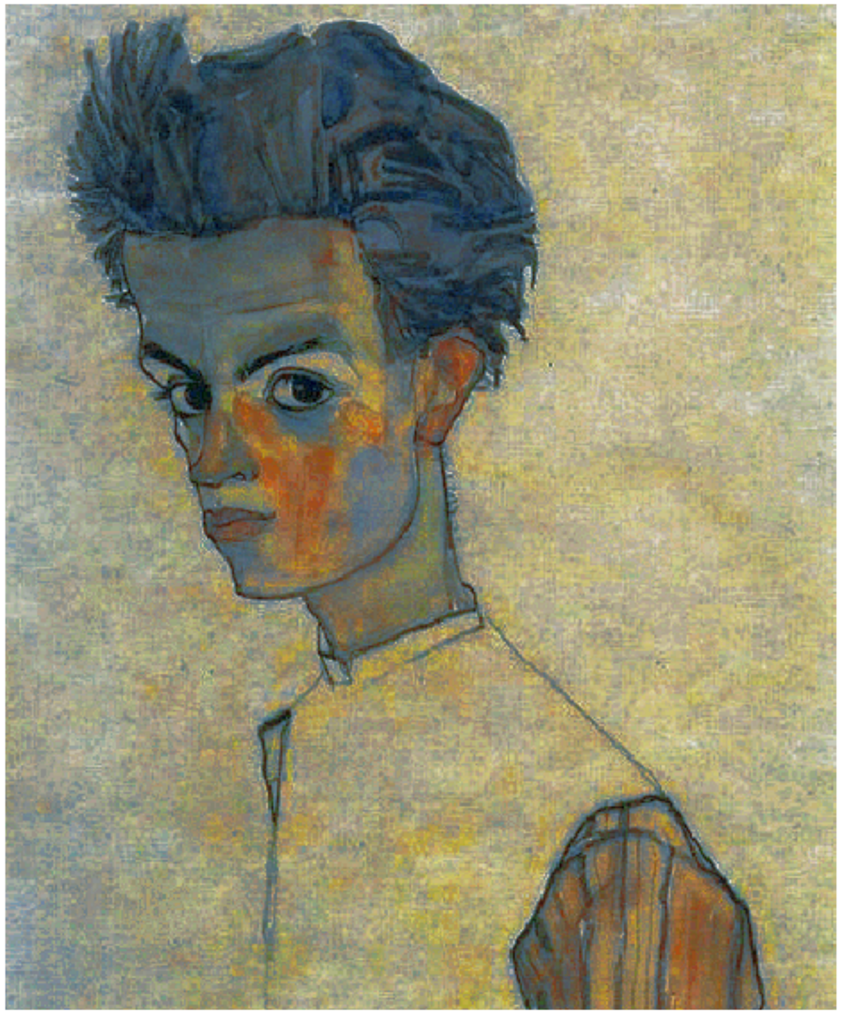
Let μ and ν be two probability measures over $\mathbb{R}^d$.

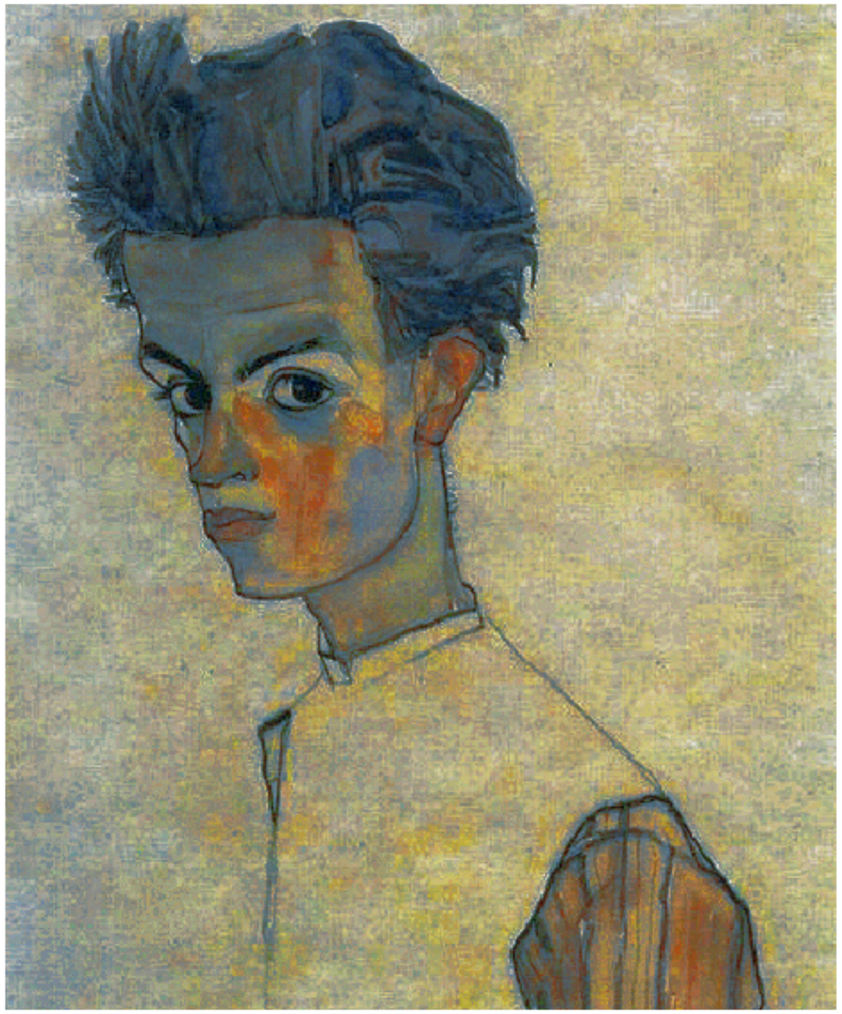
$$\inf_{T_\sharp \mu = \nu} \int \|x - T(x)\|^2 d\mu(x)$$

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.

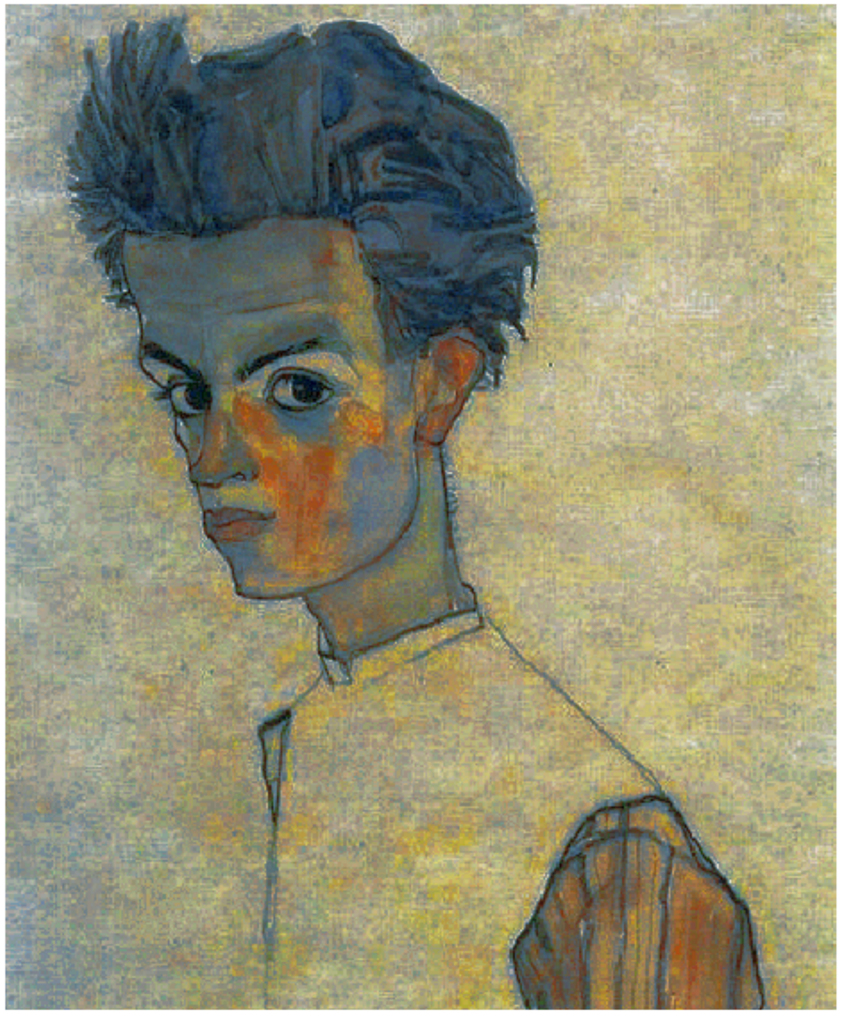
$$T = \nabla f$$

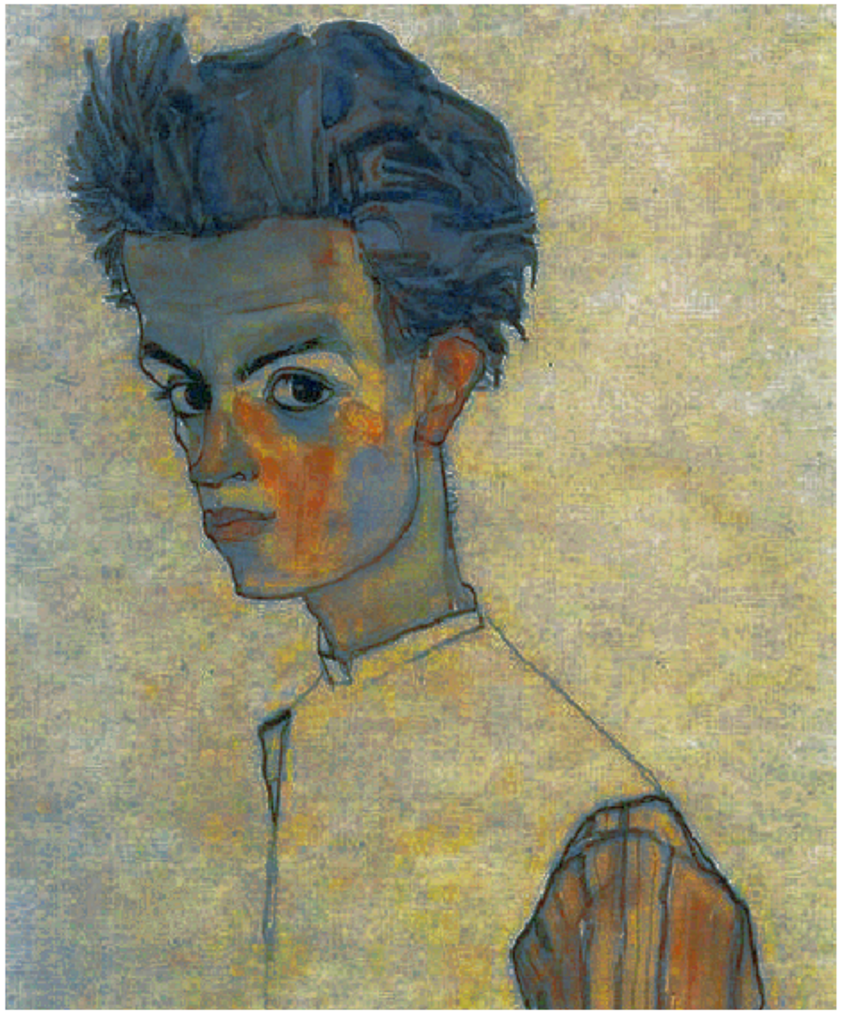



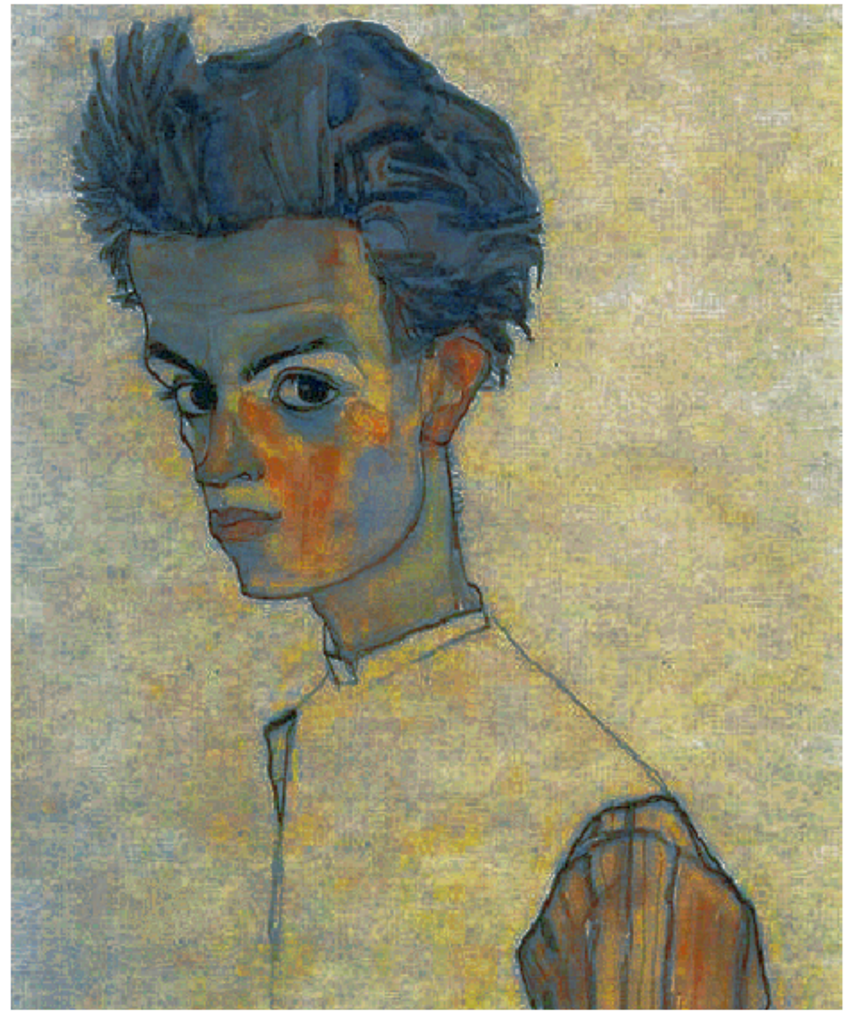
Instead of finding assumptions under which the optimal map exists and exhibits some regularity, we will enforce such existence/regularity directly in the OT problem.

Smooth and Strongly Convex Brenier Potentials



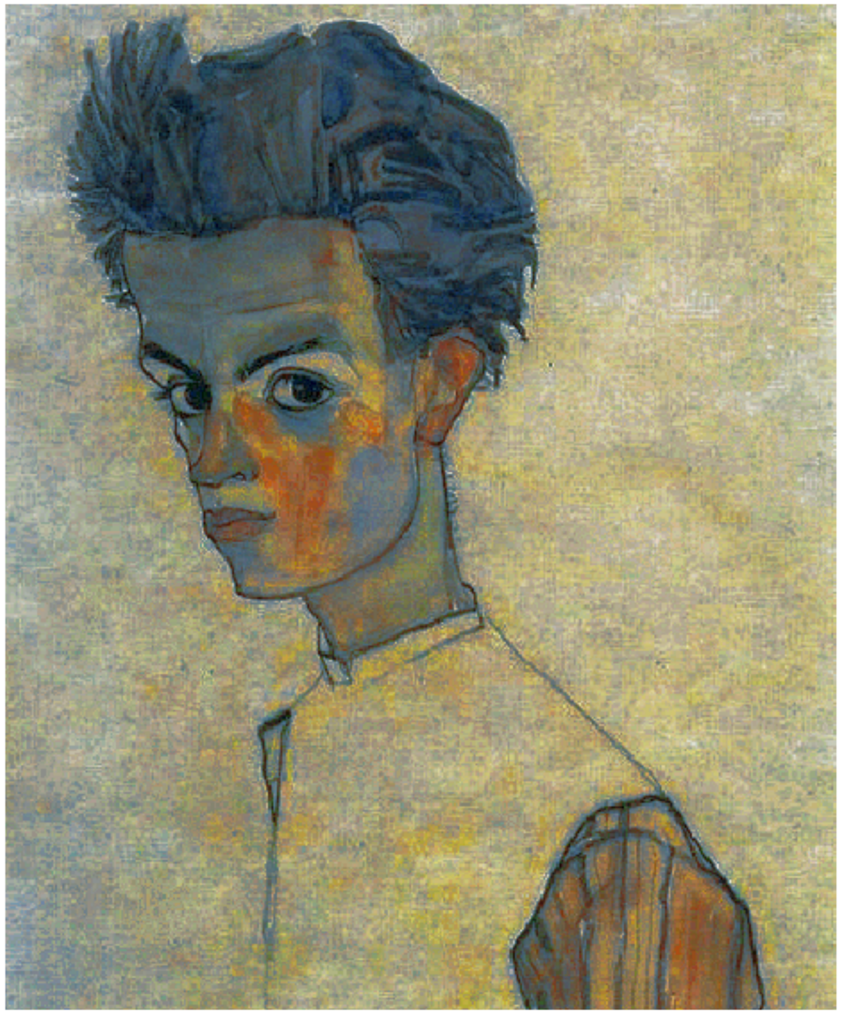
  

$$\ell\|x - y\| \leq \|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

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

We ask that $T = \nabla f$ is a bi-Lipschitz map



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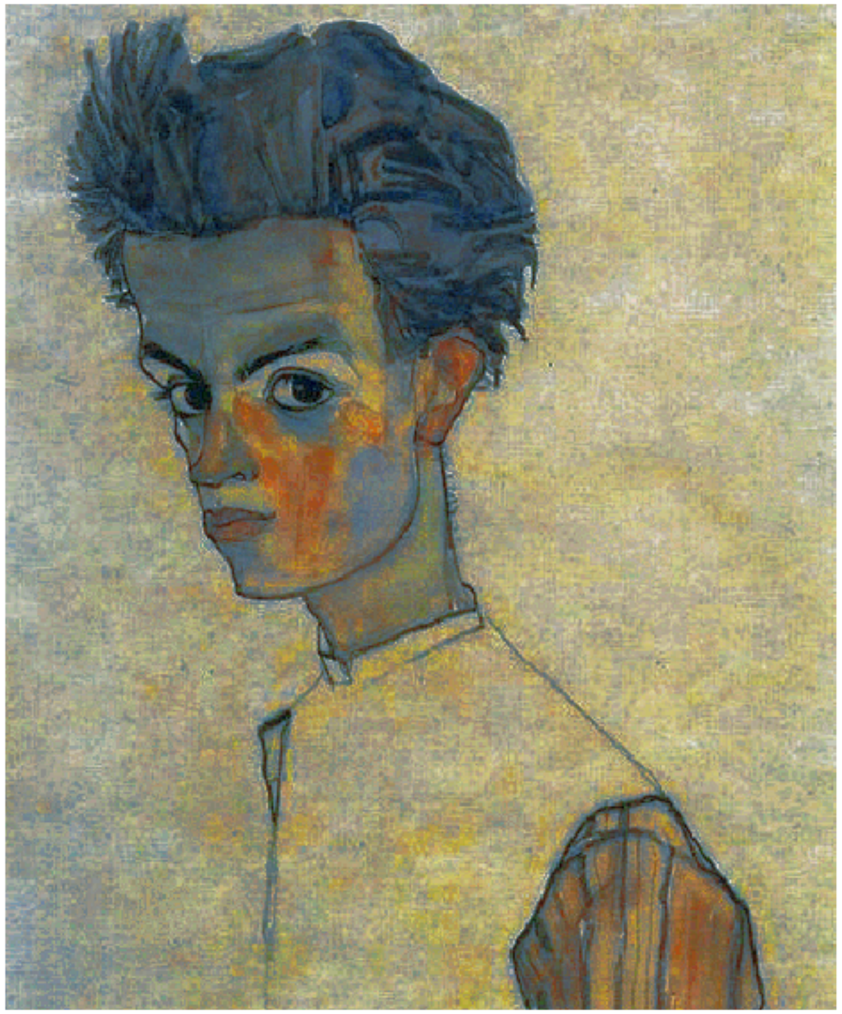
We ask that f is **smooth** and **strongly convex**

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

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

But there may not even such a regular f that is admissible for the Monge problem, *i.e.* such that $(\nabla f)_{\sharp}\mu = \nu$.

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

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<u>Smooth and Strong Convex Brenier Potentials</u>

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Finite dimensional double minimization

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

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Finite dimensional double minimization

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

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Solved by alternating minimization on f and Wasserstein computation

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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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This defines an estimator $\nabla f^\star$ of the optimal transport map sending μ to ν

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

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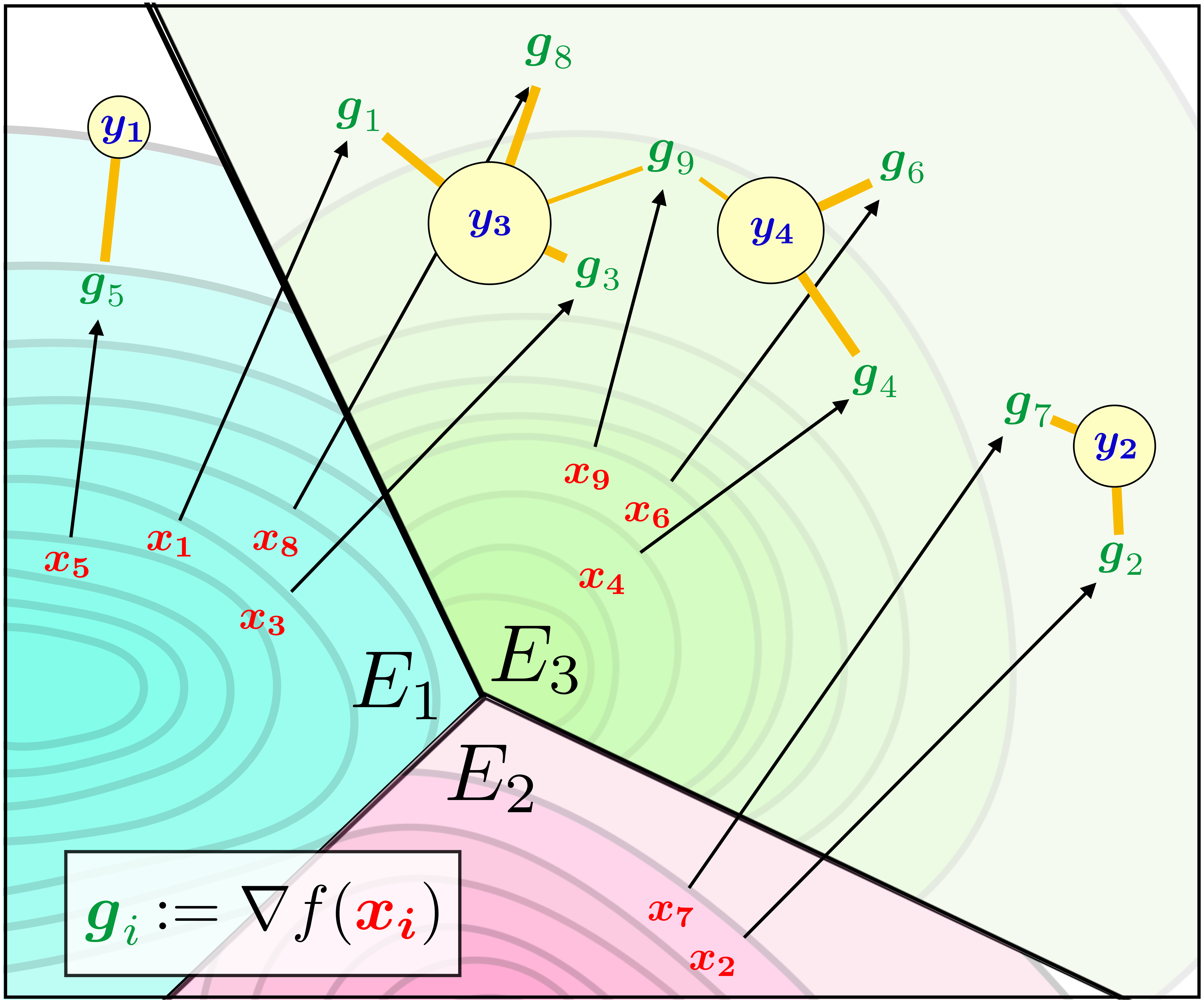
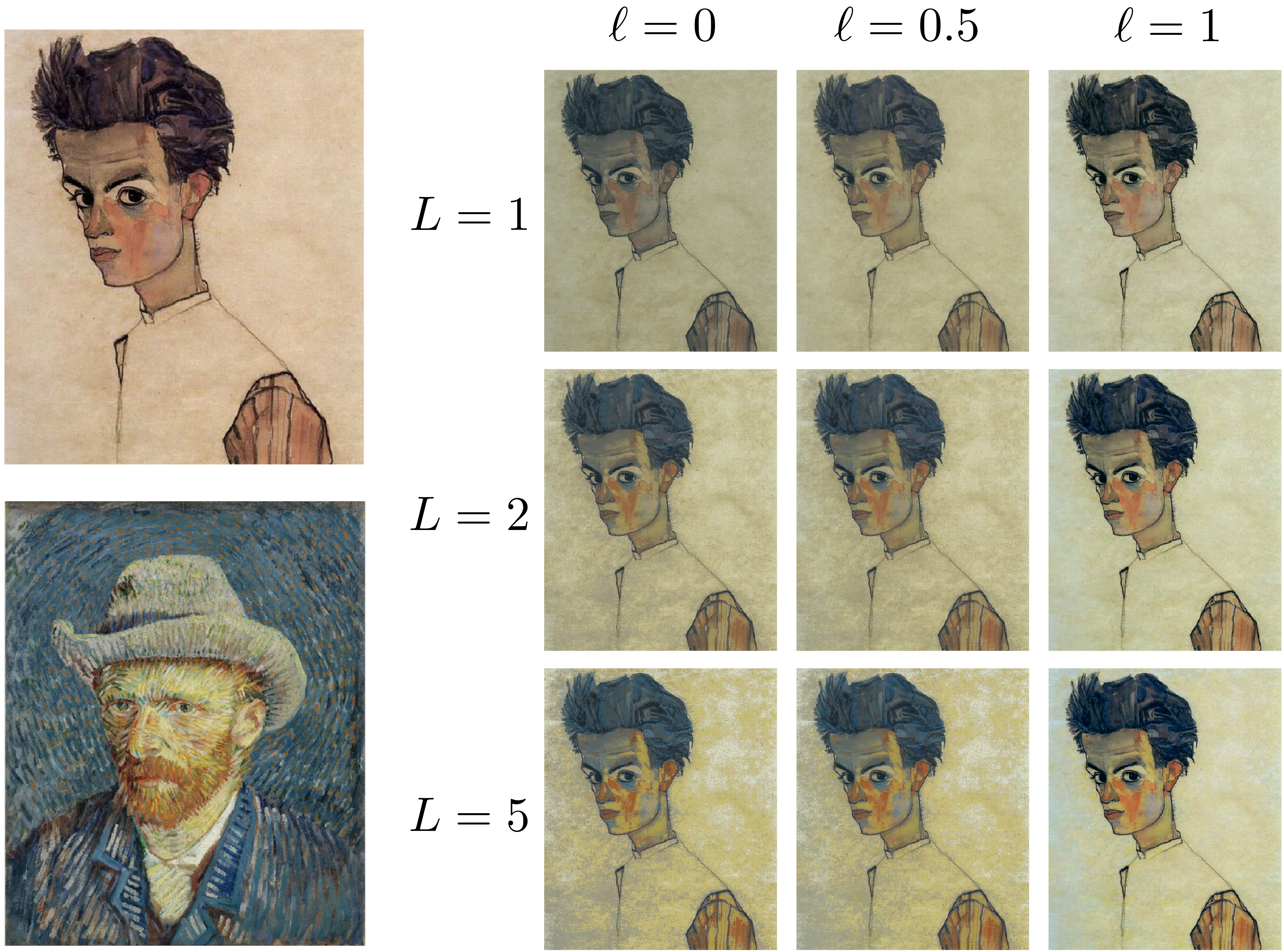
We define the *SSNB estimator* as a plug-in:

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

Regularity "by part"




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