Regularizing Optimal Transport Using Regularity Theory

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Based on a joint work with ***Alexandre d'Aspremont*** *and* ***Marco Cuturi***

ENSAE

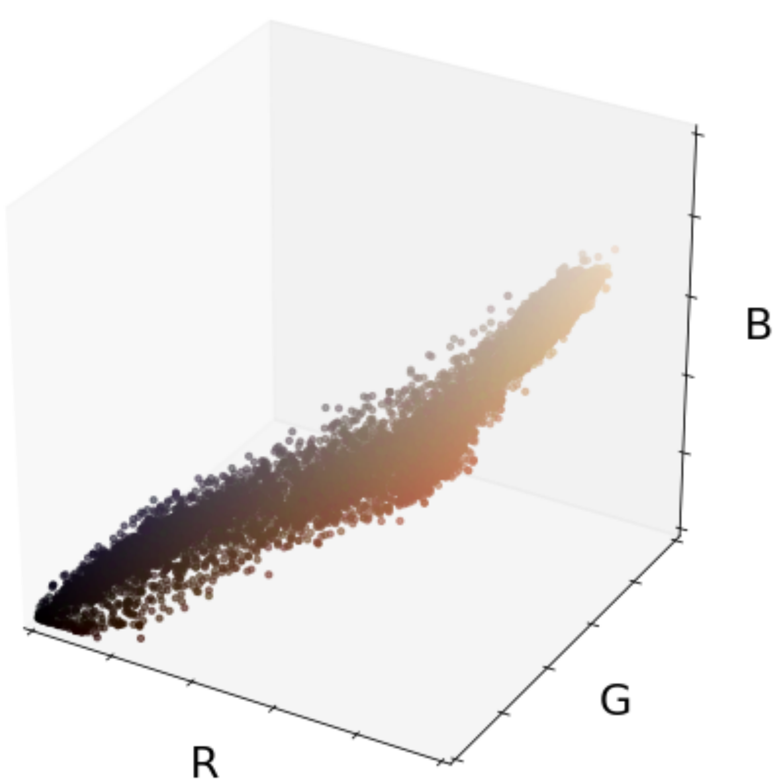
IP PARIS

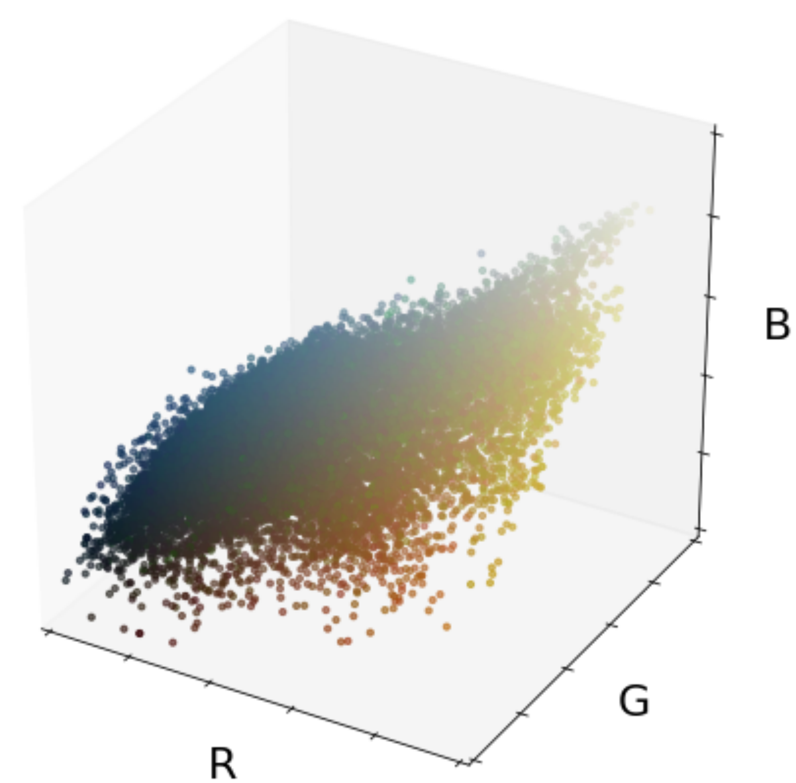
INTRODUCTION

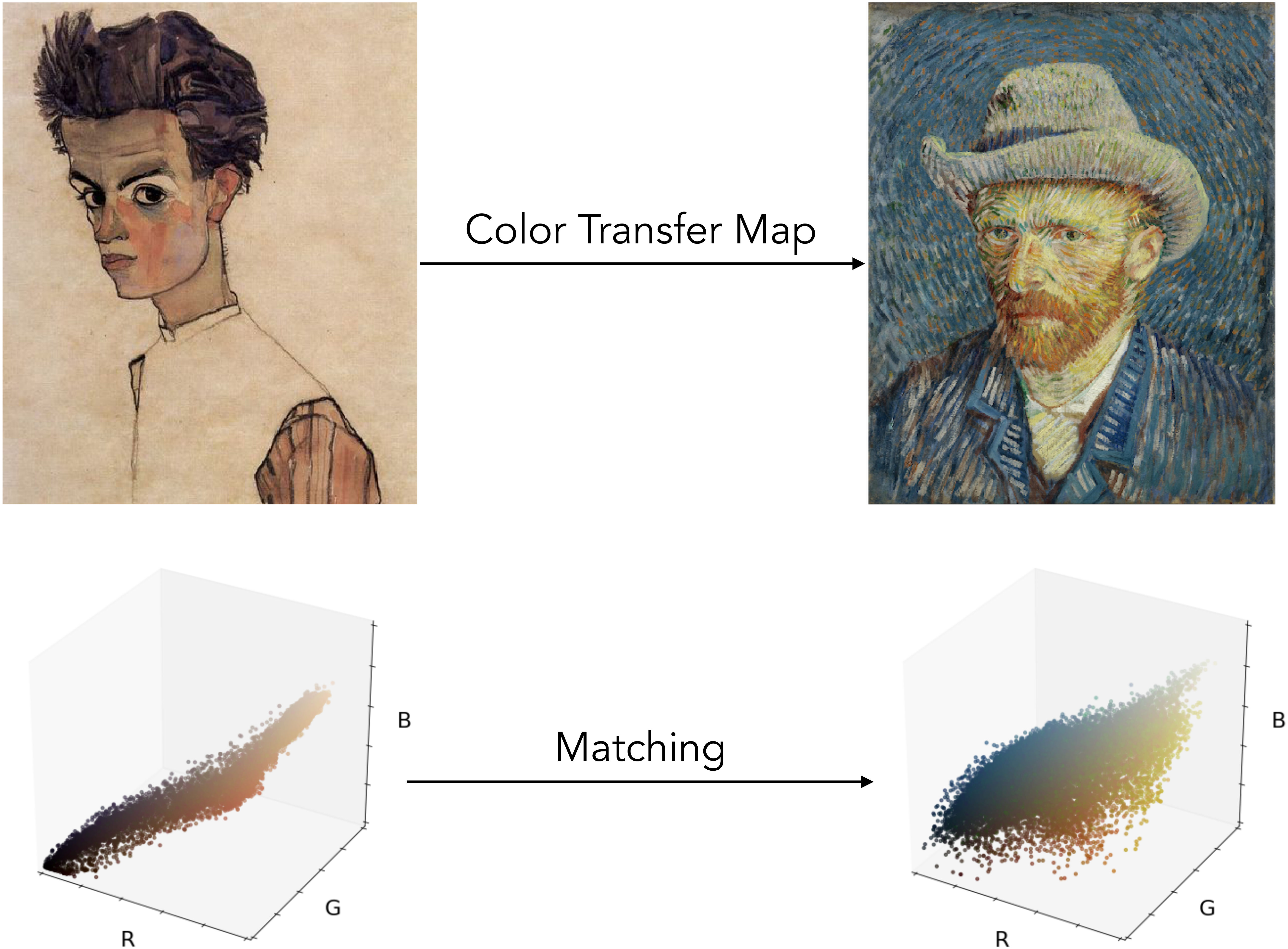
Gaspard Monge

Color Transfer Map

Color Transfer Map






Color Transfer Map
Matching
B
G
R
B
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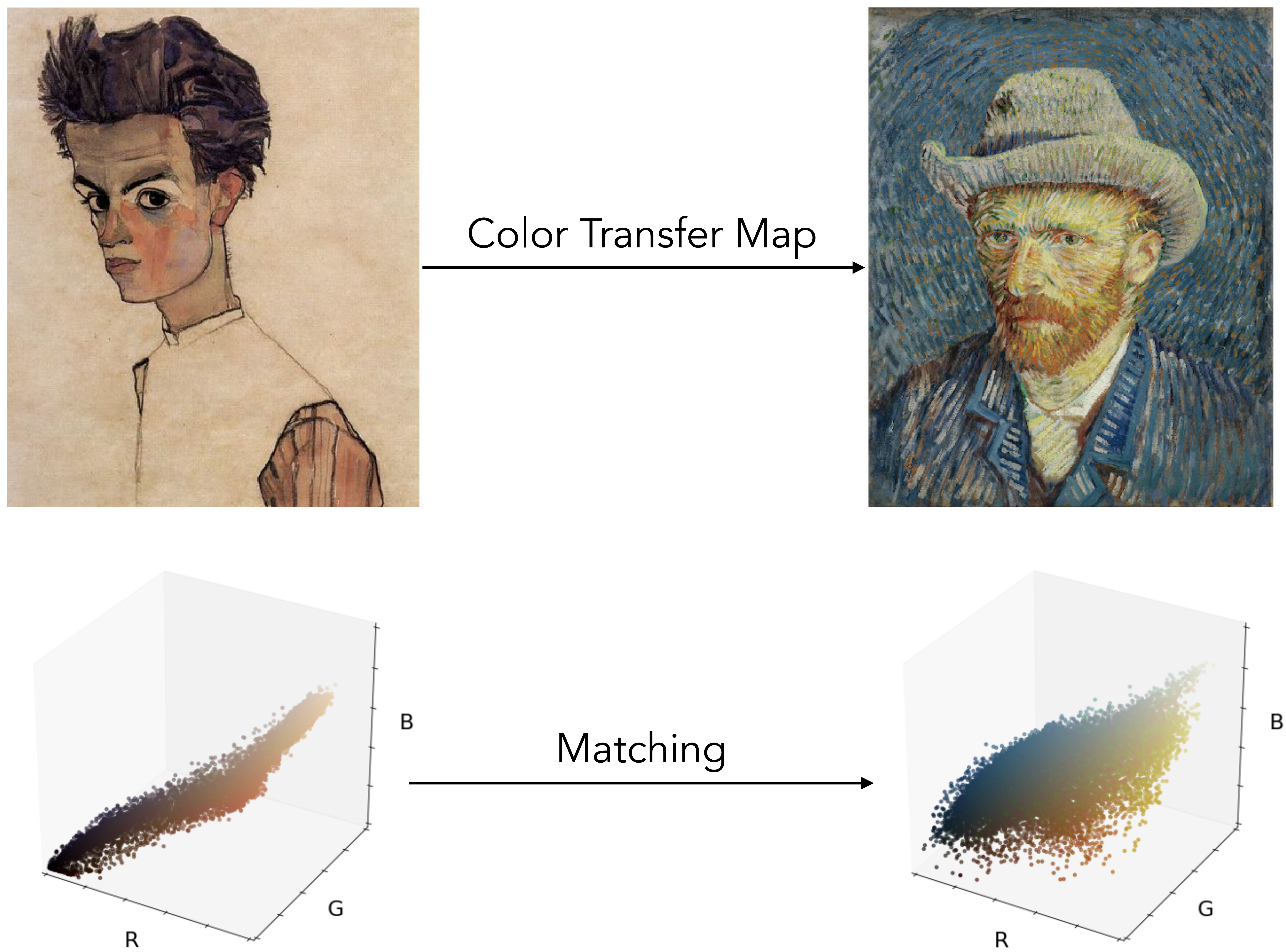
R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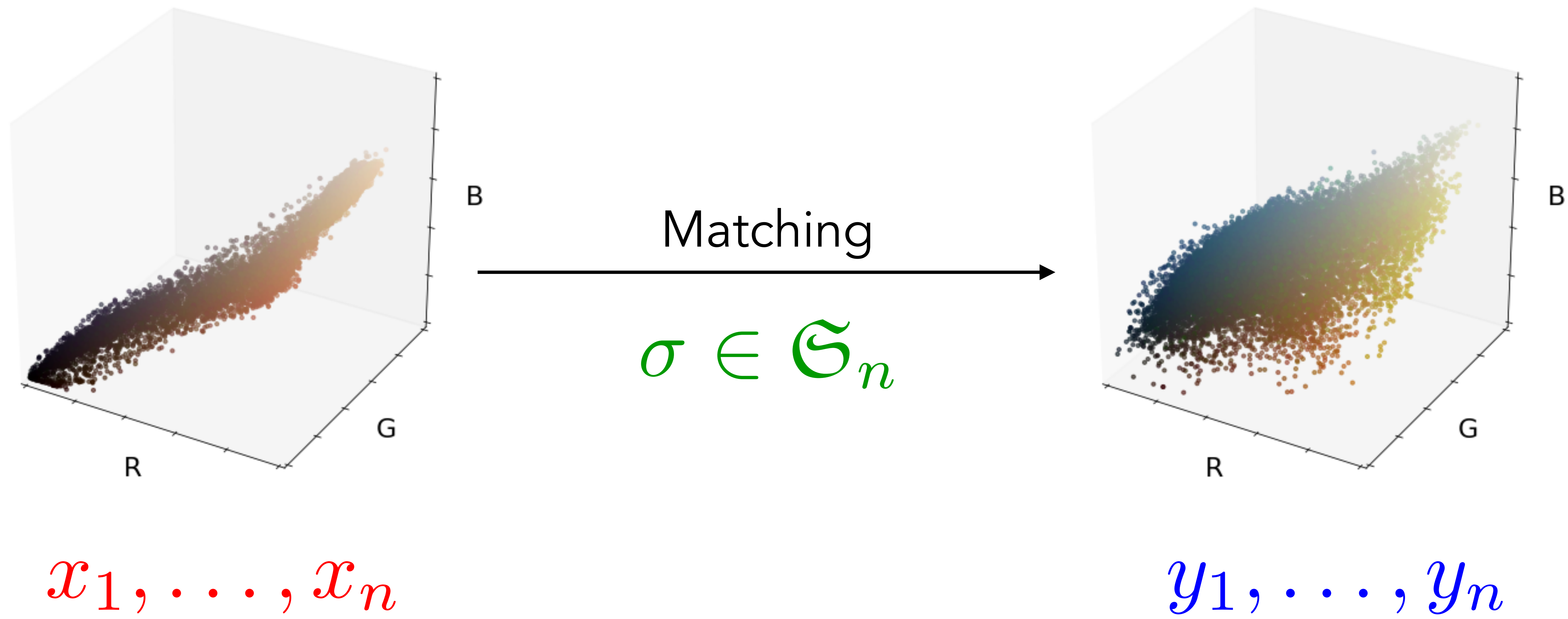
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$\sigma \in \mathfrak{S}_n$
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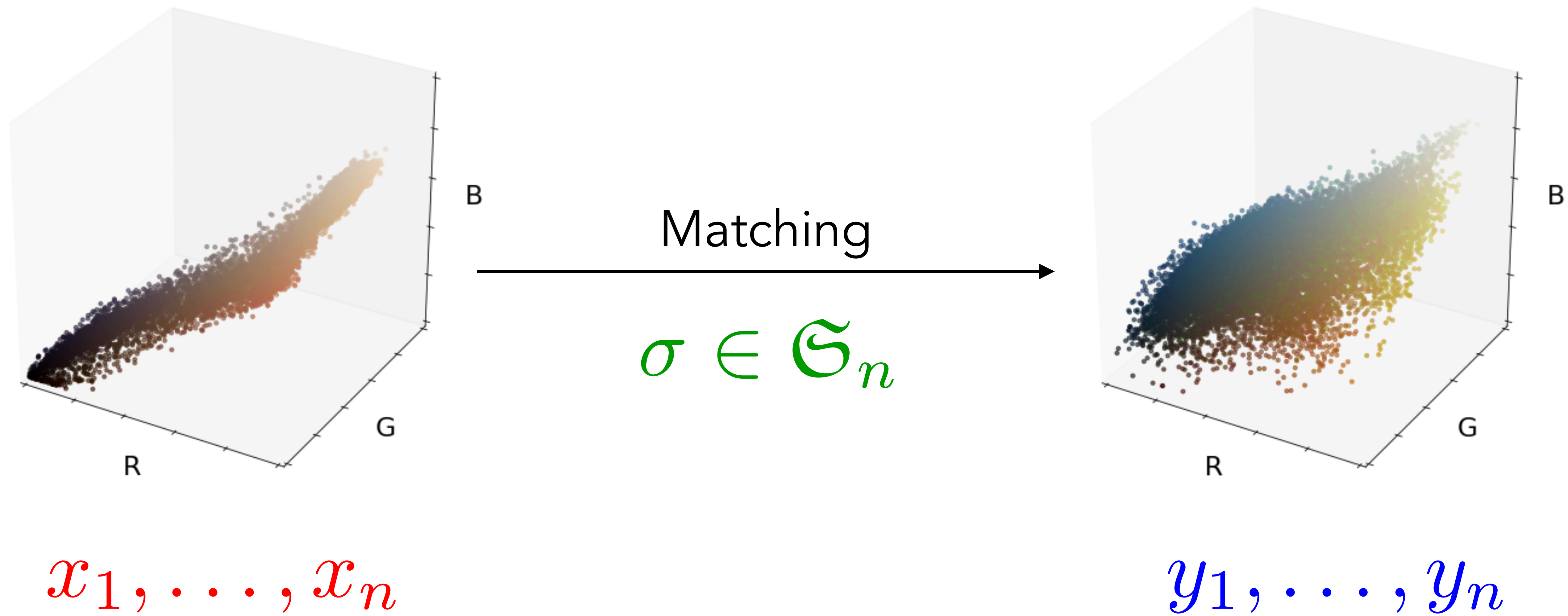
$y_1, \ldots, y_n$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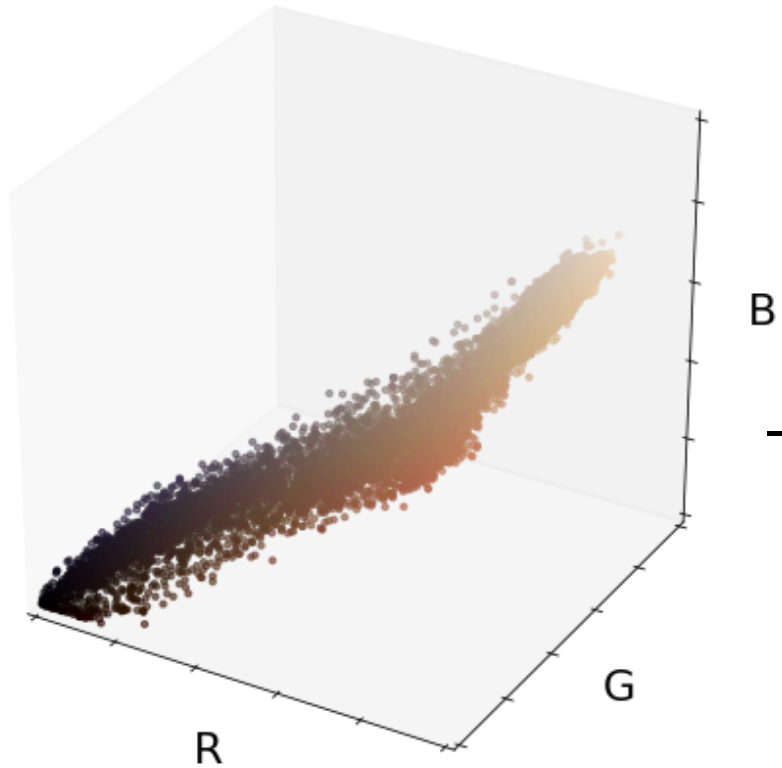

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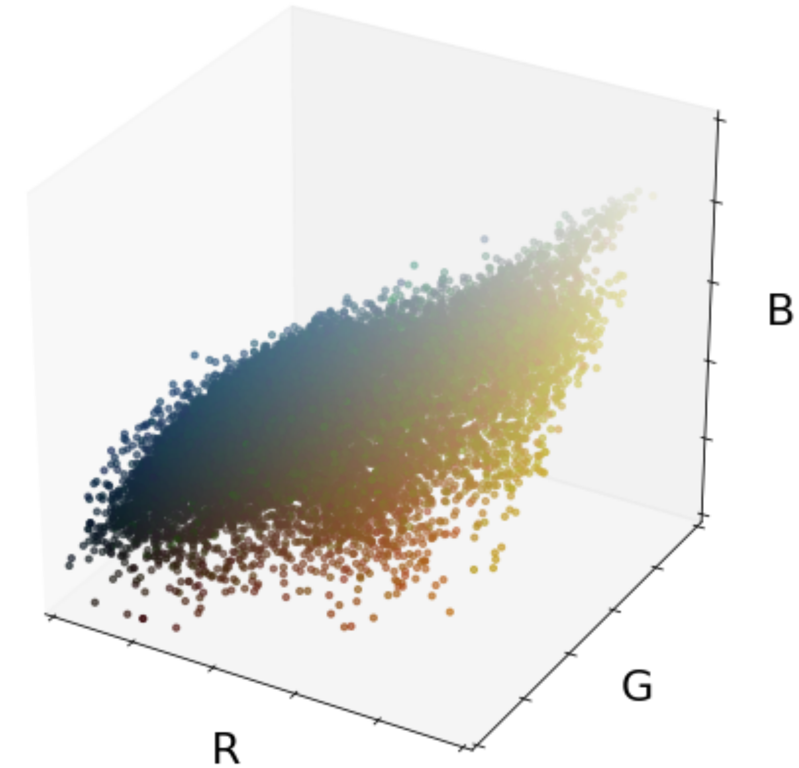
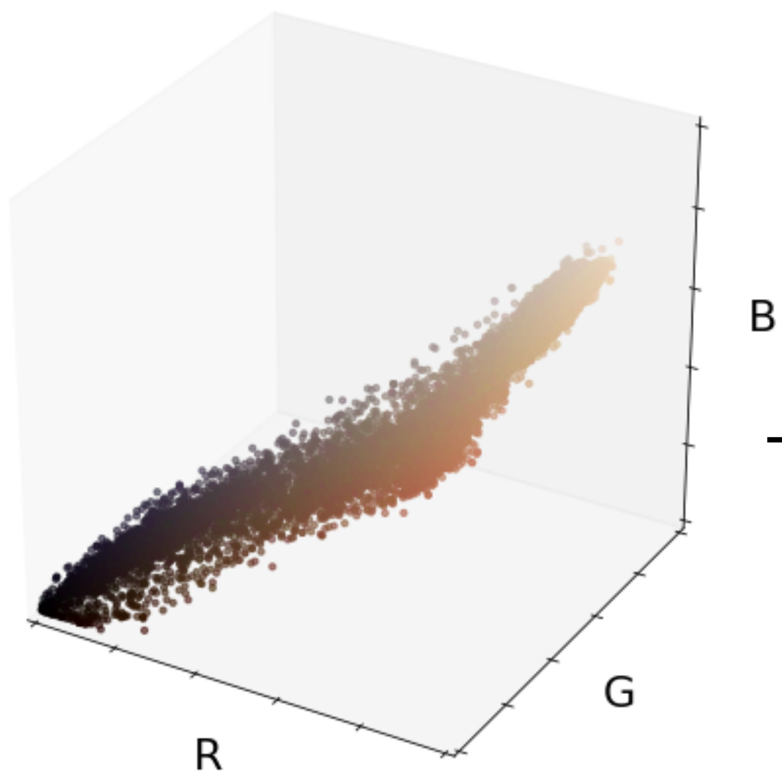


$x_1, \dots, x_n$

$y_1, \dots, y_n$

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



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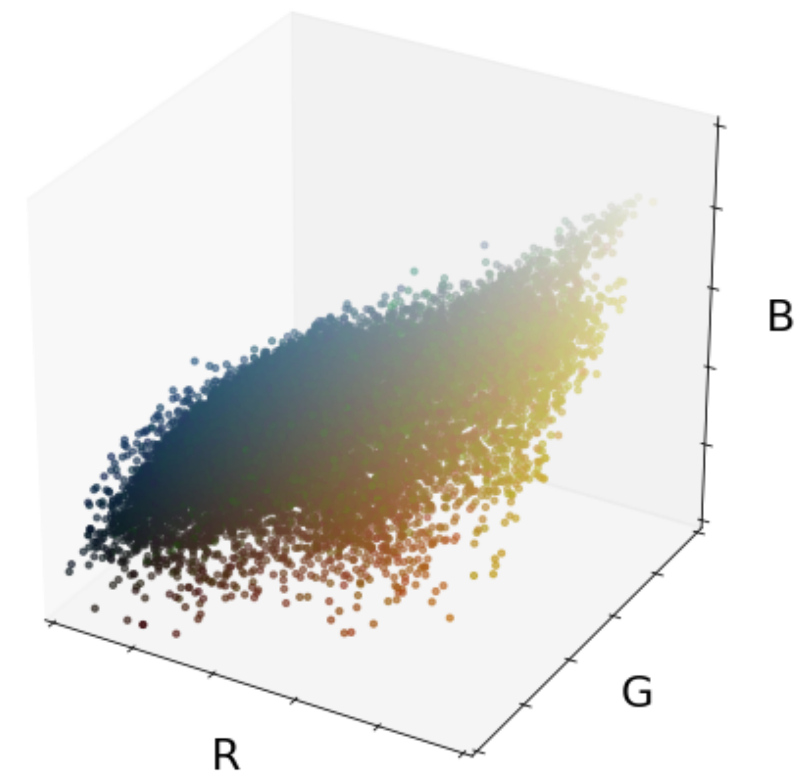

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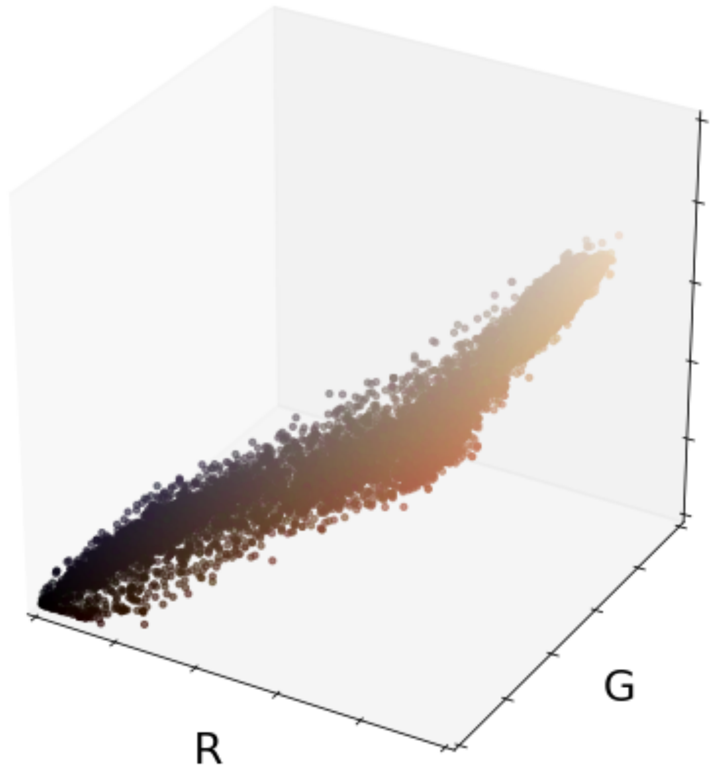

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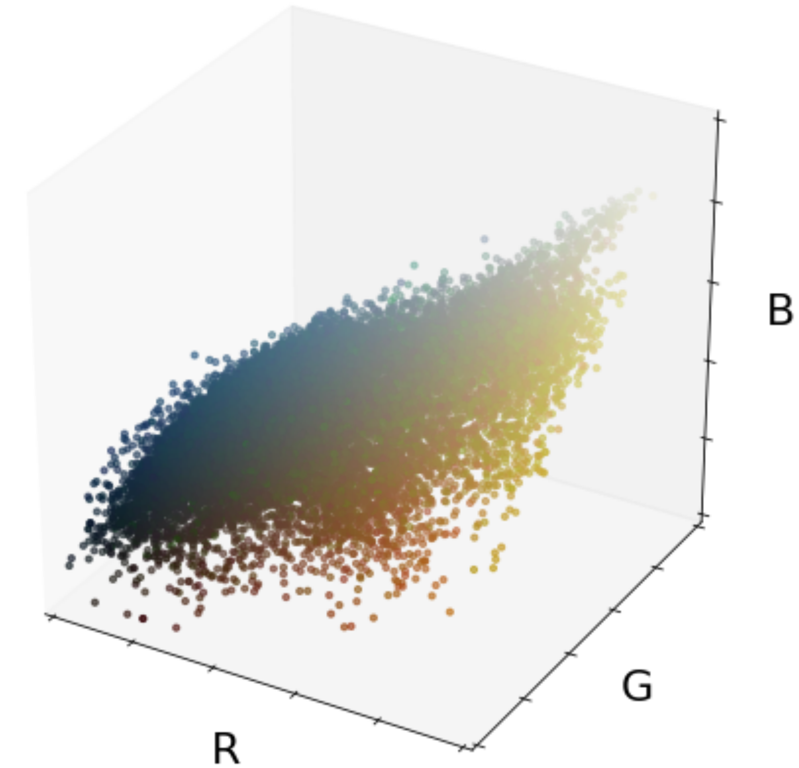

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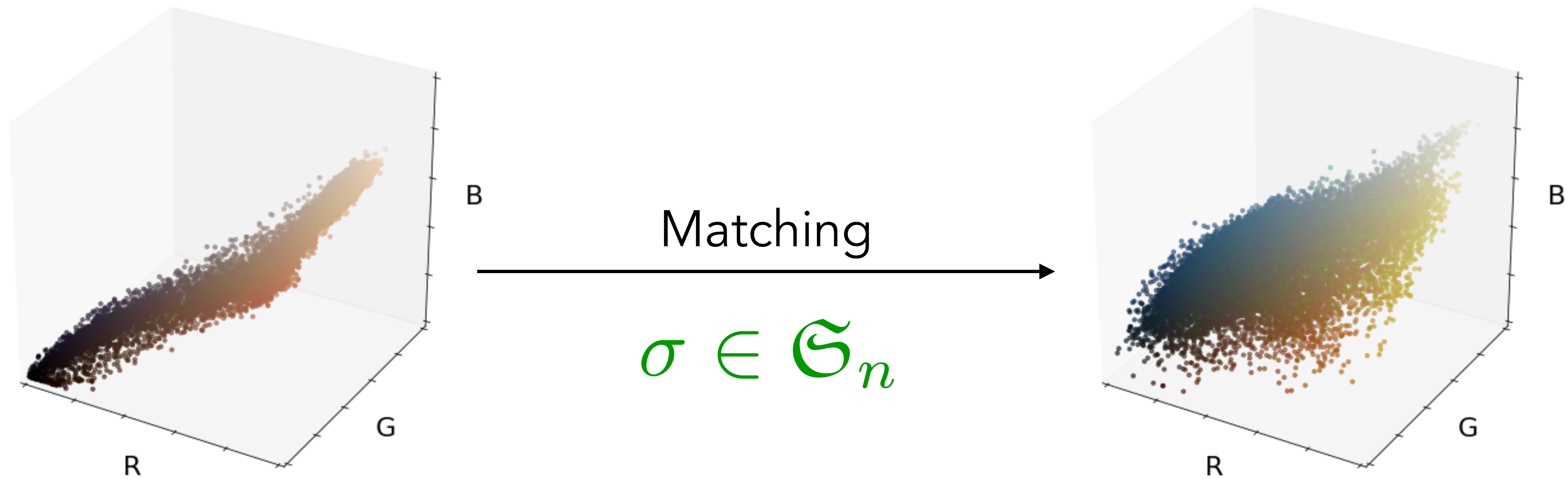

Discrete Monge Problem (1781)

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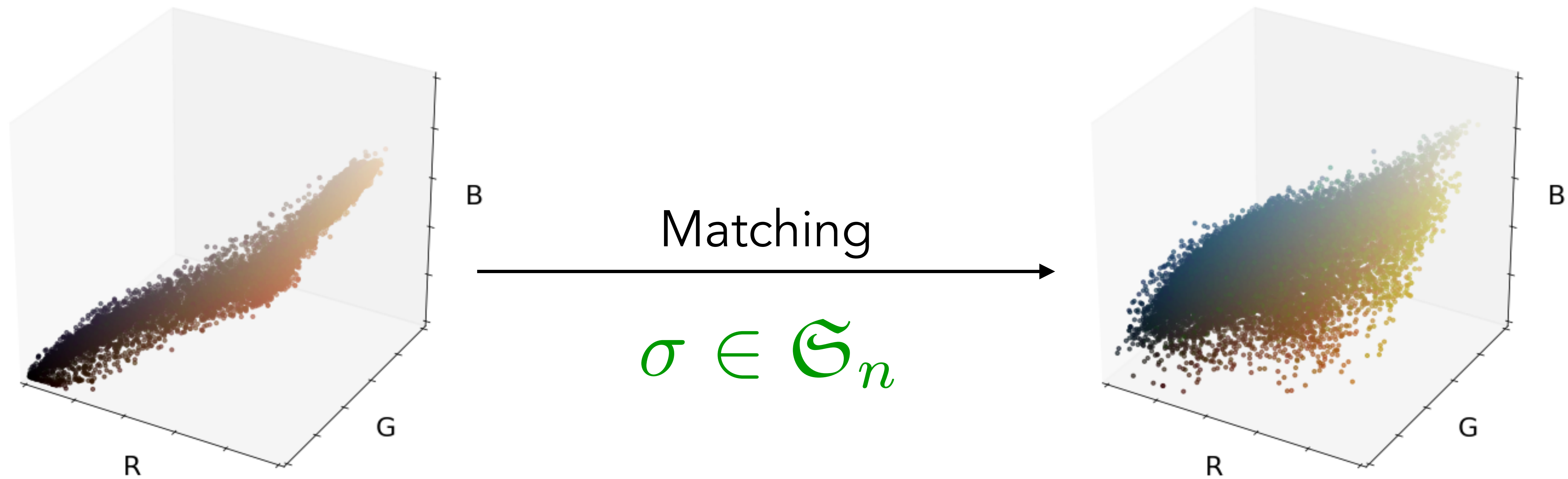

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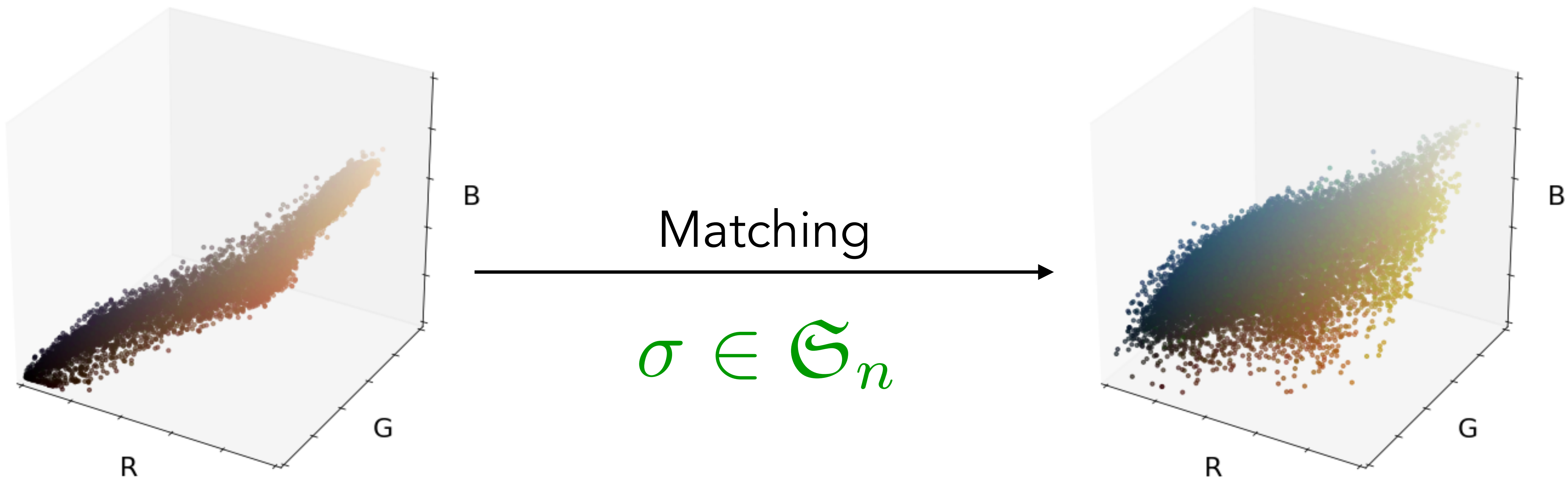

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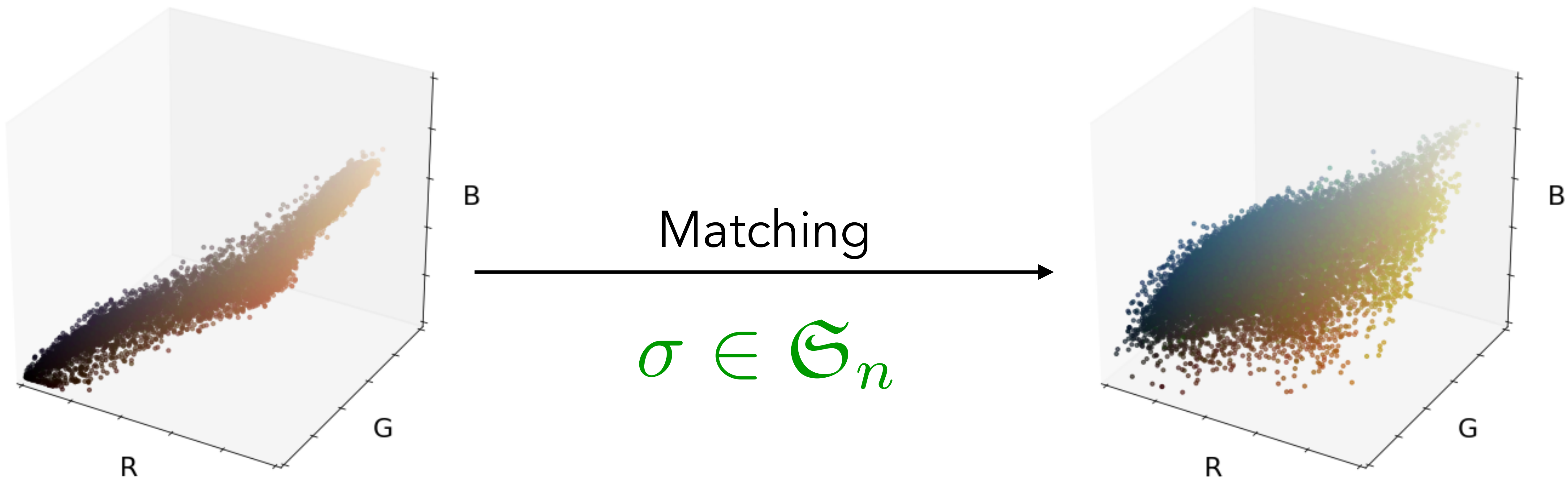

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(i) How to handle repeated points ?

(ii) How to handle different numbers of points ?

(iii) How to compute this combinatorial problem ?

OPTIMAL TRANSPORT

Leonid Kantorovich

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

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

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

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

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

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

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In statistics, we can interpret the data points as iid samples from two densities / probability measures:

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

We can define the Monge problem and the Kantorovich problem in the general case of two probability measures.

Monge and Kantorovich problems

Monge and Kantorovich problems

Kantorovich

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

$$\min_{P \in \mathfrak{U}(\mu,\nu)} \iint \|x - y\|^2 \, dP(x, y)$$

Monge and Kantorovich problems

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Monge

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

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

Given samples

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

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can we reconstruct the Wasserstein distance between the generating measures ?

A natural estimator is the Wasserstein between the empirical measures:

$$|W_2(\mu, \nu) - W_2(\hat{\mu}_n, \hat{\nu}_n)| \sim \left(\frac{1}{n}\right)^{1/d}$$

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Curse of Dimensionality

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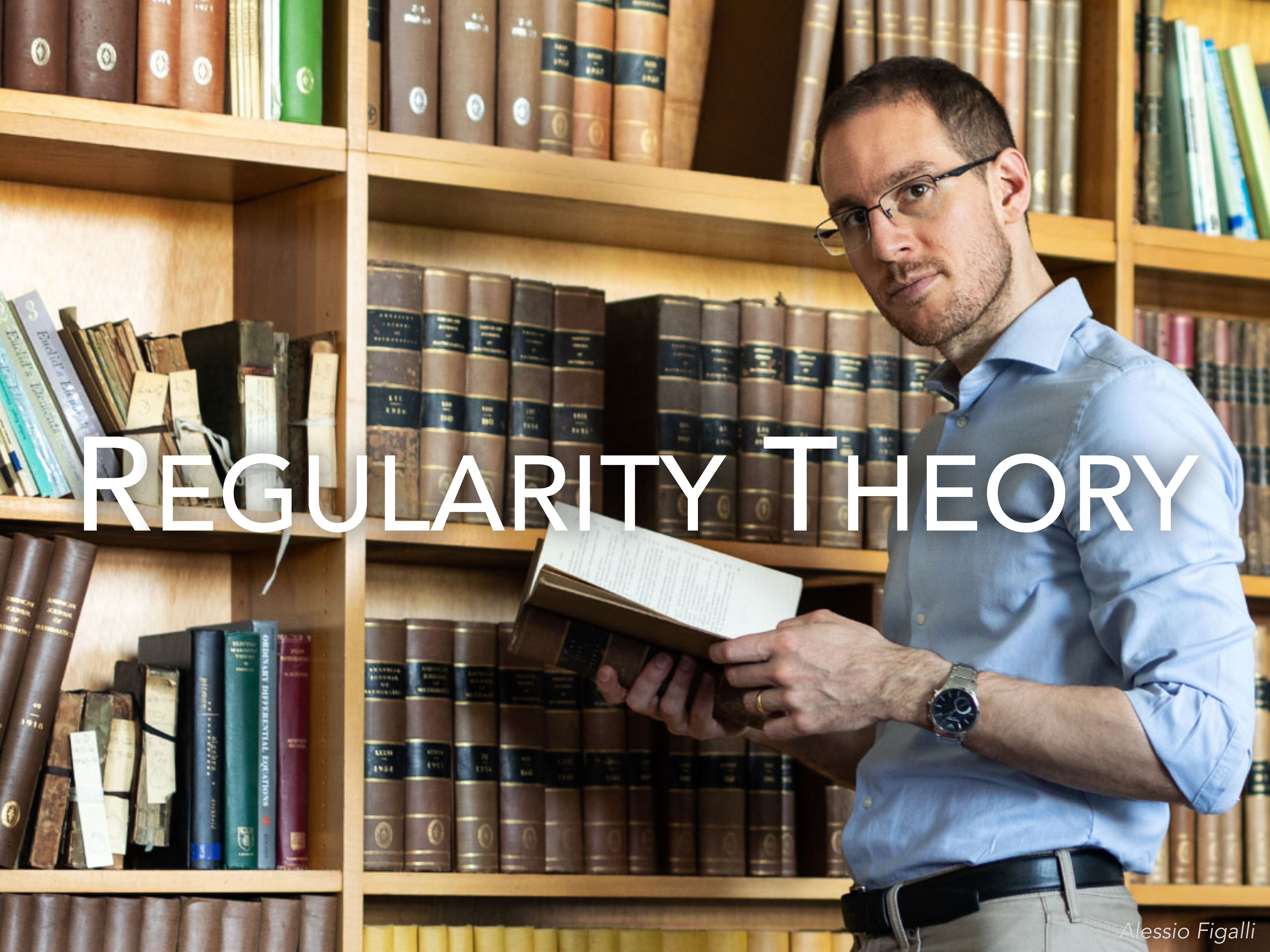
REGULARITY THEORY
Alessio Figalli

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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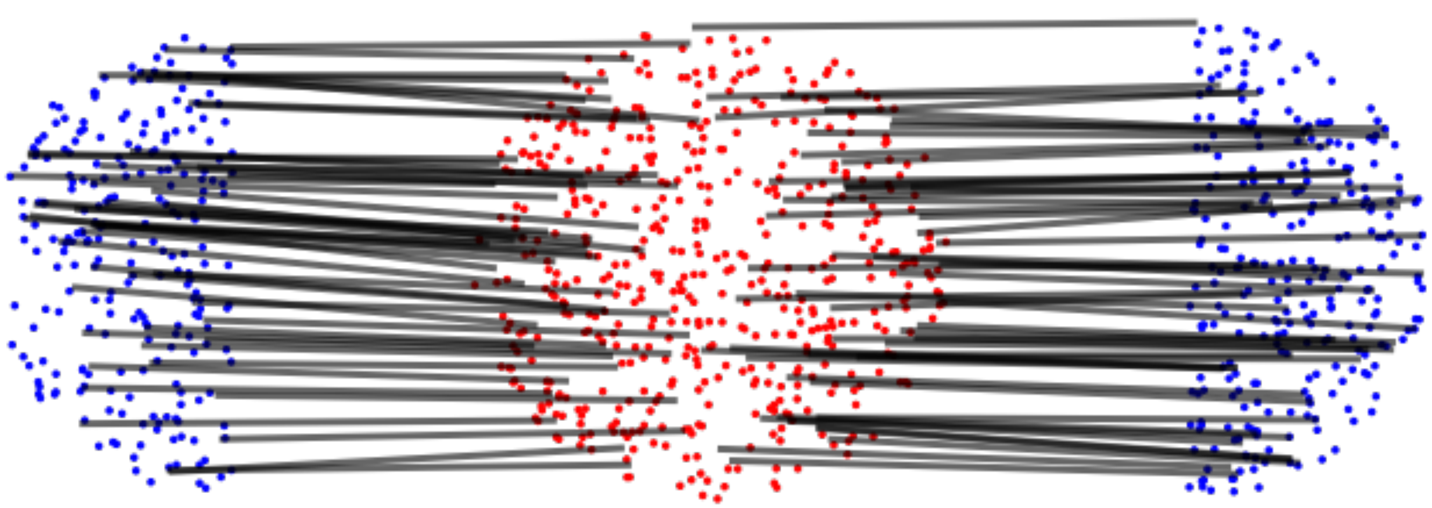
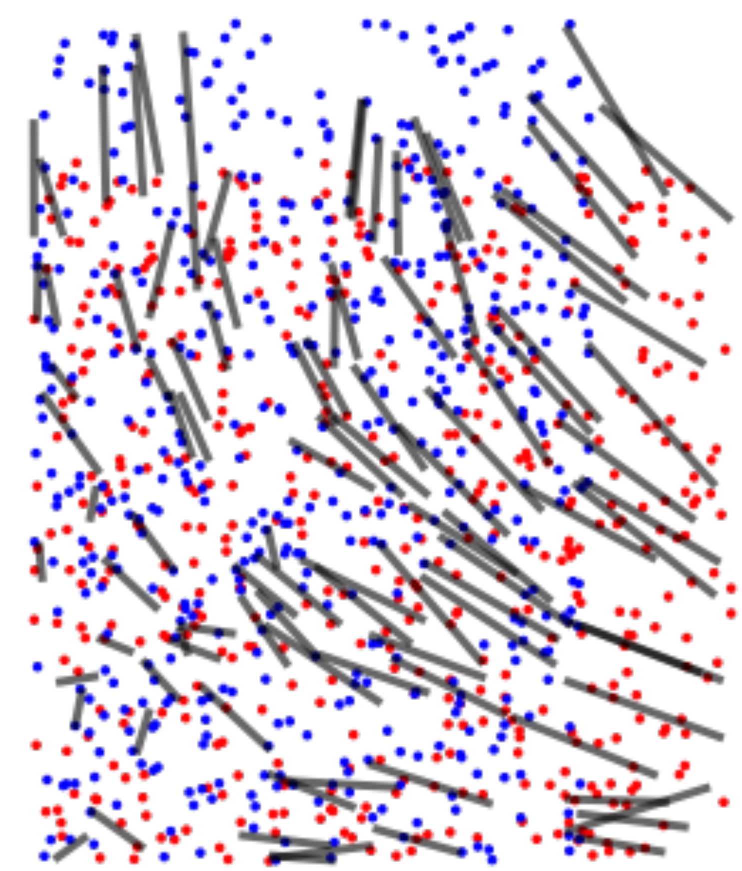
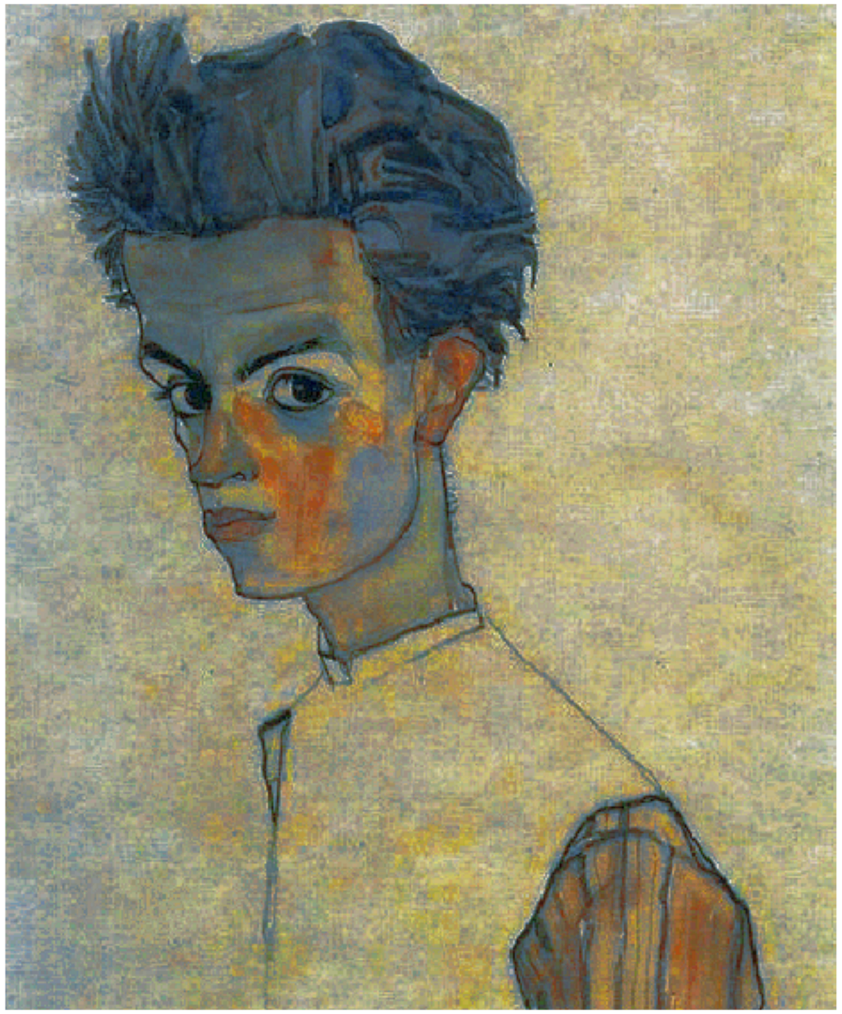
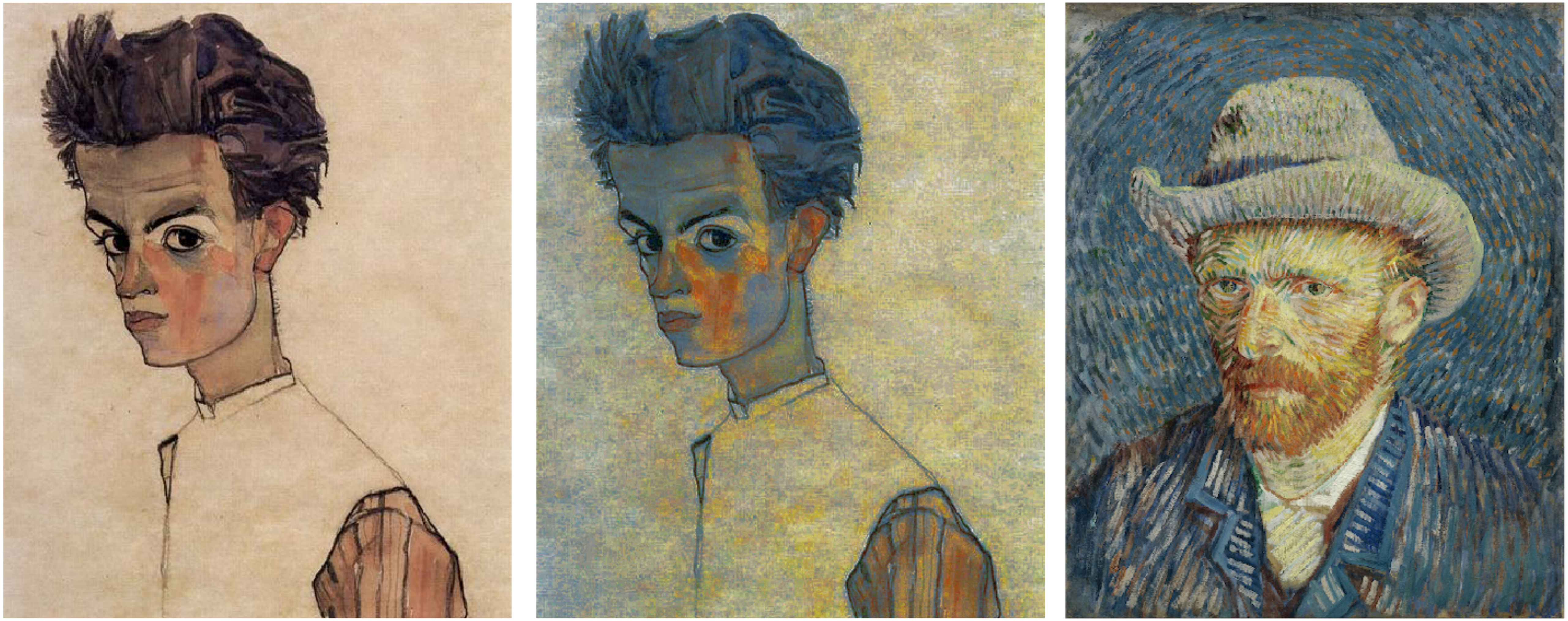




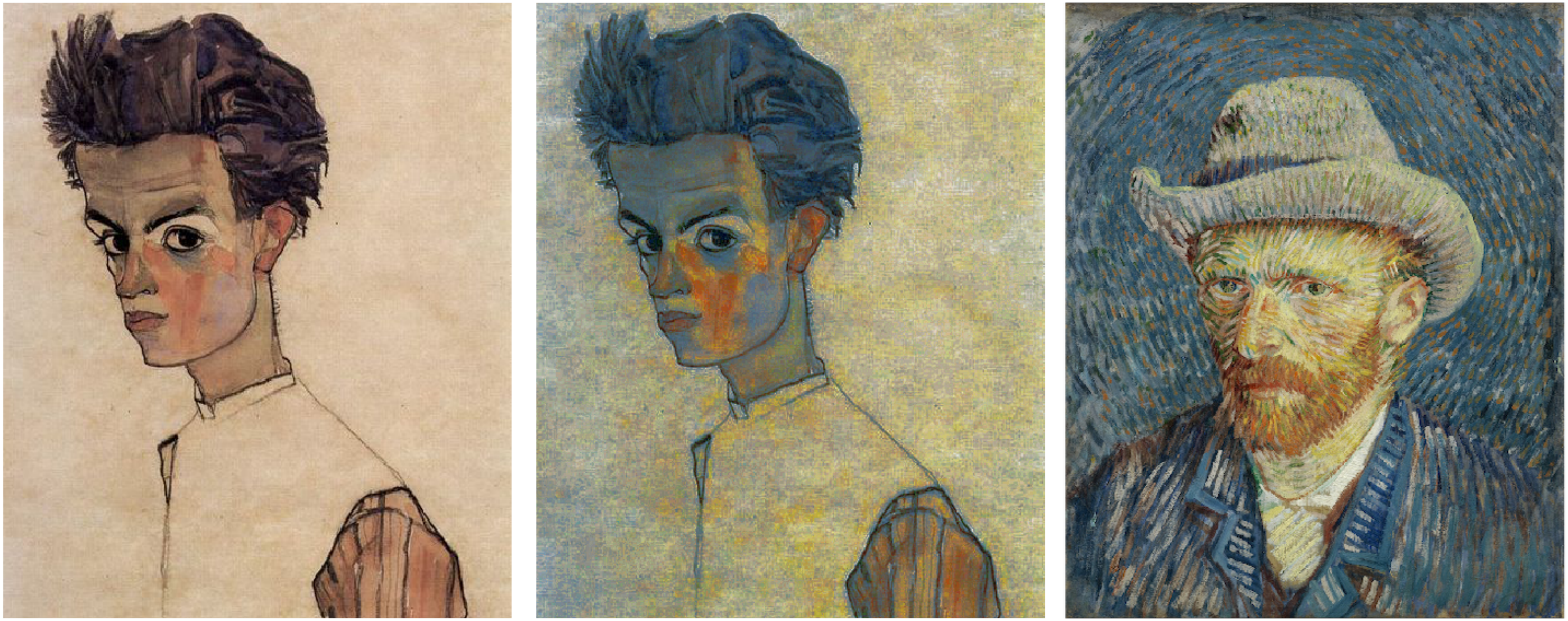


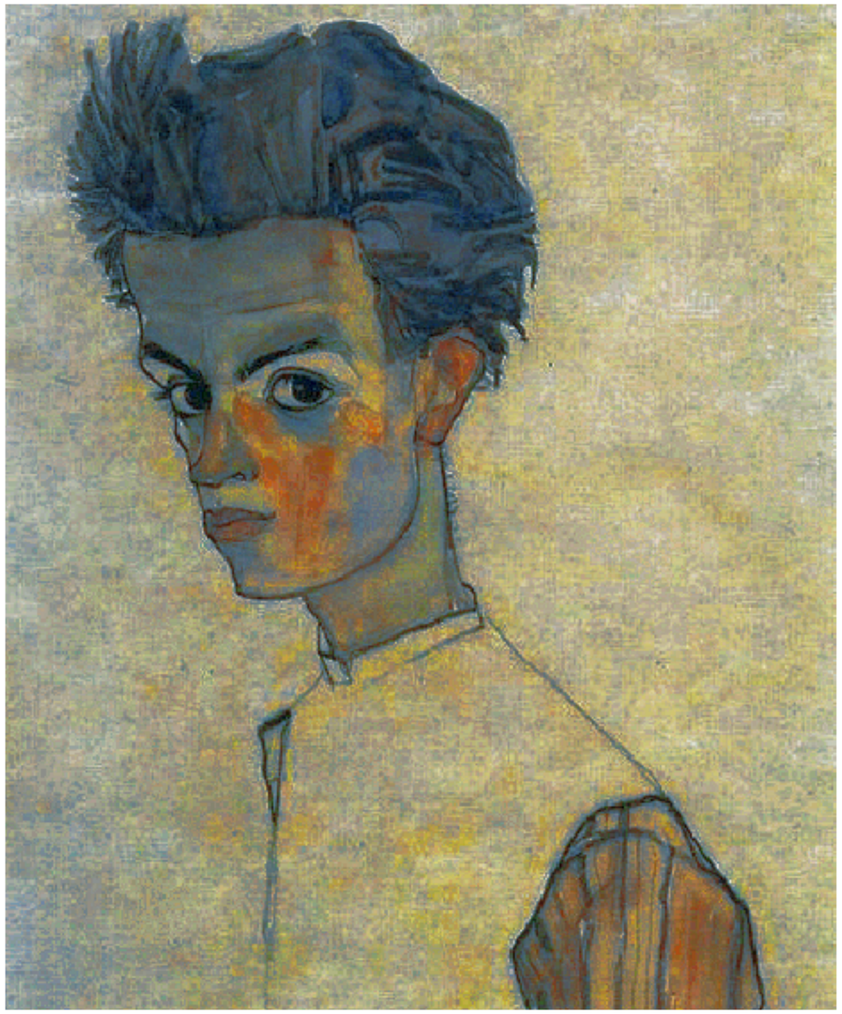


Instead of finding assumptions under which the optimal map exists and exhibits some regularity, we will enforce such regularity directly in the OT problem.

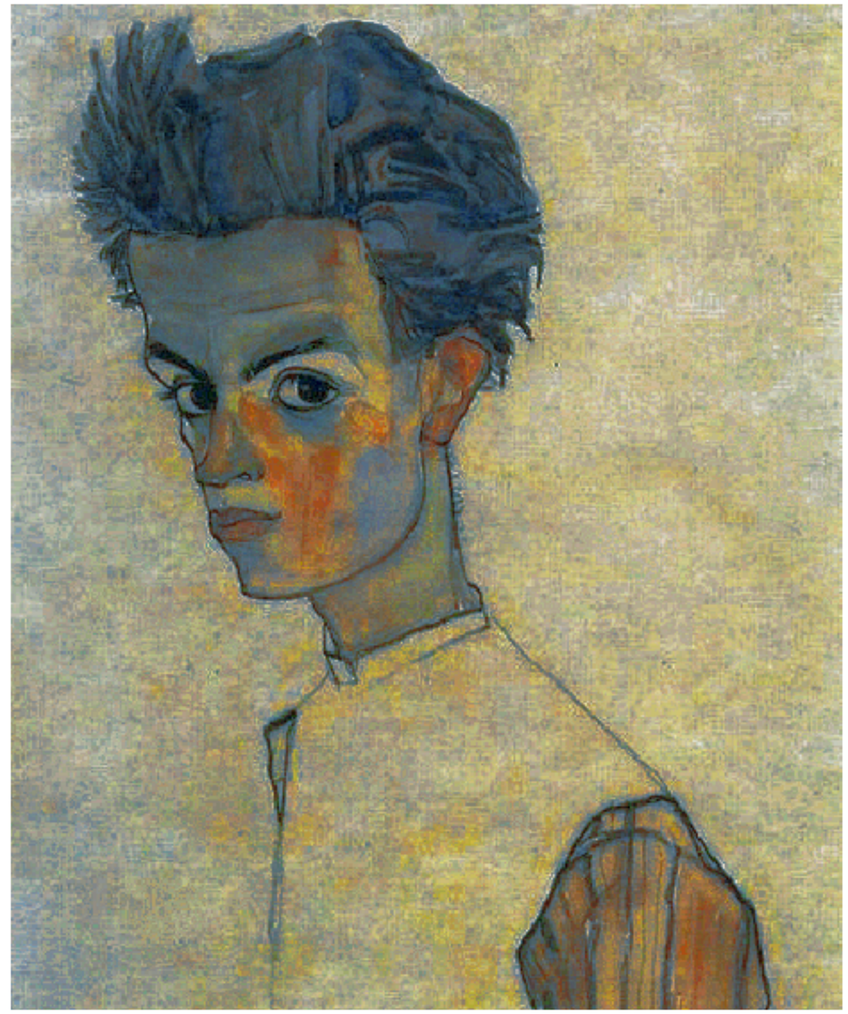
Smooth and Strongly Convex Brenier Potentials

Yann Brenier



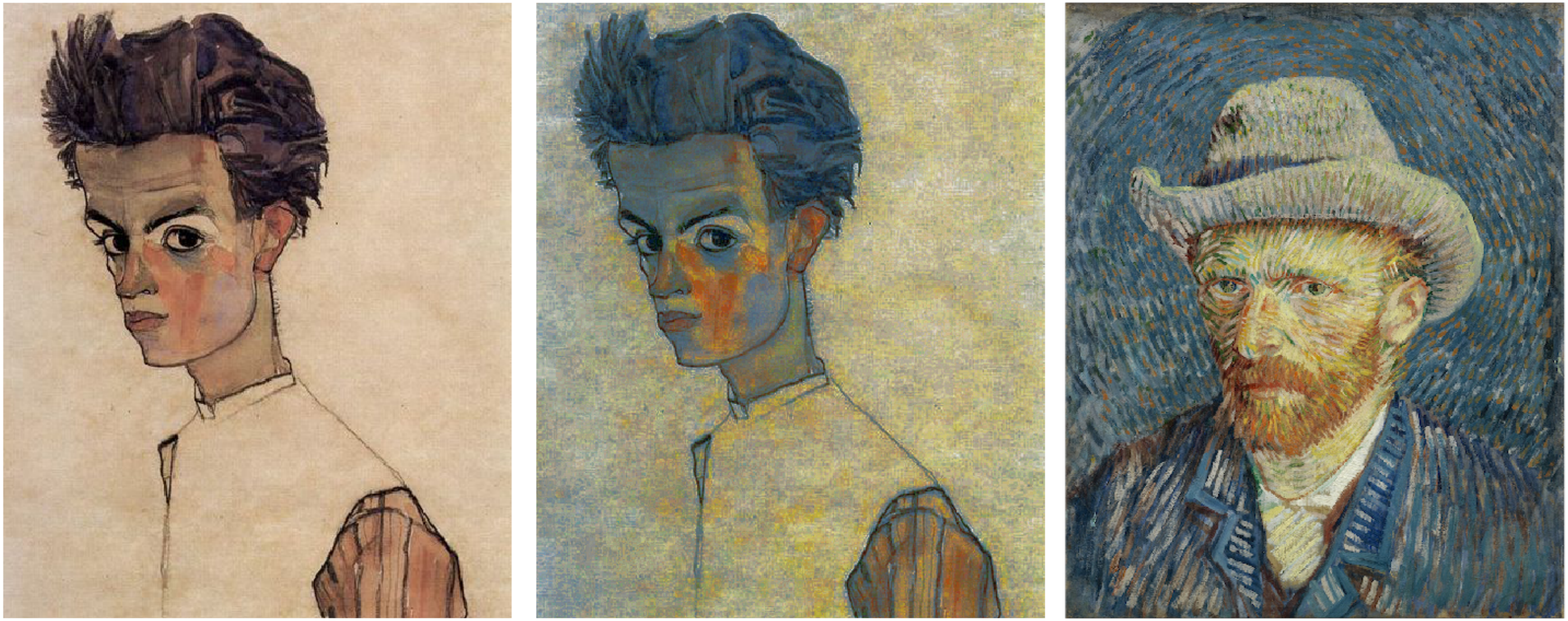


$$\ell\|x-y\| \leq \|\nabla f(x) - \nabla f(y)\| \leq L\|x-y\|$$

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

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



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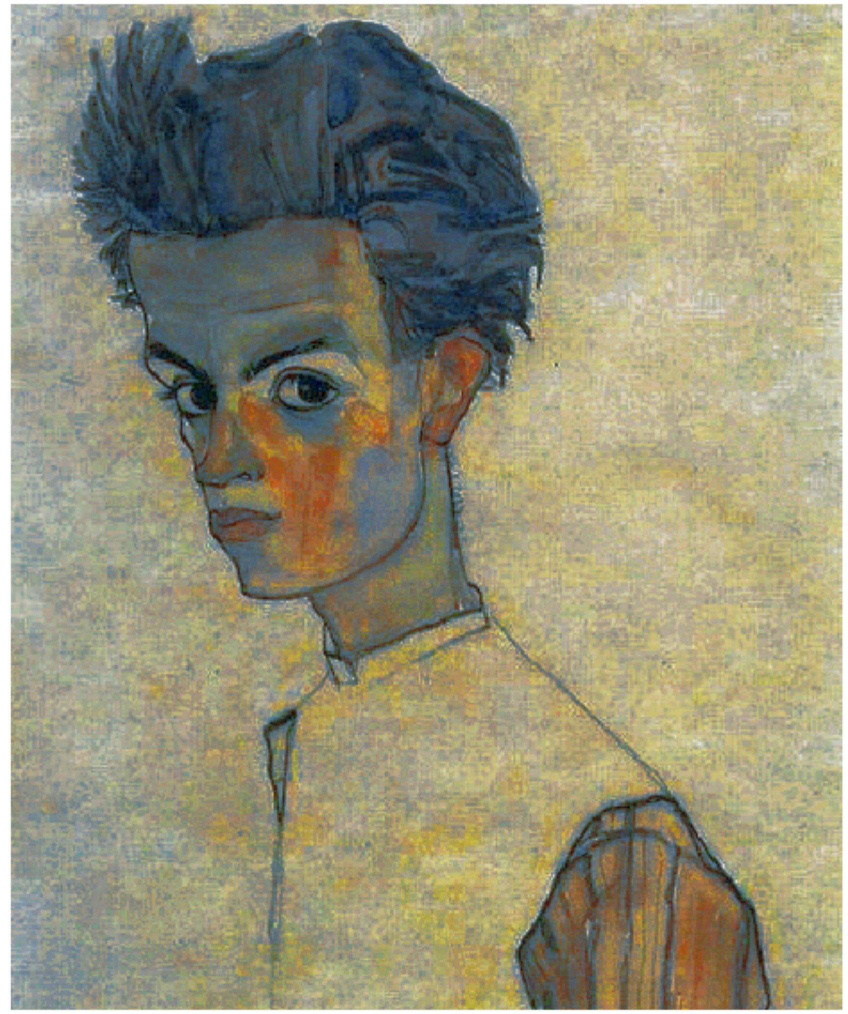
We ask that f is **smooth** and **strongly convex**

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

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

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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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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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$z_1^\star, \ldots, z_n^\star, u^\star$

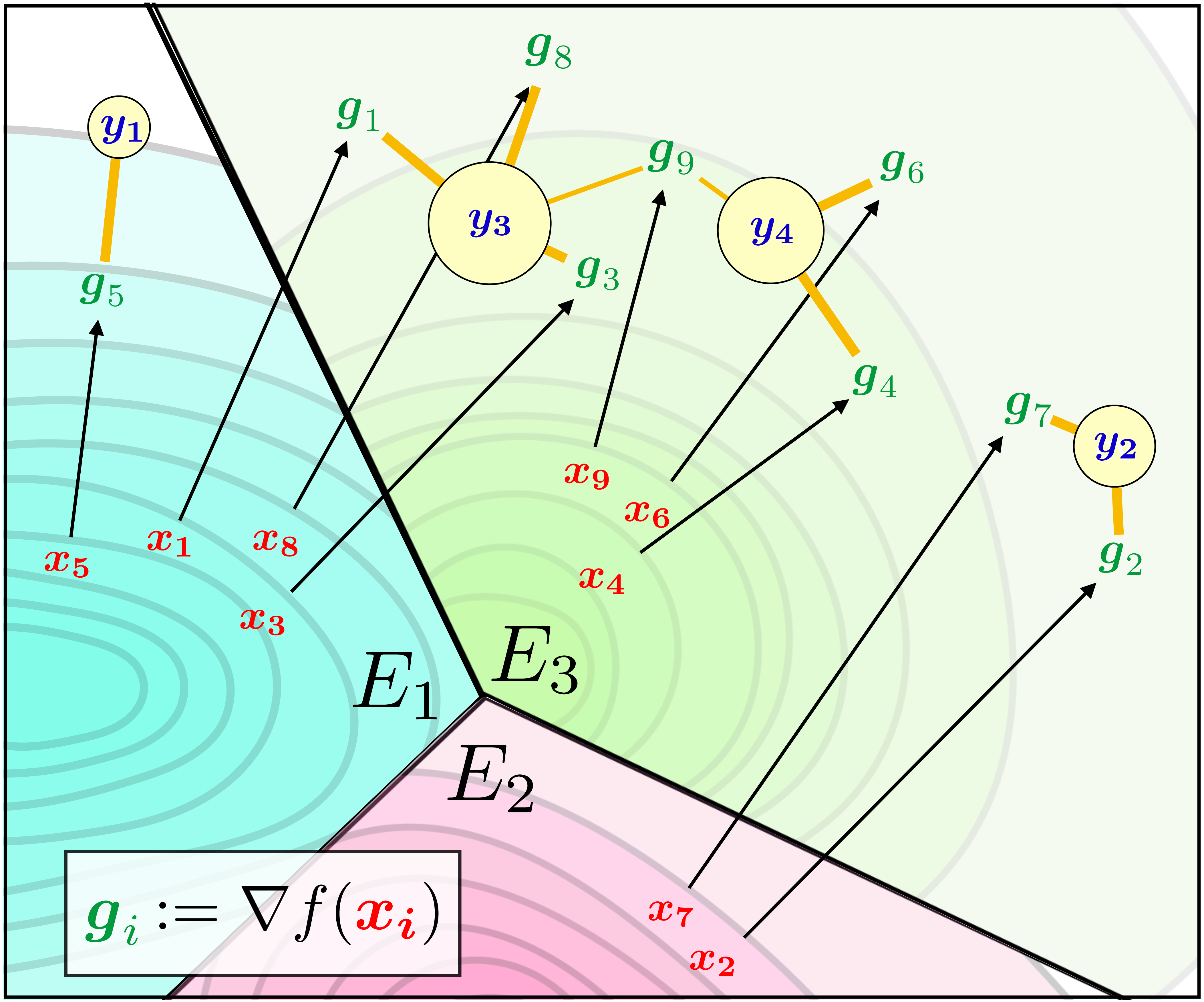
We can easily compute the map on any new point x by solving a cheap QCQP

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

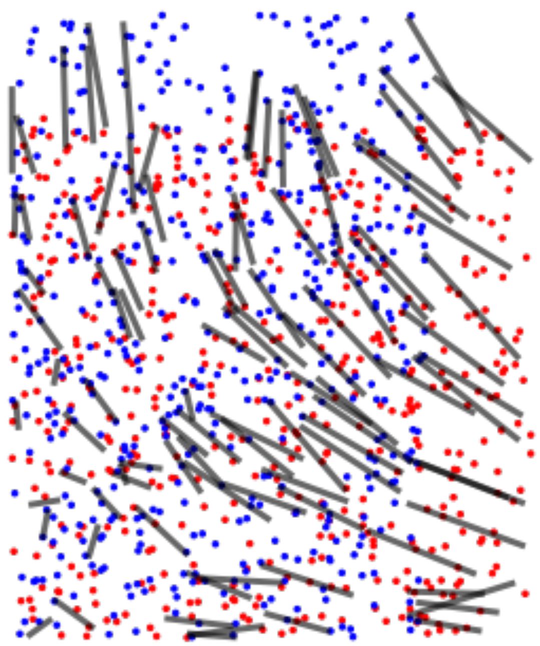
We define the *SSNB estimator* as a plug-in:

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

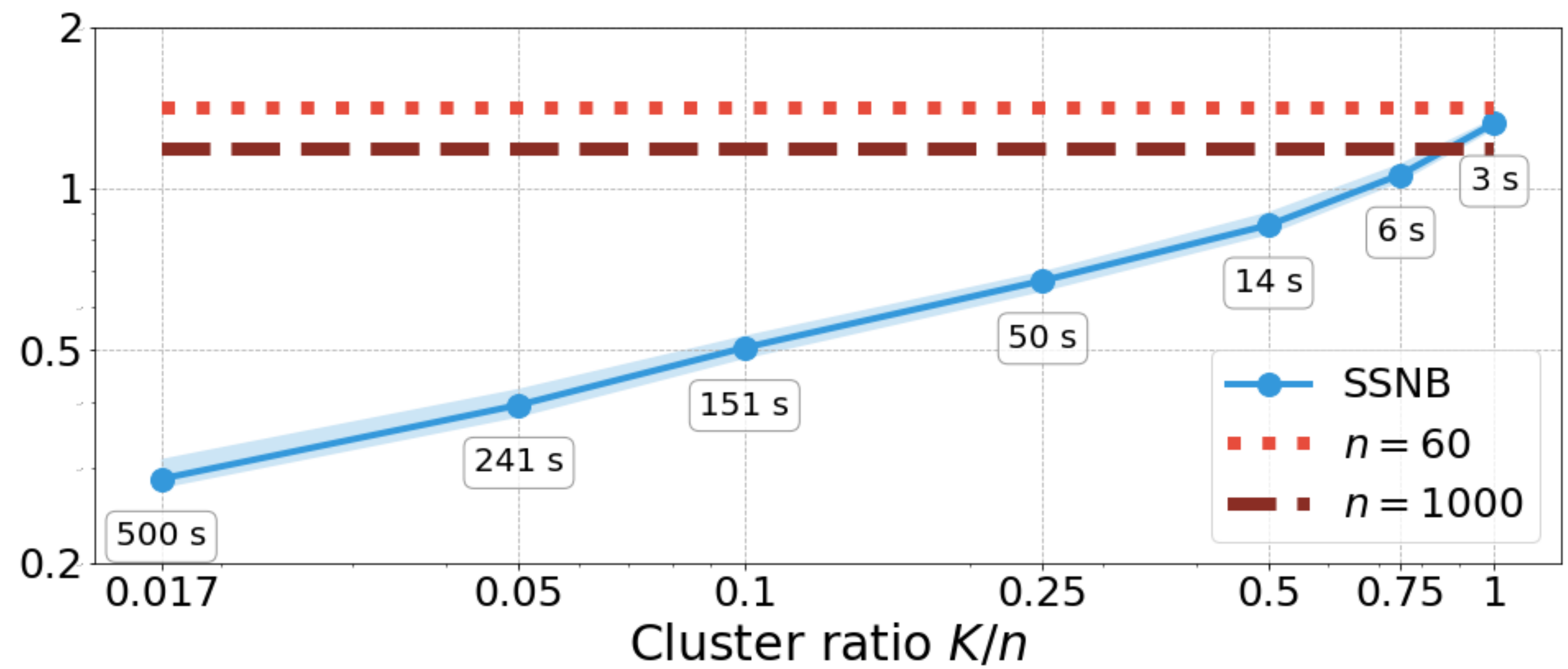
Regularity "by part"

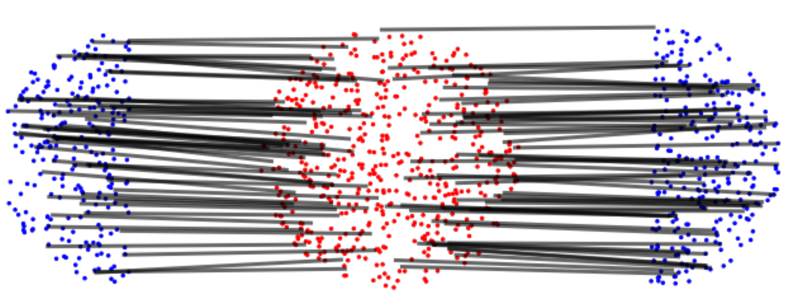


Estimation Error depending on K

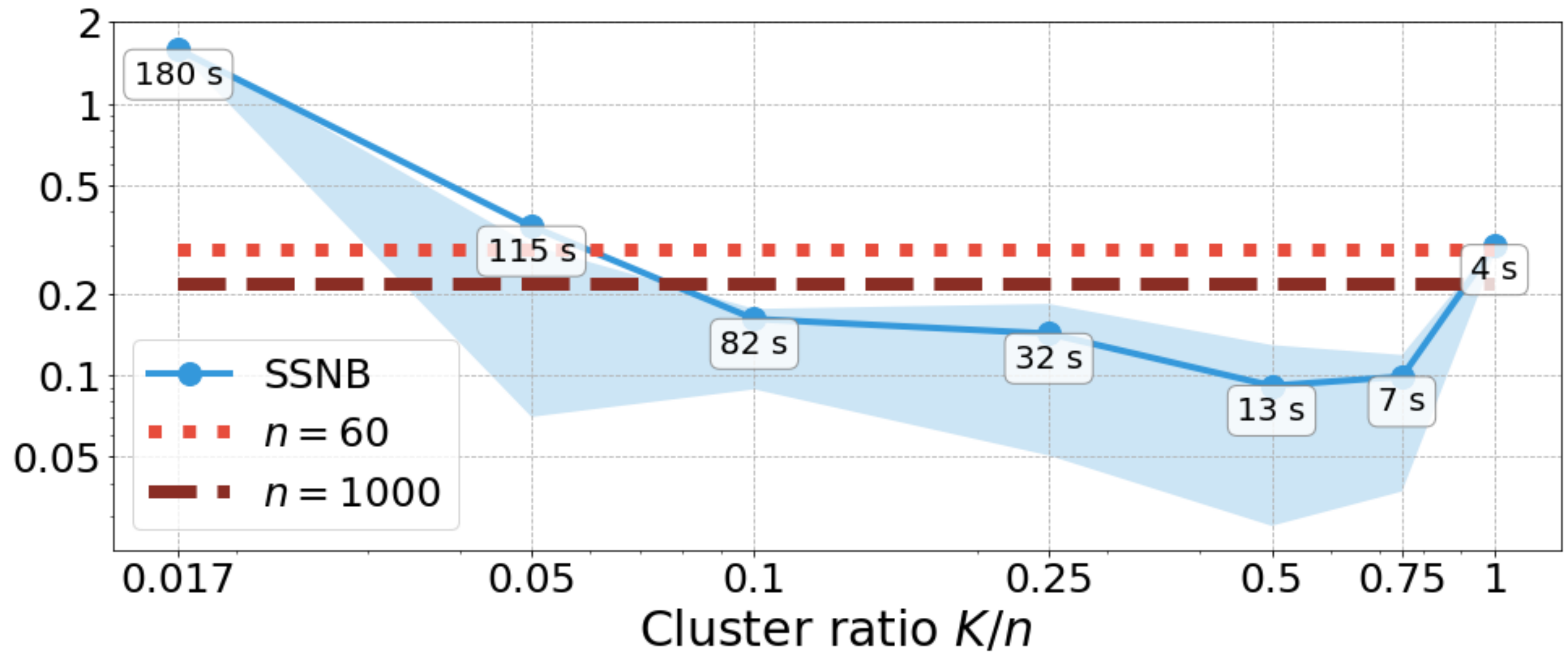


Global Regularity

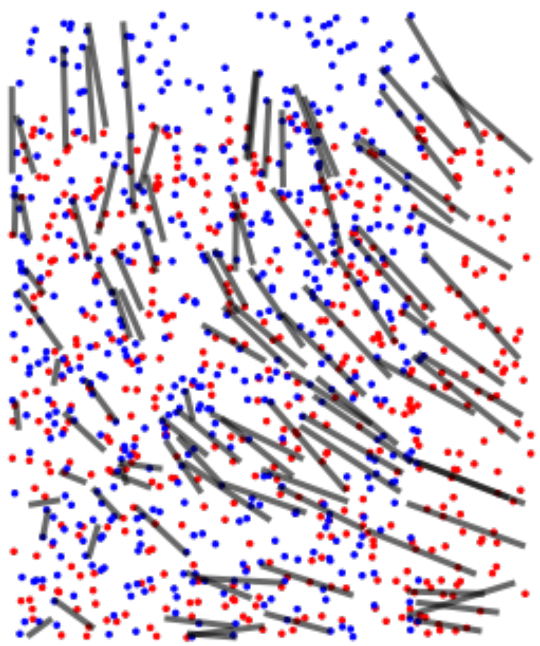




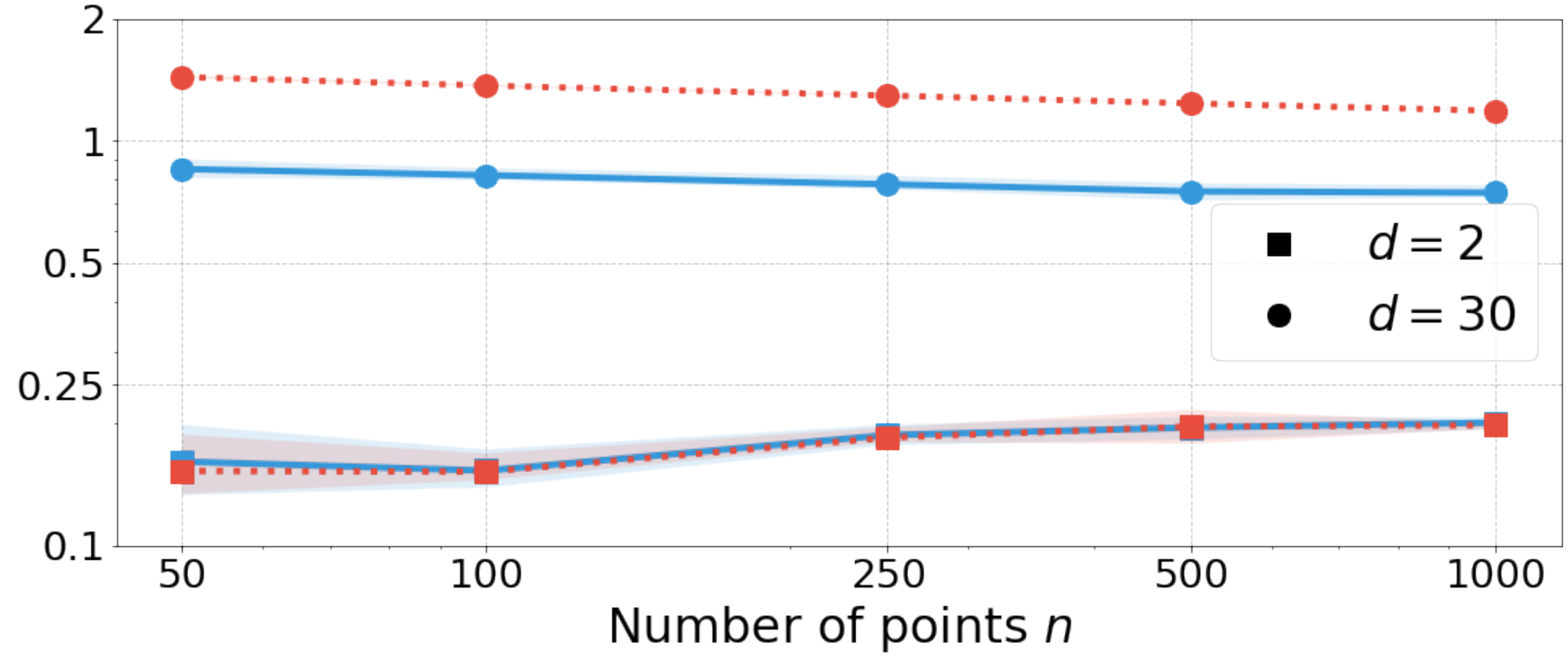
Local Regularity

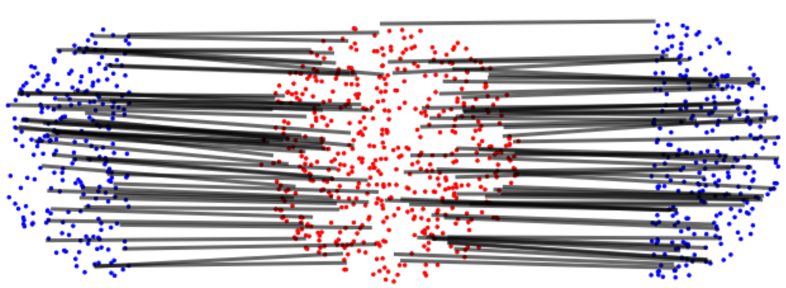


Estimation Error depending on n

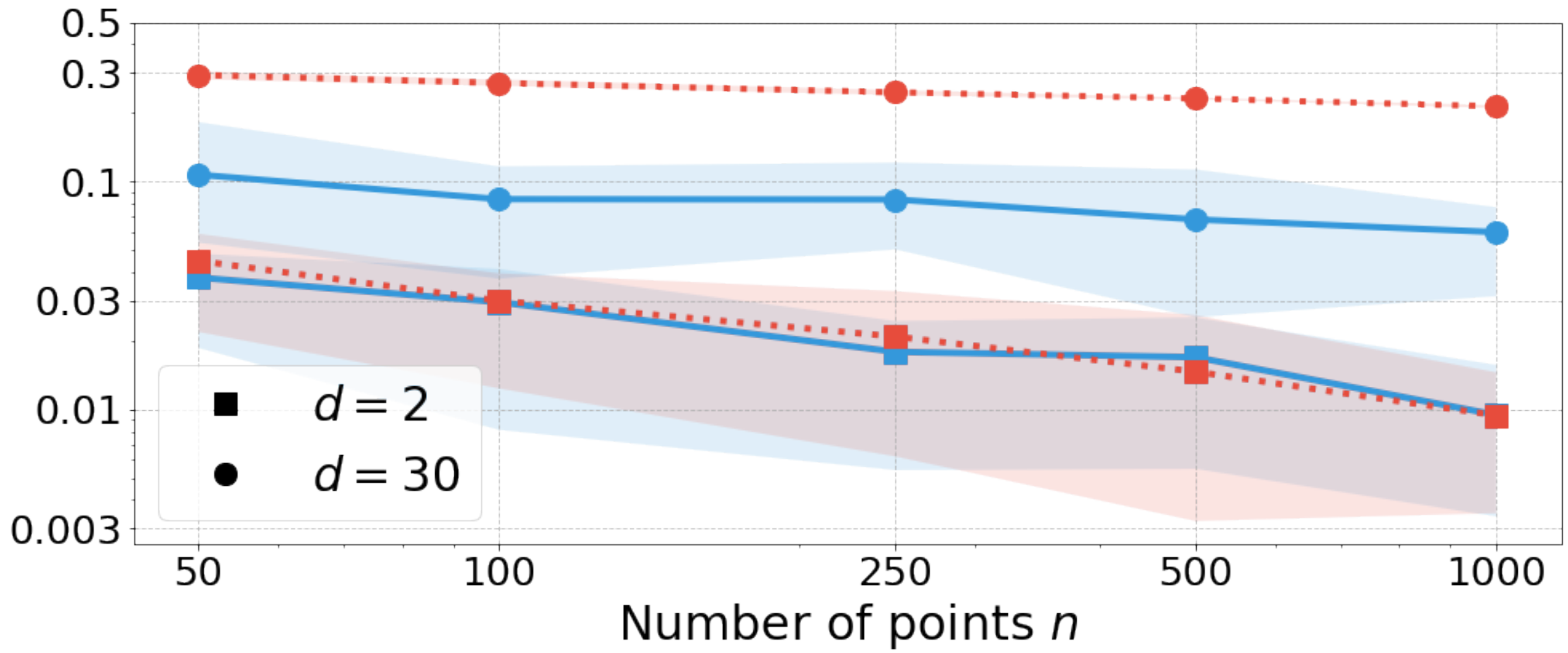


Global Regularity

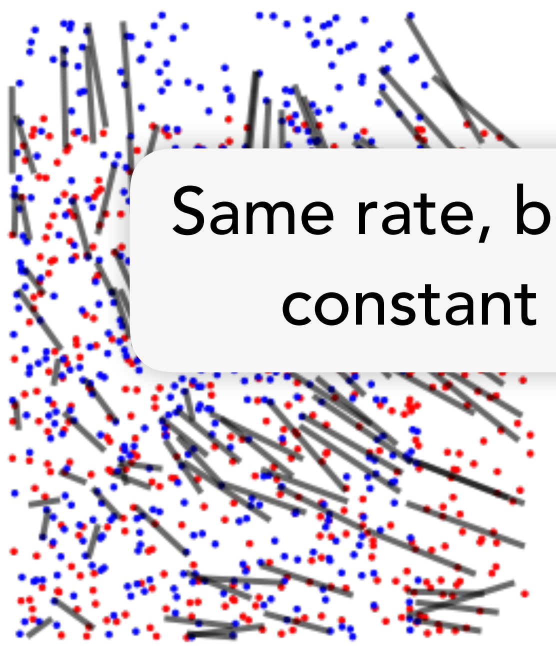




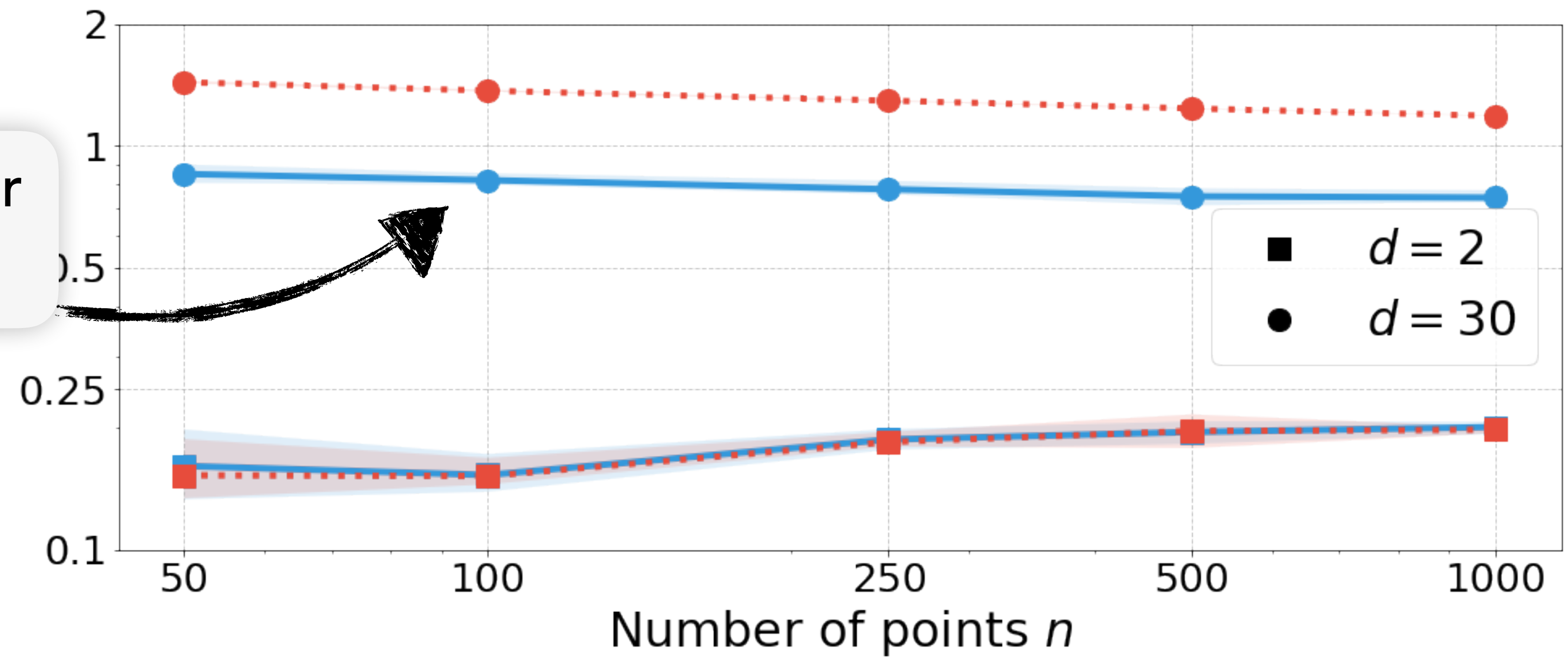
Local Regularity



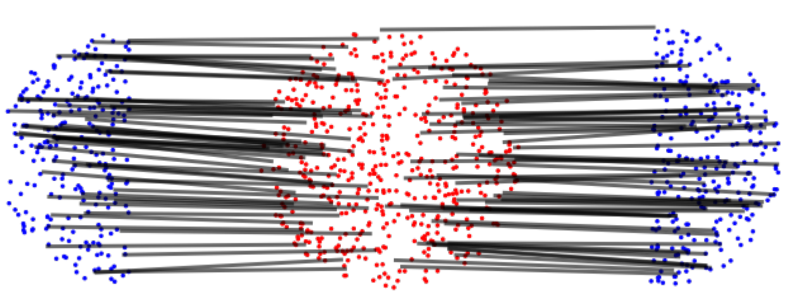
Estimation Error depending on n



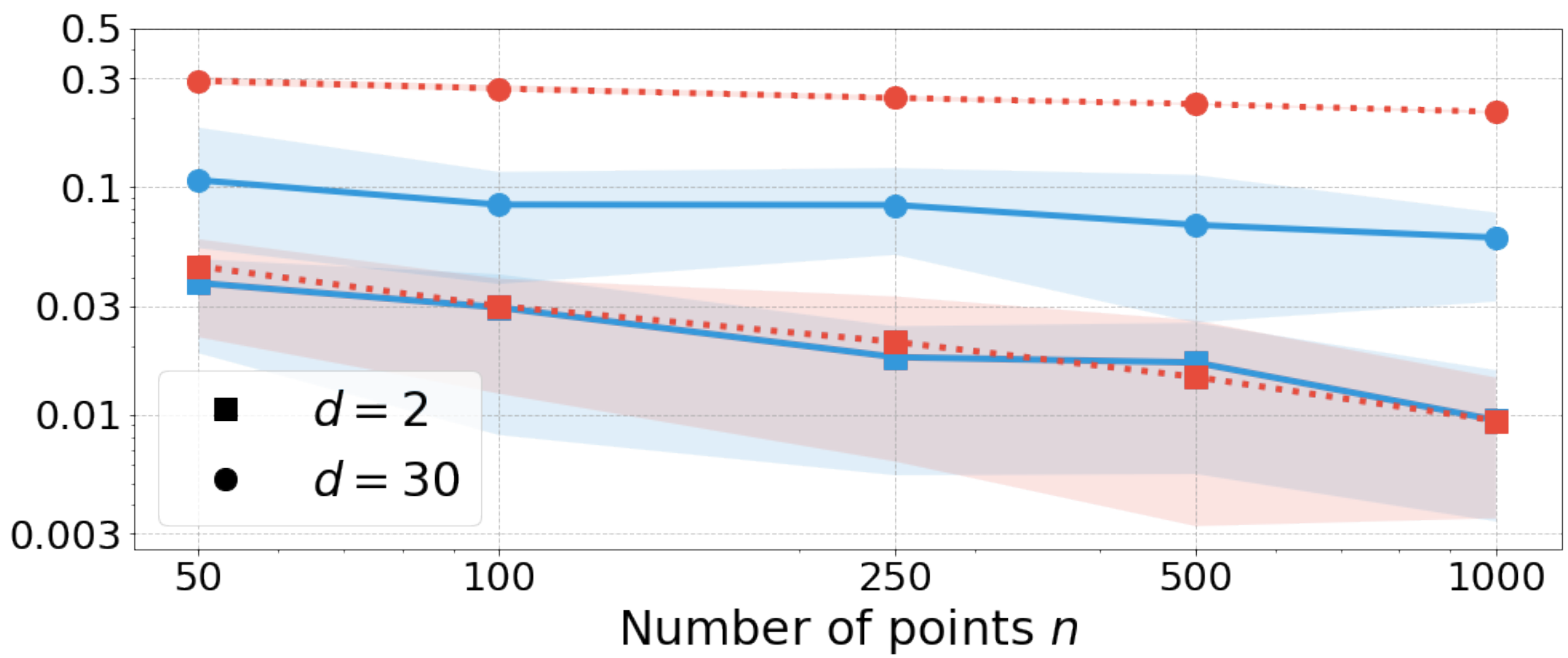
Same rate, better constant ?

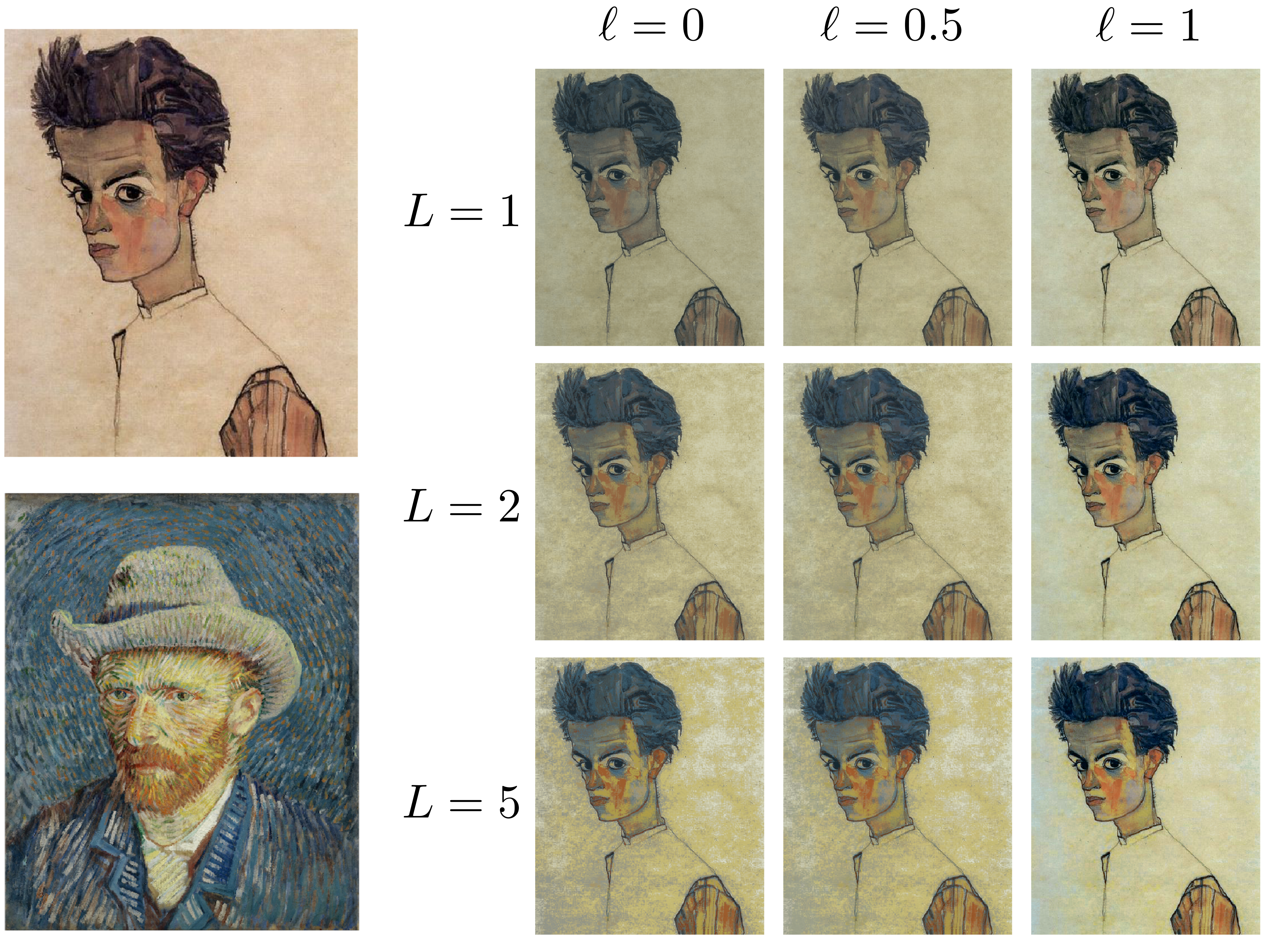


Global Regularity



Local Regularity





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


QUESTIONS ?
Cédric Villani