

**Question :** How precisely do WGANs solve the OT problem?

## Background on Optimal Transport .

For distributions  $\mathbb{P}, \mathbb{Q}$  on  $\mathbb{R}^D$  the Monge's form of the Wasserstein-1 distance is

$$\mathbb{W}_1(\mathbb{P}, \mathbb{Q}) = \min_{T: \mathbb{P} \rightarrow \mathbb{Q}} \int \|x - T(x)\|_2 d\mathbb{P}(x).$$

The Kantorovich's relaxation is given by

$$\mathbb{W}_1(\mathbb{P}, \mathbb{Q}) = \min_{\pi \in \Pi(\mathbb{P}, \mathbb{Q})} \int_{\mathbb{R}^D \times \mathbb{R}^D} \|x - y\|_2 d\pi(x, y).$$

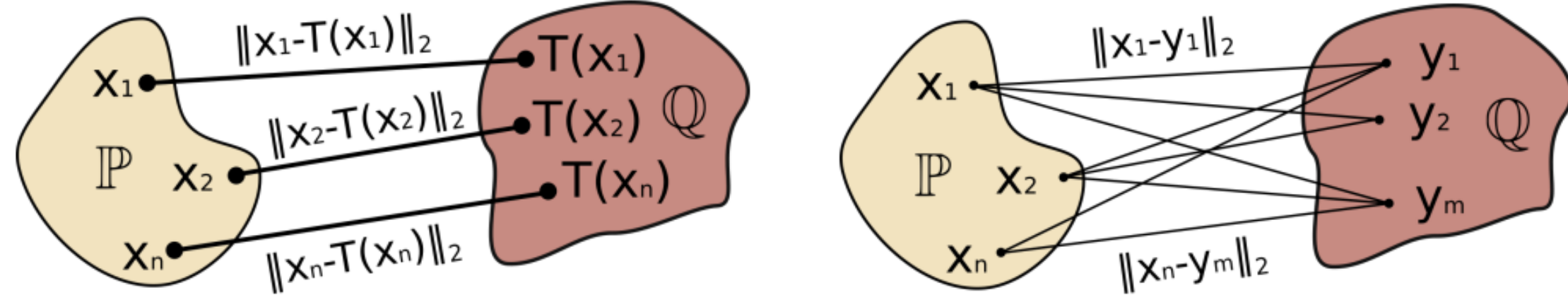


Figure 1. Monge's and Kantorovich's OT formulations.

## Dual formulation of $\mathbb{W}_1$ .

For distributions  $\mathbb{P}, \mathbb{Q}$ , the dual formulation of  $\mathbb{W}_1$  is given by

- Conventional ([LS]):

$$\mathbb{W}_1(\mathbb{P}, \mathbb{Q}) = \max_{f \oplus g \leq \|\cdot\|_2} \int f(x) d\mathbb{P}(x) + \int g(y) d\mathbb{Q}(y);$$

- c-transform ([MM:B], [MM:Bv2], [MM], [MM:R]):

$$\mathbb{W}_1(\mathbb{P}, \mathbb{Q}) = \max_f \int f(x) d\mathbb{P}(x) + \int \min_{y \in \mathbb{R}^D} \{ \|x - y\|_2 - f(y) \} d\mathbb{Q}(y);$$

- 1-Lipschitz constraint ([WC], [GP], [LP], [SN], [SO]):

$$\mathbb{W}_1(\mathbb{P}, \mathbb{Q}) = \max_{\|f\|_L \leq 1} \int f(x) d\mathbb{P}(x) - \int f(y) d\mathbb{Q}(y).$$

Typically, the dual potential is recovered with neural nets which are trained with SGD.

## Optimal Transport in GANs .

Let  $\mathbb{P} = \mathbb{P}_\alpha$  is a parametric distribution and  $\mathbb{Q}$  is the data distribution. Typically,  $\mathbb{P}_\alpha = G_\alpha \# \mathbb{S}$  obtained by a generator network  $G_\alpha$  from a fixed latent  $\mathbb{S}$ .

The loss function for the generator  $G_\alpha$  is

$$\mathbb{W}_1(\mathbb{P}_\alpha, \mathbb{Q}) = \int_z f^*(G_\alpha(z)) d\mathbb{S}(z) - \int f^*(y) d\mathbb{Q}(y).$$

The derivative of the loss is

$$\frac{\partial \mathbb{W}_1(\mathbb{P}_\alpha, \mathbb{Q})}{\partial \alpha} = \int_z J_\alpha G_\alpha(z)^T \nabla f^*(G_\alpha(z)) d\mathbb{S}(z).$$

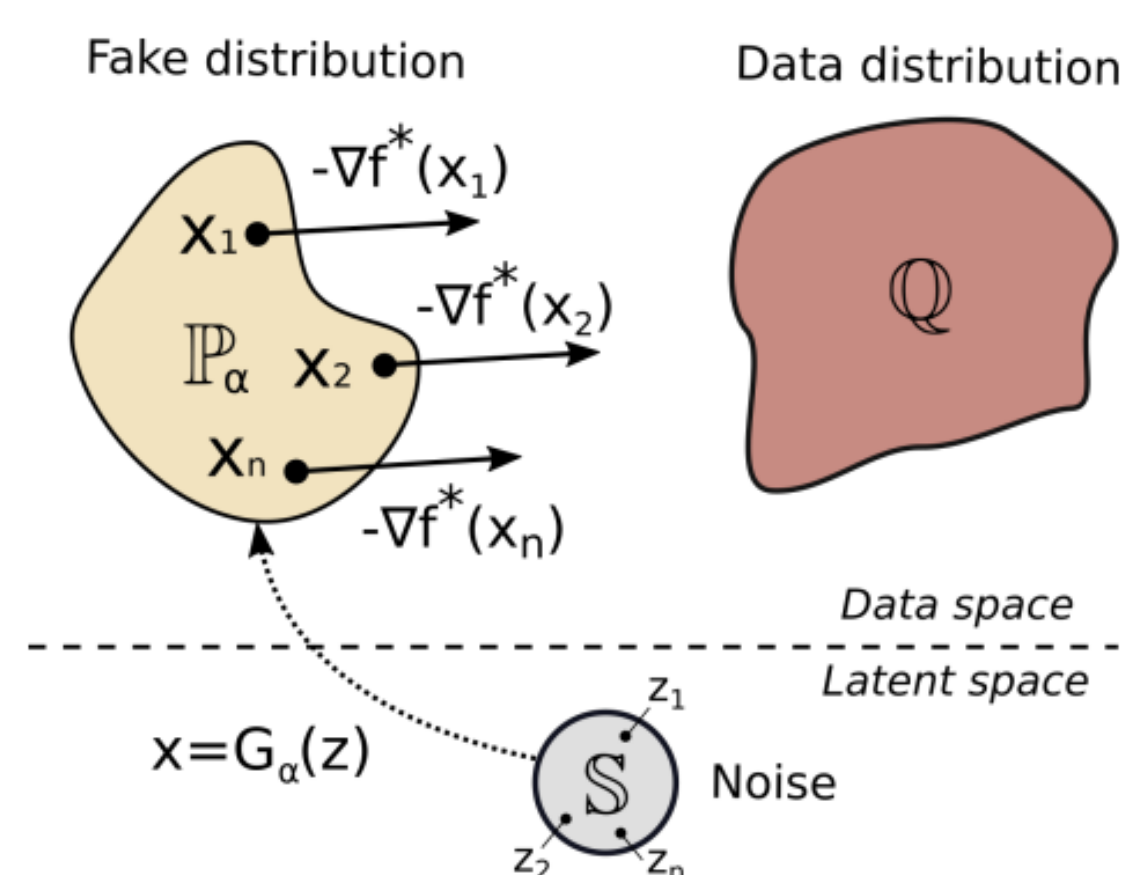


Figure 2. The anti-gradient  $-\nabla f^*(x)$  shows where to move the mass of each  $x = G_\alpha(z)$  to make the generated  $\mathbb{P}_\alpha$  closer to  $\mathbb{Q}$  in  $\mathbb{W}_1$ .

**Problem:** There are no non-trivial pairs  $\mathbb{P}, \mathbb{Q}$  with known OT gradient  $\nabla f^*$ .

## Constructing benchmark pairs.

We propose a way to construct pairs of  $\mathbb{P}, \mathbb{Q}$  with a known OT map, cost, gradient.

### 1: Definition

For a 1-Lipschitz function  $u: \mathbb{R}^D \rightarrow \mathbb{R}$ , we say that a transport plan  $\pi \in \Pi(\mathbb{P}, \mathbb{Q})$  is *u-ray monotone* (decreasing) if  $u(x) - u(y) = \|x - y\|_2$  holds  $\pi$ -almost surely for  $x, y \in \mathbb{R}^D$ .

### 2: Proposition

Let  $\pi \in \Pi(\mathbb{P}, \mathbb{Q})$  be a *u-ray monotone* transport plan for a 1-Lipschitz function  $u$ . Then it is an optimal plan between  $\mathbb{P}, \mathbb{Q}$ .

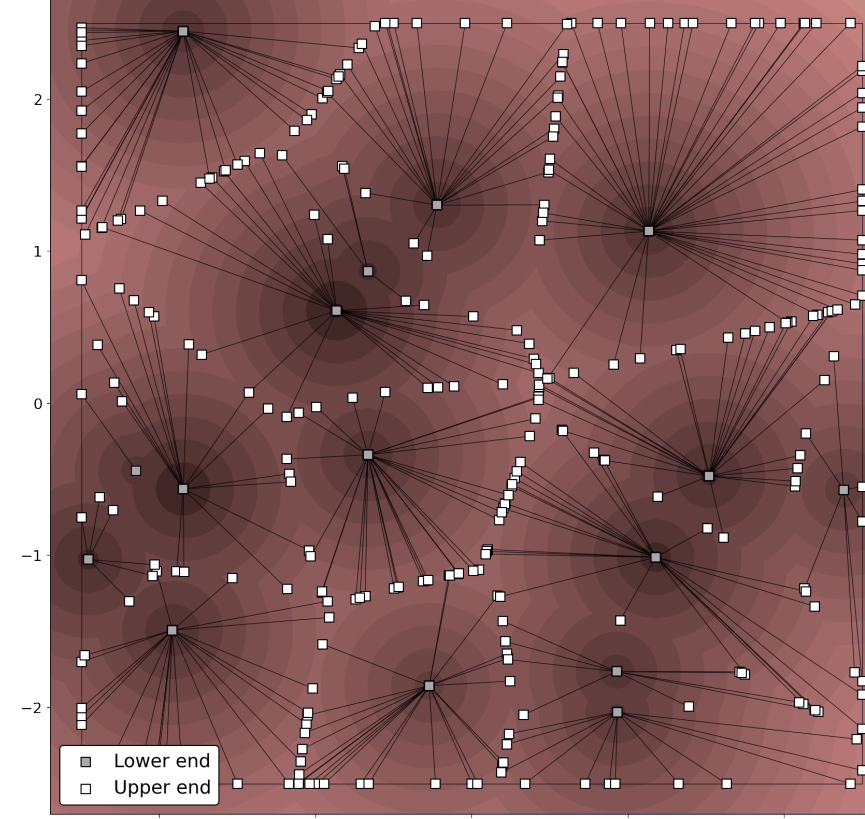


Figure 3. Truncated transport rays of a random MinFunnel  $N = 16, D = 2$ .

### Parameterizing 1-Lipschitz functions:

$u: \mathbb{R}^D \rightarrow \mathbb{R}$ , we employ the following 1-Lipschitz *MinFunnel* functions

$$u(x) = \min_n \{ \|x - a_n\|_2 + b_n \}.$$

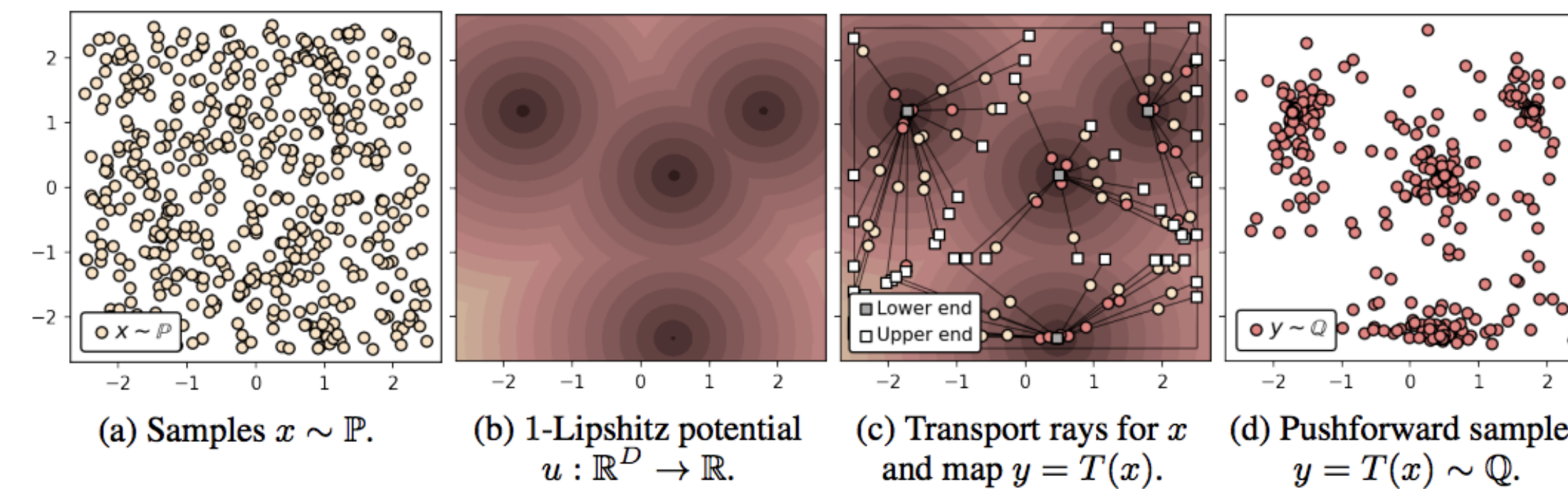


Figure 4. The pipeline of constructing of benchmark pairs.

### The construction pipeline:

- Pick absolutely continuous distribution  $\mathbb{P}$ .
- Take 1-Lipschitz MinFunnel function  $u(x)$ .
- Find  $u$ 's transport rays,  $u$ -forward map.
- Move samples from  $\mathbb{P}$  to  $\mathbb{Q}$  by the map.

## High-dimensional and images benchmark pairs.

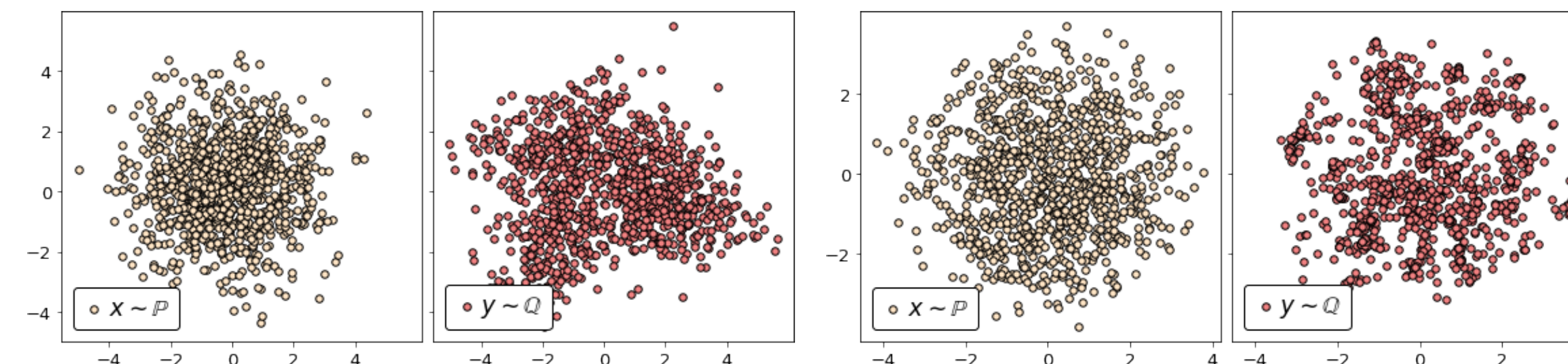


Figure 5. The pair with  $N = 4, D = 32$ .

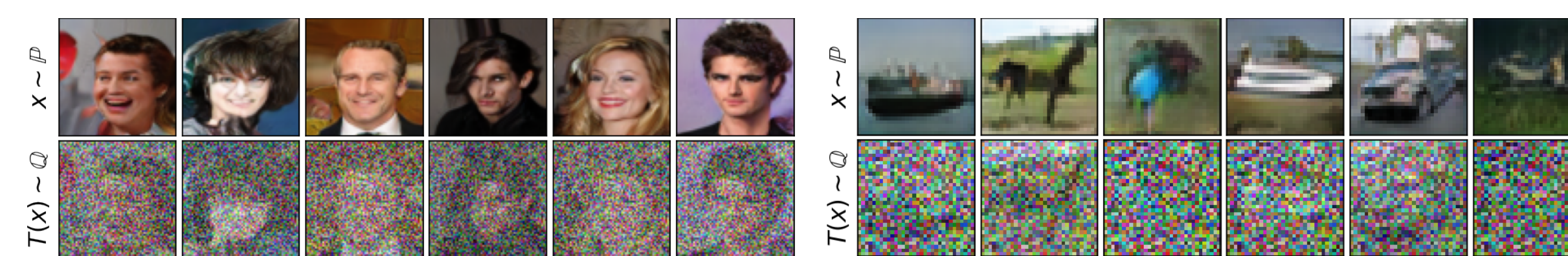


Figure 6. The pair with  $N = 64, D = 4$ .

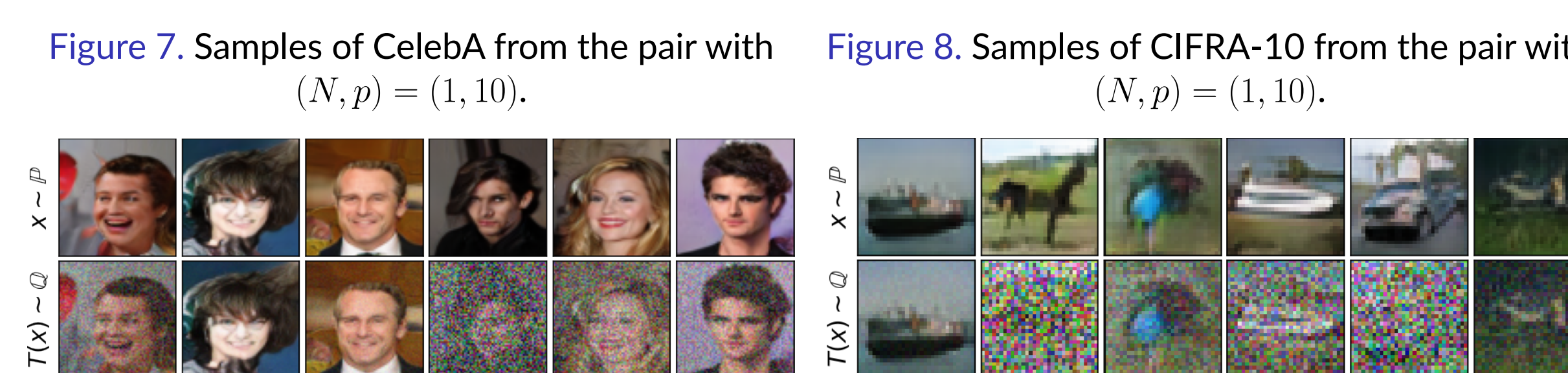


Figure 7. Samples of CelebA from the pair with  $(N, p) = (1, 10)$ .

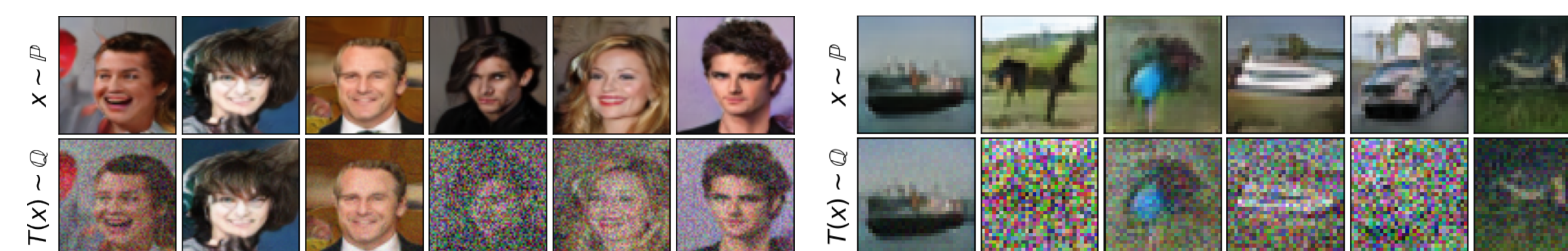


Figure 8. Samples of CIFAR-10 from the pair with  $(N, p) = (1, 10)$ .



Figure 9. Samples of CelebA from the pair with  $(N, p) = (16, 100)$ .



Figure 10. Samples of CIFAR-10 from the pair with  $(N, p) = (16, 100)$ .

## Evaluating dual surfaces in 2D.

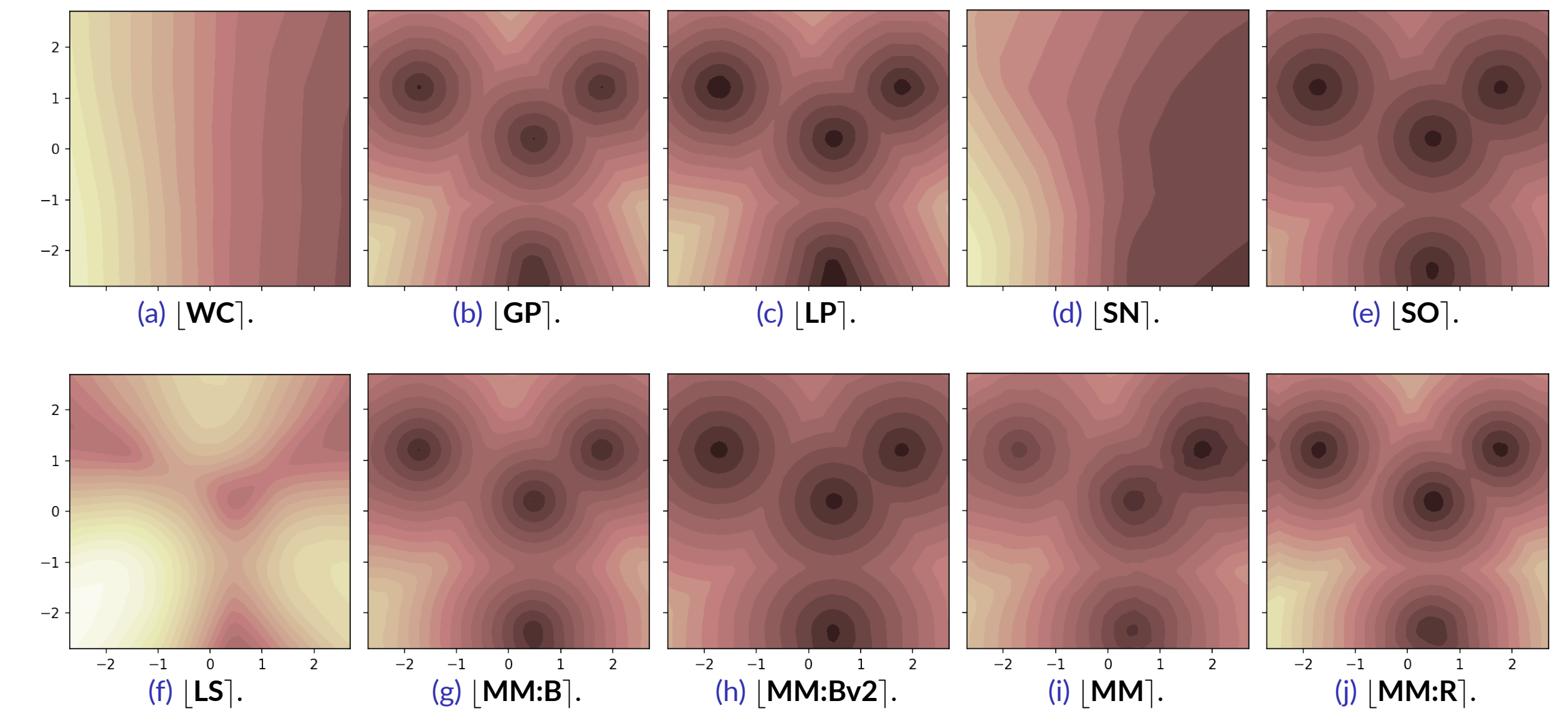


Figure 11. Surfaces of potentials  $f_\theta$  learned by OT solvers on the pair with  $D = 2, N = 4$ . The ground truth optimal potential is in Figure 4.

## Qualitative comparison of dual solvers.

- $\mathcal{L}^2$  - metric:

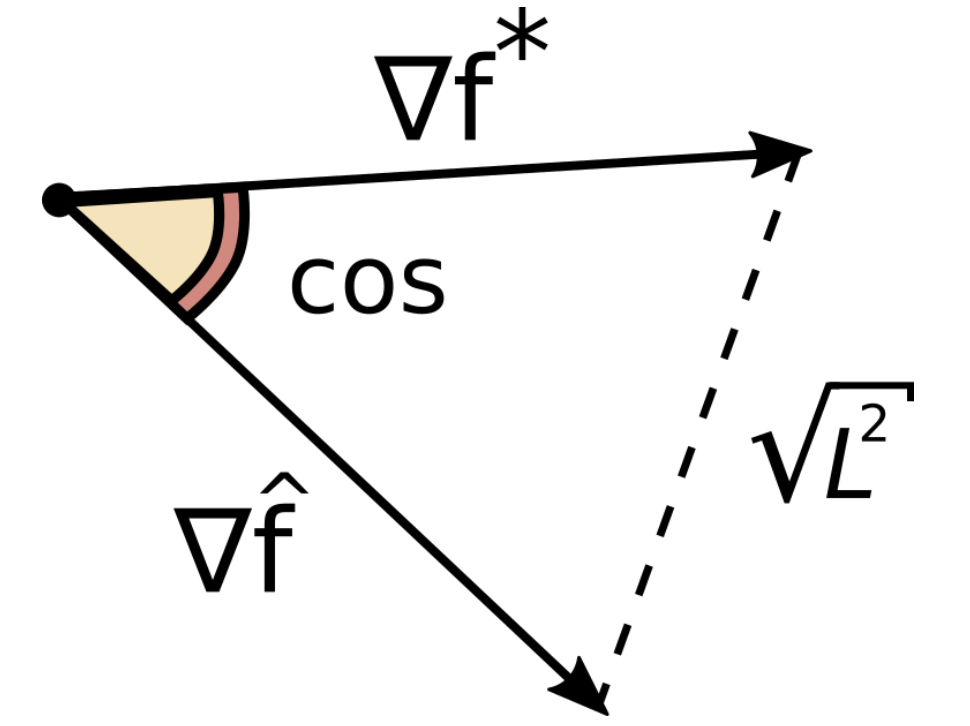
$$\mathcal{L}^2(\nabla \hat{f}, \nabla f^*) = \|\nabla \hat{f} - \nabla f^*\|_2^2;$$

- Cosine similarity:

$$\cos(\nabla \hat{f}, \nabla f^*) = \frac{\langle \nabla \hat{f}, \nabla f^* \rangle}{\|\nabla \hat{f}\|_2 \|\nabla f^*\|_2};$$

- Deviation of  $\hat{\mathbb{W}}_1$  from  $\mathbb{W}_1$ :

$$\text{dev} = 100\% \cdot \frac{|\mathbb{W}_1 - \hat{\mathbb{W}}_1|}{\mathbb{W}_1}.$$



## Results.

	[WC]	[GP]	[LP]	[SN]	[SO]	[LS]	[MM:B]	[MM:Bv2]	[MM]	[MM:R]
HD	0.11	0.56	0.56	0.09	0.61	-0.51	-0.54	0.45	0.53	0.31
Img	0.33	0.92	0.92	0.35	-	0.36	0.38	0.09	0.46	0.91

Table 1. The top row demonstrates *cos* for dual solvers for pairs with  $N = 256, D = 128$ , while the bottom row shows *cos* for image pairs  $N = 16, p = 100$

	[WC]	[GP]	[LP]	[SN]	[SO]	[LS]	[MM:B]	[MM:Bv2]	[MM]	[MM:R]
HD	>>10	0.89	0.9	1.57	0.77	2.07	1.98	>>10	0.73	1.38
Img	>>10	1.34	1.12	3.32	-	1.87	1.28	>>10	0.16	0.95

Table 2. The top row demonstrates  $\mathcal{L}^2$  metric for dual solvers for pairs with  $N = 256, D = 128$ , while the bottom row shows  $\mathcal{L}^2$  metric for image pairs  $N = 16, p = 100$

	[WC]	[GP]	[LP]	[SN]	[SO]	[LS]	[MM:B]	[MM:Bv2]	[MM]	[MM:R]
HD	0.36	0.67	0.69	0.12	0.8	-0.32	-0.32	2.61	0.79	1.02
Img	>>100	36.16	36.75	13.26	-	5.24	4.21	24.36	>>100	23.46

Table 3. The top row demonstrates *dev* metric for dual solvers for pairs with  $N = 64, D = 128$ , while the bottom row shows *dev* for image pairs  $N = 16, p = 100$

## Conclusion.

- All the solvers should **not** be considered as **meaningful estimators of  $\mathbb{W}_1$** .
- The gradient  $\nabla \hat{f}$  recovered by some solvers shows **positive** *cos* with the ground-truth gradient  $\nabla f^*$ , but mostly they provide **poor**  $\mathcal{L}^2$  metric.

More details and code are represented in GitHub page.



<https://github.com/justkolesov/Wasserstein1Benchmark>