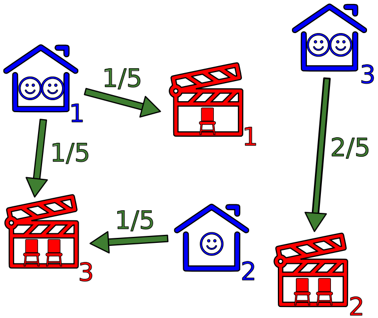
Properties of Discrete Sliced Wasserstein Losses

Eloi Tanguy, Rémi Flamary, Julie Delon

MAP5, Université Paris-Cité

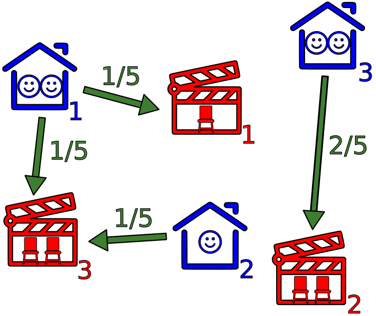
27 May 2024

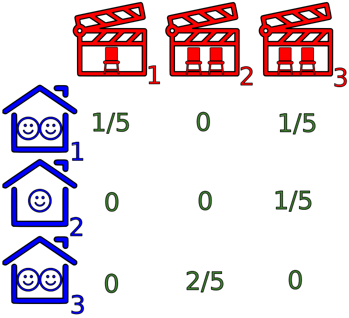
Discrete Optimal Transport



	1	2	3
1	1/5	0	1/5
2	0	0	1/5
3	0	2/5	0

Discrete Optimal Transport





Assignment Cost:

$$\frac{1}{5} \times c(x_1, y_1) + \frac{1}{5} \times c(x_1, y_3) + \frac{1}{5} \times c(x_2, y_3) + \frac{2}{5} \times c(x_3, y_2).$$

Constraints on $\pi \in \mathbb{R}_+^{3\times 3}$: $\pi \mathbf{1} = (2/5, 1/5, 2/5)$, $\pi^\top \mathbf{1} = (1/5, 2/5, 2/5)$.

$$\text{Optimal Transport Cost}: \min_{\pi} \sum_{i,j} c(x_i, y_j)\pi_{i,j}.$$

2-Wasserstein Distance: $c(x, y) = \|x - y\|_2^2$

Measures $\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$, $\nu = \frac{1}{m}\sum_{j=1}^{m} \delta_{y_j}$.

$$\mathrm{W}_2^2(\mu, \nu) = \min_{\substack{\pi \in \mathbb{R}_+^{n\times m} \\ \pi \mathbf{1} = a,\ \pi^\top \mathbf{1} = b}} \sum_{i=1}^{n}\sum_{j=1}^{m} \|x_i - y_j\|_2^2 \pi_{i,j}.$$

2-Wasserstein Distance: $c(x,y) = \|x-y\|_2^2$

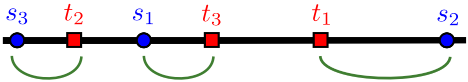
Measures $\mu = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}, \ \nu = \frac{1}{m}\sum_{j=1}^m \delta_{y_j}.$

$$\mathrm{W}_2^2(\mu,\nu) = \min_{\substack{\pi \in \mathbb{R}_+^{n\times m} \\ \pi\mathbf{1}=a,\ \pi^\top\mathbf{1}=b}} \sum_{i=1}^n\sum_{j=1}^m \|x_i - y_j\|_2^2 \pi_{i,j}.$$

Continuous case: $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$,

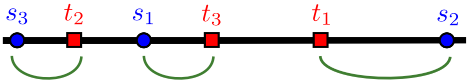
$$\mathrm{W}_2^2(\mu,\nu) = \min_{\pi \in \Pi(\mu,\nu)} \int_{\mathbb{R}^{2d}} \|x-y\|_2^2 \mathrm{d}\pi(x,y) = \min_{\pi\in\Pi(\mu,\nu)} \mathbb{E}_{(X,Y)\sim\pi}\left[\|X-Y\|_2^2\right].$$

1D Wasserstein and Sliced Wasserstein

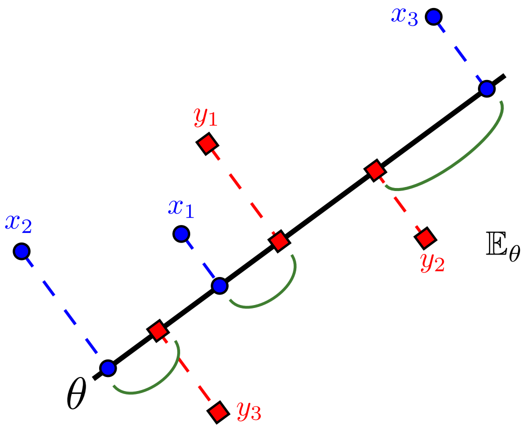


$$\mathrm{W}_2^2(\gamma_S, \gamma_T) = \frac{1}{n}\sum_{i=1}^{n} \left| s_{\sigma(i)} - t_{\tau(i)} \right|^2$$

1D Wasserstein and Sliced Wasserstein



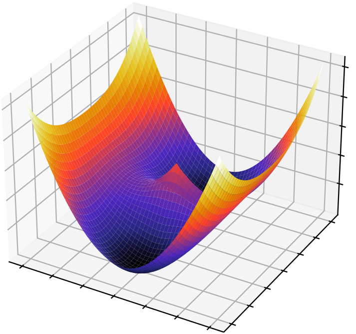
$$\mathrm{W}_2^2(\gamma_S, \gamma_T) = \frac{1}{n}\sum_{i=1}^{n} \left| s_{\sigma(i)} - t_{\tau(i)} \right|^2$$



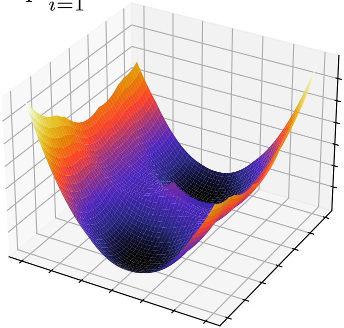
$$\mathrm{SW}_2^2(\gamma_X, \gamma_Y) = \mathbb{E}_{\theta \sim \mathcal{U}(\mathbb{S}^d)} \left[\mathrm{W}_2^2(\theta \# \gamma_X, \theta \# \gamma_Y) \right]$$

Monte-Carlo Approximation

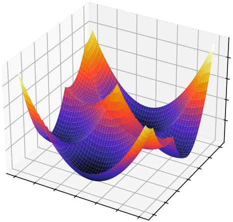
$$\mathcal{E}(X) = \mathbb{E}_{\theta\sim\mathcal{U}(\mathbb{S}^d)}\left[\mathrm{W}_2^2(\theta\#\gamma_X, \theta\#\gamma_Y)\right]$$



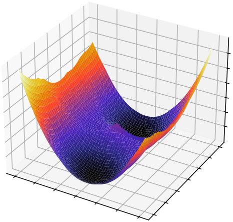
$$\mathcal{E}_p(X) := \frac{1}{p}\sum_{i=1}^{p}\mathrm{W}_2^2(\theta_i\#\gamma_X, \theta_i\#\gamma_Y)$$



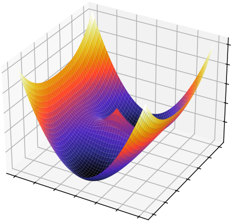
Statistical Properties



(a) $p = 3$

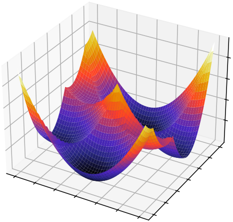


(b) $p = 10$

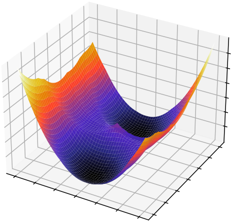


(c) $\mathcal{E}$

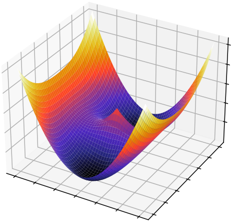
Statistical Properties



(a) $p = 3$



(b) $p = 10$

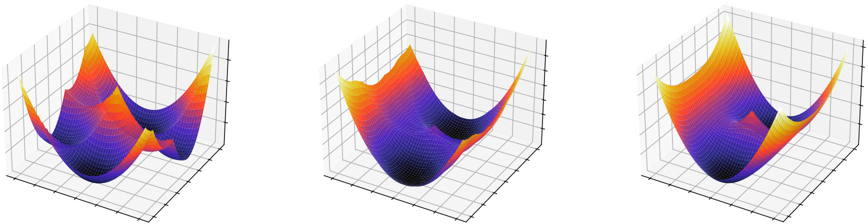


(c) $\mathcal{E}$

Uniform Convergence [5]

For $\mathcal{K} \subset \mathbb{R}^{n\times d}$ compact, $\mathbb{P}\left(\|\mathcal{E}_p - \mathcal{E}\|_{\infty,\mathcal{K}} \xrightarrow[p\to+\infty]{} 0\right) = 1.$

Statistical Properties



(a) $p = 3$ (b) $p = 10$ (c) $\mathcal{E}$

Uniform Convergence [5]

For $\mathcal{K} \subset \mathbb{R}^{n \times d}$ compact, $\mathbb{P}\left(\|\mathcal{E}_p - \mathcal{E}\|_{\infty, \mathcal{K}} \xrightarrow[p \longrightarrow +\infty]{} 0 \right) = 1.$

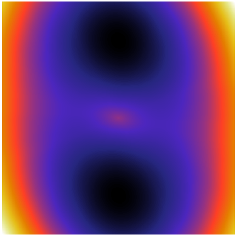
Uniform Central Limit Theorem [5]

For $\mathcal{K} \subset \mathbb{R}^{n \times d}$ compact, $\sqrt{p}(\mathcal{E}_p - \mathcal{E}) \xrightarrow[p \longrightarrow +\infty]{\mathcal{L},\ \ell^\infty(\mathcal{K})} G.$

Global Optima

- SW_2 is a distance:

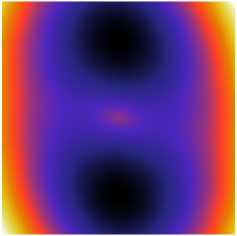
$$\underset{X\in\mathbb{R}^{n\times d}}{\operatorname{argmin}}\ \mathcal{E}(X) = \underset{X\in\mathbb{R}^{n\times d}}{\operatorname{argmin}}\ \mathrm{SW}_2^2(\gamma_X, \gamma_Y)$$
$$= \{Y \text{ up to a permutation}\}$$



Global Optima

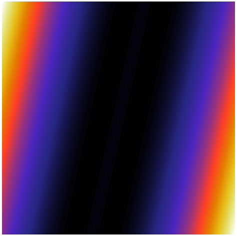
- SW_2 is a distance:

$$\underset{X \in \mathbb{R}^{n\times d}}{\mathrm{argmin}}\ \mathcal{E}(X) = \underset{X \in \mathbb{R}^{n\times d}}{\mathrm{argmin}}\ \mathrm{SW}_2^2(\gamma_X, \gamma_Y)$$
$$= \{Y \text{ up to a permutation}\}$$



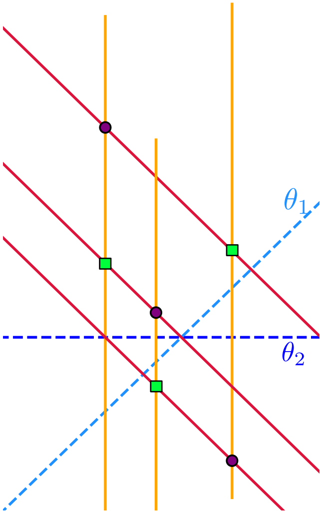
- $\widehat{\mathrm{SW}}_{2,p}$ is **not** a distance:

$$\widehat{\mathrm{SW}}_{2,p}(\gamma, \gamma_Y) = 0 \iff \forall i \in [\![1, p]\!],\ \theta_i\#\gamma = \theta_i\#\gamma_Y .$$

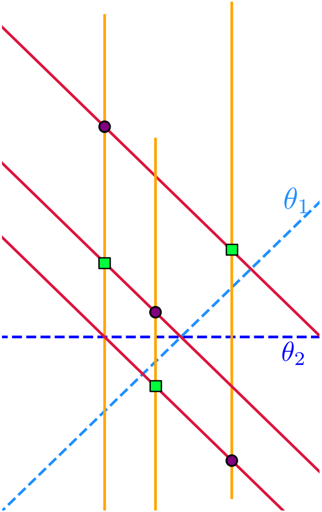


$\mathcal{E}_p$ with $p = 1$.

Reconstruction Problem



Reconstruction Problem



For $P_i : \mathbb{R}^d \longrightarrow \mathbb{R}^{d_i}$,
$$(\mathrm{RP}) : \ \forall i \in [\![1, p]\!],\ P_i\#\gamma = P_i\#\gamma_Y.$$

a.s. Reconstruction [4]

If $\sum_i d_i > d$, for $Y \in \mathbb{R}^{n\times d}$ fixed, $\mathcal{S}_{\mathrm{RP}} = \{\gamma_Y\}$, almost-surely, for random (P_i).

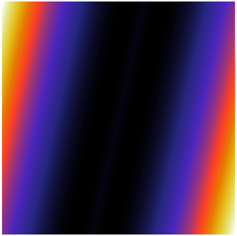
Consequences of the Reconstruction Problem on $\mathcal{E}_p$

If $p \leq d$,

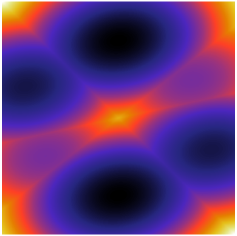
$$\mathcal{E}_p(X) = 0 \not\Longrightarrow X \in \{Y \text{ up to a permutation}\}.$$

If $p > d$, almost-surely,

$$\mathcal{E}_p(X) = 0 \Longrightarrow X \in \{Y \text{ up to a permutation}\}.$$



$\mathcal{E}_p$ with $p = 1$.



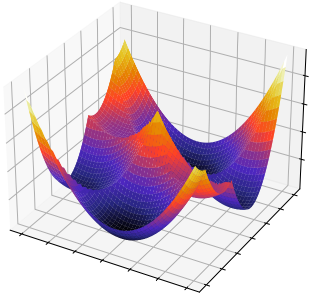
$\mathcal{E}_p$ with $p = 3$.

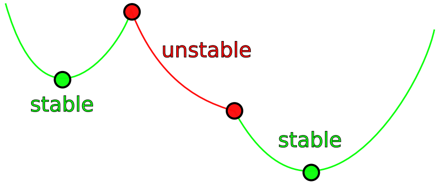
$\mathcal{E}_p$ Cell Decomposition

$$\mathcal{E}_p(X) = \frac{1}{p}\sum_{i=1}^{p} \mathrm{W}_2^2(\theta_i\#\gamma_X, \theta_i\#\gamma_Y) = \min_{(\sigma_1,\cdots,\sigma_p)\in\mathfrak{S}_n^p} \frac{1}{np}\sum_{i=1}^{p}\sum_{k=1}^{n}(\theta_i^T(x_k - y_{\sigma_i(k)}))^2.$$

$\mathcal{E}_p$ Cell Decomposition

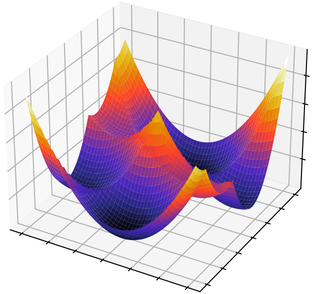
$$\mathcal{E}_p(X) = \frac{1}{p}\sum_{i=1}^{p} \mathrm{W}_2^2(\theta_i\#\gamma_X, \theta_i\#\gamma_Y) = \min_{(\sigma_1,\cdots,\sigma_p)\in\mathfrak{S}_n^p} \frac{1}{np}\sum_{i=1}^{p}\sum_{k=1}^{n}(\theta_i^T(x_k - y_{\sigma_i(k)}))^2.$$

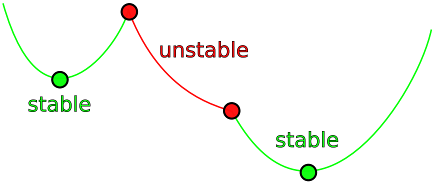




$\mathcal{E}_p$ Cell Decomposition

$$\mathcal{E}_p(X) = \frac{1}{p}\sum_{i=1}^{p} \mathrm{W}_2^2(\theta_i\#\gamma_X, \theta_i\#\gamma_Y) = \min_{(\sigma_1,\cdots,\sigma_p)\in\mathfrak{S}_n^p} \frac{1}{np}\sum_{i=1}^{p}\sum_{k=1}^{n}(\theta_i^T(x_k - y_{\sigma_i(k)}))^2.$$



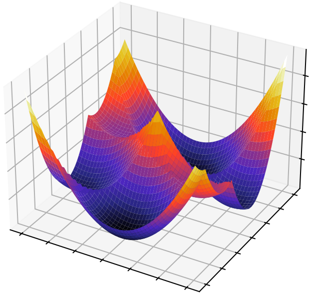


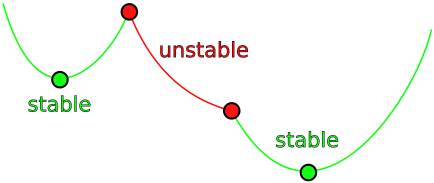
Cell Optima [5]

$\nabla\mathcal{E}_p(X) = 0 \iff X$ is min of a stable cell $\iff X$ is a local min.

$\mathcal{E}_p$ Cell Decomposition

$$\mathcal{E}_p(X) = \frac{1}{p}\sum_{i=1}^{p} \mathrm{W}_2^2(\theta_i\#\gamma_X, \theta_i\#\gamma_Y) = \min_{(\sigma_1,\cdots,\sigma_p)\in\mathfrak{S}_n^p} \frac{1}{np}\sum_{i=1}^{p}\sum_{k=1}^{n}(\theta_i^T(x_k - y_{\sigma_i(k)}))^2.$$



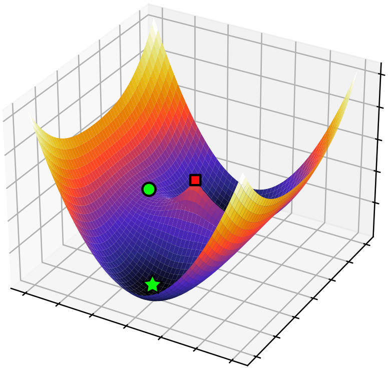


Cell Optima [5]

$\nabla\mathcal{E}_p(X) = 0 \iff X$ is min of a stable cell $\iff X$ is a local min.

As $p \longrightarrow +\infty$, $\mathcal{E}_p \approx \mathcal{E}$, more local optima but better optimisation.

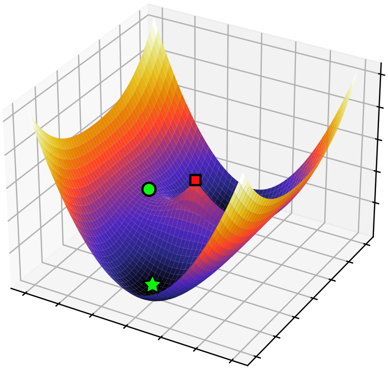
$\mathcal{E}$ Differentiable Critical Points



Critical Points of $\mathcal{E}$ [5]

$$\forall X \in \mathcal{D}_{\mathcal{E}},$$
$$\nabla \mathcal{E}(X) = 0 \iff F(X) = X$$

$\mathcal{E}$ Differentiable Critical Points



Critical Points of $\mathcal{E}$ [5]

$$\forall X \in \mathcal{D}_{\mathcal{E}},$$
$$\nabla \mathcal{E}(X) = 0 \iff F(X) = X$$

Critical Point Approximation [5]

For X_p critical points of $\mathcal{E}_p$, $\quad X_p - F(X_p) \xrightarrow[p \longrightarrow +\infty]{\mathbb{P}} 0.$

1. The Discrete Sliced Wasserstein Distance
2. Optimisation Properties
3. **SGD Convergence**
4. SGD for Training SW Neural Networks

Convergence of Interpolated Trajectories

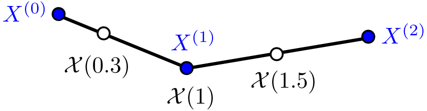
SGD on $\mathbb{E}_{\theta\sim\mathcal{U}(\mathbb{S}^d)}\left[\underbrace{\mathrm{W}_2^2(\theta\#\gamma_X, \theta\#\gamma_Y)}_{w_\theta(X)}\right]$:

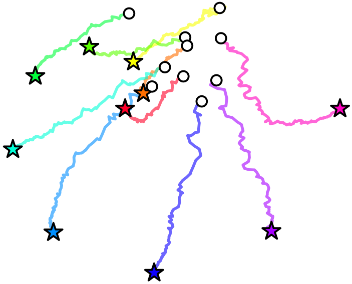
$$X^{(k+1)} = X^{(k)} - \alpha\nabla w_{\theta^{(k+1)}}(X^{(k)})$$

Convergence of Interpolated Trajectories

SGD on $\mathbb{E}_{\theta\sim\mathcal{U}(\mathbb{S}^d)}\left[\underbrace{\mathrm{W}_2^2(\theta\#\gamma_X, \theta\#\gamma_Y)}_{w_\theta(X)}\right]$:

$$X^{(k+1)} = X^{(k)} - \alpha\nabla w_{\theta^{(k+1)}}(X^{(k)})$$

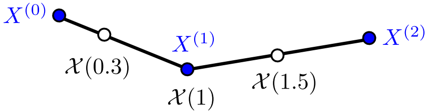


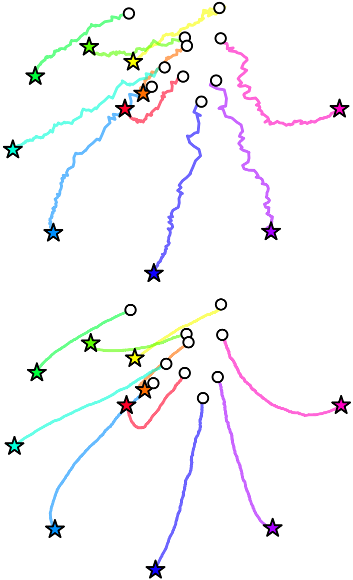


Convergence of Interpolated Trajectories

SGD on $\mathbb{E}_{\theta \sim \mathcal{U}(\mathbb{S}^d)}\left[\underbrace{\mathrm{W}_2^2(\theta \# \gamma_X, \theta \# \gamma_Y)}_{w_\theta(X)}\right]$:

$$X^{(k+1)} = X^{(k)} - \alpha \nabla w_{\theta^{(k+1)}}(X^{(k)})$$





Interpolations Converge [5]

$$d(\mathcal{X}_\alpha, \mathcal{S}) \xrightarrow[\alpha \to 0]{\mathbb{P}} 0.$$

With $\mathcal{S} = \left\{ \mathcal{X} \;\middle|\; \frac{\mathrm{d}\mathcal{X}}{\mathrm{d}t}(t) \in -\partial_C \mathcal{E}(\mathcal{X}(t)) \right\}$.

Using results from Bianchi et al. [1]

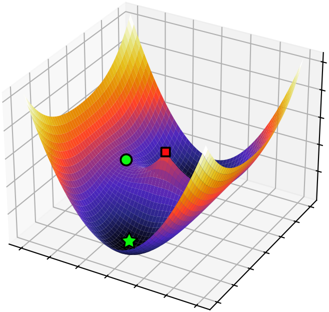
Convergence of Noised Trajectories

Noised SGD: $X^{(k+1)} = X^{(k)} - \alpha \nabla w_{\theta^{(k+1)}}(X^{(k)}) + \alpha \varepsilon^{(k+1)}$.

Convergence of Noised SGD [5]

$$\overline{\lim_{k \longrightarrow +\infty}} d(X_\alpha^{(k)}, \mathcal{Z}) \xrightarrow[\alpha \longrightarrow 0]{\mathbb{P}} 0.$$

With $\mathcal{Z} = \left\{ X \in \mathbb{R}^{n \times d} \mid 0 \in -\partial_C \mathcal{E}(X) \right\}$.



Using results from Bianchi et al. [1]

Convergence of Decreasing-Step Noised Trajectories

$$X^{(k+1)} = X^{(k)} - \alpha^{(k)}\nabla w_{\theta^{(k+1)}}(X^{(k)}) + \alpha\varepsilon^{(k+1)}.$$

Steps $\alpha^{(k)} \geq 0$ with $\sum_{k=0}^{+\infty} \alpha^{(k)} = +\infty$ and $\sum_{k=0}^{+\infty} (\alpha^{(k)})^2 < +\infty$.

Convergence of Decreasing-Step Noised SGD [5]

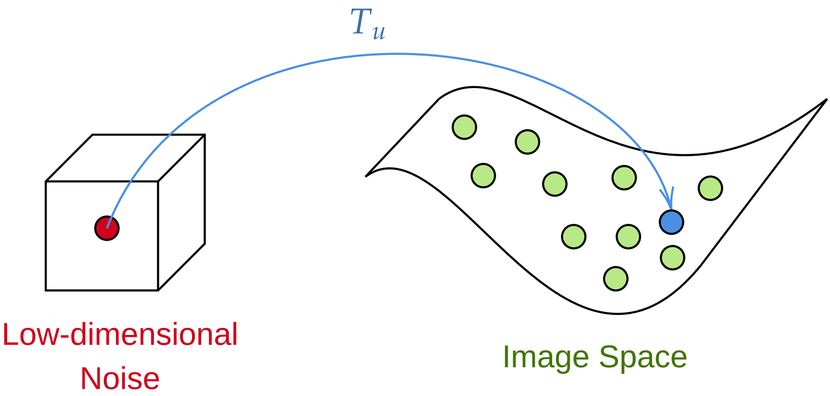
If $(X^{(k)})$ is a.s. bounded, then a.s.:

- $(\mathcal{E}(X^{(k)})_k$ converges.
- If $X^{(\varphi(k))} \xrightarrow[k \longrightarrow +\infty]{} X^\infty$, then $X^\infty \in \mathcal{Z}$.

With $\mathcal{Z} = \left\{X \in \mathbb{R}^{n\times d} \mid 0 \in -\partial_C \mathcal{E}(X)\right\}$.

Using results from Davis et al. [2]

Generative Modelling



Problem Statement

Goal: approximate $T_u \# \mathbb{x} \approx \mathbb{y}$.
Loss sample:

$$f(u, X, Y, \theta) = \mathrm{W}_2^2(\theta \# T_u \# \gamma_X, \theta \# \gamma_Y), \quad X \sim \mathbb{x}^{\otimes n},\ Y \sim \mathbb{y}^{\otimes n},\ \theta \sim \sigma.$$

Population loss:

$$F(u) = \mathop{\mathbb{E}}_{X,Y,\theta}\left[\mathrm{W}_2^2(\theta \# T_u \# \gamma_X, \theta \# \gamma_Y)\right] = \mathop{\mathbb{E}}_{X,Y}\left[\mathrm{SW}_2^2(T_u \# \gamma_X, \gamma_Y)\right].$$

Convergence Results [3]

Under technical assumptions:

- Approximation of (Clarke) gradient flows
- Convergence in the parameters $u^{(t)}$ for a modified SGD scheme

Thank You

[1] Pascal Bianchi, Walid Hachem, and Sholom Schechtman.
Convergence of constant step stochastic gradient descent for non-smooth non-convex functions.
Set-Valued and Variational Analysis, 30(3):1117–1147, 2022.

[2] Damek Davis, Dmitriy Drusvyatskiy, Sham Kakade, and Jason D Lee.
Stochastic subgradient method converges on tame functions.
Foundations of computational mathematics, 20(1):119–154, 2020.

[3] Eloi Tanguy.
Convergence of sgd for training neural networks with sliced Wasserstein losses.
Transactions on Machine Learning Research, October 2023.

[4] Eloi Tanguy, Rémi Flamary, and Julie Delon.
Reconstructing discrete measures from projections. consequences on the empirical sliced Wasserstein distance.
arXiv preprint arXiv:2304.12029, 2023.

[5] Eloi Tanguy, Rémi Flamary, and Julie Delon.
Properties of discrete sliced Wasserstein losses.