Shedding a PAC-Bayesian Light on Adaptive Sliced-Wasserstein Distances

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Abstract

The Sliced-Wasserstein distance (SW) is a computationally efficient and theoretically grounded alternative to the Wasserstein distance. Yet, the literature on its statistical properties – or, more accurately, its generalization properties – with respect to the distribution of slices, beyond the uniform measure, is scarce. To bring new contributions to this line of research, we leverage the PAC-Bayesian theory and a central observation that SW may be interpreted as an average risk, that yields maximally discriminative SW, by optimizing our theoretical bounds, and iii) empirical illustrations of our theoretical findings.

1. Introduction

The Wasserstein distance is a metric between probability distributions and a key notion of the optimal transport framework (Villani, 2009; Peyré & Cuturi, 2019). Over the past years, it has received a lot of attention from the machine learning community because of its theoretical grounding and the increasing number of problems relying on the computation of distances between measures (Solomon et al., 2014; Froger et al., 2015; Montavon et al., 2016; Kolouri et al., 2017; Courty et al., 2016; Schmitz et al., 2018), such as the learning of deep generative models (Arjovsky et al., 2017; Bousquet et al., 2017; Tolstikhin et al., 2017). As the measures μ and ν to be compared are usually unknown, the Wasserstein distance $W(\mu, \nu)$ is estimated through an “empirical” version $W(\mu_n, \nu_n)$, where $\mu_n = \{x_1, \ldots, x_n\}$ and $\nu_n = \{y_1, \ldots, y_n\}$ are i.i.d. samples from $\mu$ and $\nu$, respectively (without loss of generality, samples will be assumed to have the same size $n$). Due to its unfavorable $O(n^3 \log n)$ computational complexity, the Wasserstein distance scales badly on large datasets (Peyré & Cuturi, 2019) and alternatives have been devised to overcome this limitation, such as the Sinkhorn algorithm (Cuturi, 2013; Cuturi & Peyré, 2016), multi-scale (Oberman & Ruan, 2015) or sparse approximations approaches (Schmitzer, 2016).

The Sliced-Wasserstein distance (SW) (Rabin et al., 2012) is another computationally efficient alternative, which takes advantage of the closed-form and fast computation of the one-dimensional Wasserstein distance. For $d$-dimensional ($d > 1$) samples $\{x_1, \ldots, x_n\}$ and $\{y_1, \ldots, y_n\}$, the computation of $SW(\mu_n, \nu_n)$ is done by uniformly sampling $m$ projection directions $\{\theta_1, \ldots, \theta_m\}$ and by averaging the $m$ one-dimensional Wasserstein distances $W(\langle \theta_j, x_1 \rangle, \ldots, \langle \theta_j, x_n \rangle; \langle \theta_j, y_1 \rangle, \ldots, \langle \theta_j, y_n \rangle)$ for $j = 1, \ldots, m$. SW has been analyzed theoretically (Bonnotte, 2013; Nadjahi et al., 2019; Bayraktar & Guo, 2021; Nadjahi et al., 2020b), refined to gain additional efficiency (Nadjahi et al., 2021) and to handle “nonlinear” projections (Kolouri et al., 2019a, 2020), and it has been successfully used in a variety of machine learning tasks (Bonneel et al., 2015; Kolouri et al., 2016; Carriere et al., 2017; Lutkus et al., 2019; Deshpande et al., 2018; Kolouri et al., 2018; 2019b; Nadjahi et al., 2020a; Bonet et al., 2021; Rakotomamonjy & Ralaivola, 2021). A direction to yet improve SW consists in adapting $\rho$, the distribution $\{\theta_i\}_{i=1}^m$ in a data-dependent manner, as done by maximum SW (max-SW, Deshpande et al., 2019), which aims at finding a unique slice $\theta_*$ (or equivalently, the Dirac measure $\delta_{\theta_*}$) that maximizes the one-dimensional Wasserstein distance, or distributional SW (DSW) (Nguyen et al., 2021), which seeks for a maximally discriminative distribution on the unit sphere. These works fall into the class of what we refer as adaptive Sliced-Wasserstein distances and denote $SW(\cdot; \rho)$, overloading the $SW(\cdot, \cdot)$ notation to make explicit the dependence on $\rho$.

A question of interest in adaptive SW, which has not been explicitly addressed in previous work, is whether one can learn a distribution $\rho^*(\mu_n, \nu_n)$ from training data, such that $SW_\rho(\mu, \nu; \rho^*(\mu_n, \nu_n))$ is guaranteed to be highly discrimin-
inative. In our work, we address this problem by measuring the “generalization” gap between $SW_p^P(\mu_n, \nu_n; \rho)$ and $SW_p^P(\mu, \nu; \rho)$. Bounds on this gap can be derived from existing results for max-SW [Lin et al. 2021; Niles-Weed & Rigollet 2022]. However, it is unclear how these bounds are able to accommodate distributions $\rho$ that are not reduced to Dirac measures. To go that direction, we propose the first connection between adaptive SW and PAC-Bayesian theory and we derive a novel set of flexible PAC-Bayesian generalization bounds. Our bounds state that with probability $1 - \delta$, the following holds for all measures (with non-discrete support) $\rho$ on the $d$-dimensional unit sphere: $SW(\mu, \nu; \rho) \geq SW(\mu_n, \nu_n; \rho) - \varepsilon(n, \rho, \delta)$, where $\varepsilon$ can be written explicitly and captures the properties of $\mu, \nu$, and allows us to control the tightness of the bound via $\rho$.

Three key reasons make the PAC-Bayesian theory [McAllester 1999; Catoni 2007; Alquier 2021] particularly suited to characterize the generalization properties of adaptive SW. First, from a general perspective, the literature shows this framework allows the derivation of tight bounds that can be converted into effective learning procedures [Ambroladze et al. 2007; Laviolette et al. 2006; Germain et al. 2009; Zantedeschi et al. 2021]. Second, PAC-Bayesian bounds deal with the generalization ability of learned distributions; while those distributions usually lie on spaces of predictors, the distributions $\rho$ of interest in our case are the distributions of slices. Lastly, a key quantity of PAC-Bayesian bounds is the average empirical risk which, as we will show, can naturally be interpreted as $SW_p^P(\mu_n, \nu_n; \rho)$, our main focus.

The paper is organized as follows. In Section 2, we recall essential notions of Sliced-Wasserstein distances and PAC-Bayesian theory. We then delve into our contributions: i) a generic PAC-Bayesian bound for adaptive Sliced-Wasserstein distances and refinements to specific settings (Section 3), ii) a theoretically-grounded procedure to train a maximally discriminative Sliced-Wasserstein distances (Section 4) and iii) illustrations of the soundness of our theoretical results through numerical experiments, conducted on both toy and real-world datasets (Section 5).

Notations. Let $d \in \mathbb{N}^*$ with $\mathbb{N}^* = \mathbb{N} \setminus \{0\}$. For $x, y \in \mathbb{R}^d$, $(x, y)$ denotes the dot product between $x$ and $y$, and $\|x\|$ is the Euclidean norm of $x$. For $X \subset \mathbb{R}^d$, $\mathcal{P}(X)$ is the set of probability measures supported on $X$, and $\mathcal{P}_n(X)$ is the set of probability measures supported on $X$ with finite moment of order $q$. $\mathcal{U}(X)$ is the uniform distribution on $X$, and $\delta_x$ is the Dirac measure with mass on $x \in X$. For $\mu \in \mathcal{P}(X)$ and $n \in \mathbb{N}^*$, $\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$ is the empirical measure supported on $n$ samples $\{x_1, \ldots, x_n\}$ i.i.d. from $\mu$. For $\mu \in \mathcal{P}(\mathbb{R})$, $F_\mu$ is the cumulative distribution function (c.d.f.) of $\mu$ and $F_\mu^{-1}$ is its quantile function.



## 2. Background

### 2.1. Sliced-Wasserstein Distances

Sliced-Wasserstein distances refer to a family of distances between probability measures, which was first introduced by [Rabin et al. 2012] to overcome the computational issues of the Wasserstein distance. We formally define the Wasserstein distance and SW, and explain why the latter can provide significant computational advantages over the former. In what follows, we fix $X \subset \mathbb{R}^d$.

**Definition 1** (Wasserstein distance). Let $p \in [1, +\infty)$. The Wasserstein distance of order $p$ between $\mu, \nu \in \mathcal{P}(X)$ is

$$W_p^\mu(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times X} \|x - y\|^p d\pi(x, y),$$

where $\Pi(\mu, \nu) \subset \mathcal{P}(X \times X)$ denotes the set of probability measures on $X \times X$, whose marginals with respect to the first and second variables are $\mu$ and $\nu$, respectively.

While $W_p$ has been shown to possess appealing theoretical properties, e.g. it is a metric on $\mathcal{P}_p(X)$ which metrizes the weak convergence [Villani 2009, Chapter 6], it is computationally too demanding in general. Indeed, consider two discrete distributions $\mu_n, \nu_n$, each supported on $n$ samples. Computing $W_p(\mu_n, \nu_n)$ means solving a linear program [Peyré & Cuturi 2019, Section 3.1], whose solution is not analytically available in general, but can be approximated with standard solvers from linear programming and combinatorial optimization. However, such methods have a super-cubic cost in practice, and their worst-case computational complexity scales in $O(n^3 \log n)$.

Nevertheless, if $\mu, \nu \in \mathcal{P}(\mathbb{R})$, $W_p(\mu, \nu)$ admits an analytical expression which can be efficiently approximated [Peyré & Cuturi 2019, Section 2.6]: for any $\mu, \nu \in \mathcal{P}(\mathbb{R})$,

$$W_p^\mu(\mu, \nu) = \int_0^1 |F_\mu^{-1}(t) - F_\nu^{-1}(t)|^p dt.$$

In particular, for $\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$ and $\nu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{y_i}$ such that, $\forall i \in \{1, \ldots, n\}$, $x_i, y_i \in \mathbb{R}$,

$$W_p^\mu(\mu_n, \nu_n) = \frac{1}{n} \sum_{i=1}^{n} |x_{(i)} - y_{(i)}|^p,$$

where $x_{(1)} \leq x_{(2)} \leq \cdots \leq x_{(n)}$, $y_{(1)} \leq y_{(2)} \leq \cdots \leq y_{(n)}$. Computing (1) thus consists in sorting the support points of $\mu_n$ and $\nu_n$, which induces $O(n \log n)$ operations.

Sliced-Wasserstein distances leverage the fast computation of $W_p(\mu, \nu)$ for any $\mu, \nu \in \mathcal{P}(\mathbb{R})$ to efficiently compare distributions supported on medium to high-dimensional spaces. Their formal characterization is given below.

**Definition 2** (Sliced-Wasserstein distance). Let $S^{d-1} = \{\theta \in \mathbb{R}^d : \|\theta\| = 1\}$ be the unit sphere in $\mathbb{R}^d$. For
θ ∈ S^{d−1}, denote by θ∗ : Rd → R the linear map such that for x ∈ Rd, θ∗(x) = ⟨θ, x⟩. Let p ∈ [1, +∞) and ρ ∈ P(S^{d−1}). The Sliced-Wasserstein distance of order p based on ρ is defined for μ, ν ∈ P(X) as

$$SW^p_μ(µ, ν; ρ) = \frac{1}{n} \sum_{j=1}^n W_p^p(θ_j^μ, θ_j^ν) dρ(θ),$$

where for any measurable function f and ξ ∈ P(Rd), fξ is the push-forward measure of ξ by f: for any measurable set A ⊂ R, fξ(A) = ξ(f^−1(A)), f^−1(A) = {x ∈ Rd : f(x) ∈ A}.

Computational complexity of SW. By (2), SW^p_μ(µ, ν; ρ) is obtained by computing E[W_p^p(θ_j^μ, θ_j^ν)] with E taken over θ ∼ ρ. This expectation is intractable in general, and commonly approximated with the Monte Carlo estimate

$$\tilde{SW}^p_μ(µ, ν; ρ) = \frac{1}{n} \sum_{j=1}^n W_p^p(θ_j^μ, θ_j^ν),$$

where {θ_j}^n_{j=1} are i.i.d. samples from ρ. Note that for θ ∈ S^{d−1}, θ_j^μ and θ_j^ν are one-dimensional probability measures, which can be interpreted as projections of μ and ν along θ. To illustrate this, consider μ_n = (1/n) \sum_{i=1}^n δ_{x_i} with x_i ∈ Rd for i ∈ {1, . . . , n}. By definition, θ_j^μ_n = (1/n) \sum_{i=1}^n δ_{θ(x_i)}. Therefore, computing E[W_p^p(θ_j^μ, θ_j^ν)] between μ_n and ν_n amounts to projecting {x_i}^n_{i=1} and {y_i}^n_{i=1} along θ_j ∼ ρ, then computing the one-dimensional Sliced-Wasserstein distance using (1), for j ∈ {1, . . . , m}. This scheme requires O(mdn + n log n) operations which is, in general, faster than computing W_p^p(μ_n, ν_n), especially for large n.

Theoretical properties of SW. Previous works have investigated theoretical properties of SW^p_μ(µ, ν; ρ), to explain its empirical success (Bonnitte, 2013; Bayraktar & Guo, 2021; Nadjaï et al., 2019; Lin et al., 2021; Nguyen et al., 2021). However, most results apply to ρ = U(S^{d−1}) only (which corresponds to the original definition of SW, (Kabin et al., 2012)). In particular, whether (2) is a metric for any ρ has not been established: we show in Appendix A1.1 that SW^p_μ(µ, ν; ρ) is always a pseudo-metric, and we discuss for which choices of ρ it satisfies all metric axioms.

Adaptive SW. Recent works have argued that the uniform distribution may not be the most relevant choice, depending on the task at hand. Instead, they proposed to learn ρ from the observed data. This strategy provides SW^p_μ(µ, ν; ρ) with an actual degree of freedom ρ, and motivates the term adaptive Sliced-Wasserstein distance. Specifically, (Deshpande et al. 2019) and (Nguyen et al. 2021) solve a tailored optimization problem in ρ targeting a high discriminative power of ρ, in the sense that ρ puts more mass on the θ ∈ S^{d−1} that maximize the separation of θ_j^μ and θ_j^ν. The maximum Sliced-Wasserstein distance (max-SW, (Deshpande et al., 2019)) is defined as

$$\maxSW(µ, ν) = \max_{ρ ∈ P(S^{d−1})} SW^p_ρ(µ, ν; ρ)$$

with $ρ_{maxSW}(µ, ν) = \arg \sup_{ρ ∈ P(S^{d−1})} SW^p_ρ(µ, ν; ρ)$.

While the distributional Sliced-Wasserstein distance (DSW, (Nguyen et al., 2021)) is given by

$$DSW(µ, ν) = \max_{ρ ∈ P(S^{d−1})} SW^p_ρ(µ, ν; ρ)$$

with $ρ_{DSW}(µ, ν) = \arg \sup_{ρ ∈ P(S^{d−1})} SW^p_ρ(µ, ν; ρ)$.

Where in (7), θ and θ' are independent and C > 0 is a hyperparameter. We have decoupled the search for the maximizing distances (6) and the maximum arguments (5) for reasons we clarify below.

While there exist statistical guarantees on the gap between maxSW(µ, ν) and DSW(µ, ν) (Lin et al., 2021; Niles-Weed & Rigollet, 2022) (or between DSW(µ, ν) and DSW(µ, ν_n)) (Nguyen et al., 2021), there is no explicit theoretical argument on the error entailed by the learned distribution $ρ_{maxSW}(µ, ν_n)$ (or $ρ_{DSW}(µ, ν_n)$) considered on its own, outside the optimization procedure of max-SW (or DSW). Given new samples {x_1, . . . , x_n} and {y_1, . . . , y_n} from μ and ν, with empirical distributions $µ_n$ and $ν_n$, there is no guarantee for SW^p_ρ(µ_n, ν_n; ρ_{maxSW}(µ_n, ν_n)) to be high, or in other words, there is no argument ensuring the discriminative power of $ρ_{maxSW}(µ_n, ν_n)$. One way to palliate this lack of theory and to go one step further than the max-SW and DSW cases, is to derive general results relating SW^p_ρ(µ_n, ν_n; ρ) and SW^p_ρ(µ, ν; ρ), for families of distributions ρ ∈ P(S^{d−1}). This is what we bring in the present work in the form of a generalization bound rooted in the PAC-Bayesian theory.

2.2. PAC-Bayesian Theory

PAC-Bayesian theory aims at assessing the ability of learning algorithms to generalize to unseen data, by deriving generalization bounds. Let X ⊂ Rd, q ∈ N*, and S_n = {z_i}^n_{i=1} a dataset of i.i.d. samples from an unknown probability measure ξ ∈ P(X). Consider a learning algorithm whose outputs depend on the training data S_n and a vector of parameters ω ∈ Ω. The performance of such algorithm can be assessed via a loss function ℓ : Ω × X → R_+.

Fix ω ∈ Ω. The empirical ℓ-risk $\hat{r}_\ell(ω, S_n)$ and true ℓ-risk $r_\ell(ω)$ are defined as

$$\hat{r}_\ell(ω, S_n) = \frac{1}{n} \sum_{i=1}^n ℓ(ω, z_i)$$

$$r_\ell(ω) = E_{z \sim ξ} [ℓ(ω, z)]$$

A key objective of a learning procedure is to optimize (e.g. minimize) the true risk (9), which in practice cannot be achieved, because ξ is unknown. Instead, one focuses on optimizing (8) over ω ∈ Ω, a sound strategy provided the
minimizer of $\hat{\psi}$ accurately estimates the minimizer of $\psi$; this can be assessed via PAC-Bayesian bounds.

Let $\rho \in P(\Omega)$. PAC-Bayesian theory analyzes the generalization ability of $\rho$ by measuring the gap between the average empirical $\ell$-risk $E_{X \sim \rho}[r_\ell(X, S_n)]$ and the average true $\ell$-risk $E_{X \sim \rho}[r_\ell(X)]$. A classical PAC-Bayesian bound was derived by (Catoni, 2003) and is recalled below.

**Theorem 1** ([Catoni, 2003]). Let $\rho_0 \in P(\Omega)$ be a prior distribution. Assume that $0 \leq \ell \leq C$. For all $\lambda > 0$, for any $\delta \in (0, 1)$, the following holds with probability at least $1 - \delta$ (over the draw of the dataset $S_n$): \( \forall \rho \in P(\Omega), \)

$$E_{\omega \sim \rho}[r_\ell(\omega)] \leq E_{\omega \sim \rho}[r_\ell(\omega, S_n)] + \frac{\lambda C^2}{8n} + \frac{1}{\lambda} \left( KL(\rho || \rho_0) + \log \frac{1}{\delta} \right),$$

where $KL(\rho || \rho_0)$ is the Kullback-Leibler divergence between $\rho$ and $\rho_0$; if $\rho$ is absolutely continuous with respect to $\rho_0$, $KL(\rho || \rho_0) = \int \log(\rho(\omega)/\rho_0(\omega)) \rho(\omega) \, d\omega$.

The literature on PAC-Bayes is rich of many other bounds, and we refer to (Alquier, 2021) for an extensive survey.

In our work, we focus on Catoni’s bound because it is known bounds) as are the proof techniques used to derive it (Alquier, 2021; Section 2).

**Applications.** PAC-Bayesian bounds allow to control the true risk via a function depending on the empirical risk. For example, minimizing the left-hand side term of Catoni’s bound (10) over $\rho \in P(\Omega)$ yields a data-dependent distribution which guarantees the highest generalization ability (Alquier, 2021; Section 2.1.2). PAC-Bayesian theory was also applied for specific tasks, e.g., classification (McAllister, 1999), ranking (Kalaivaola et al., 2010), density estimation (Higgs & Shawe-Taylor, 2010), deep learning (Dziugaite & Roy, 2017; Cherief-Abdellatif et al., 2022).

### 3. Generalization Bounds for Adaptive Sliced-Wasserstein Distances

In this section, we leverage the PAC-Bayesian framework to derive generalization bounds for adaptive Sliced-Wasserstein distances. Proofs are deferred to Appendix A2.

Before presenting our main results, we clarify the notion of generalization for adaptive SW. In practice, since one generally has access to data generated from unknown probability measures $\mu, \nu$, empirical estimates $SW^p_p(\mu, \nu; \rho)$ are computed instead of $SW_p^p(\mu, \nu; \rho)$. Besides, adaptive SW means that an algorithm is deployed to learn $\rho$ from $\mu_n, \nu_n$, so that $SW^p_p(\mu_n, \nu_n; \rho)$ is sufficiently discriminative (Section 2.1). In this context, the learning algorithm is said to generalize well if the distribution learned from $\mu_n, \nu_n$ (denoted by $\rho(\mu_n, \nu_n)$) is such that $SW^p_p(\cdot, \cdot; \rho(\mu_n, \nu_n))$ is discriminative, even on unseen data. More formally, given new samples $\{x'_1, \ldots, x'_n\}$ and $\{y'_1, \ldots, y'_n\}$ from $\mu$ and $\nu$, with associated empirical distributions $\mu'_n$ and $\nu'_n$, $SW^p_p(\mu'_n, \nu'_n; \rho(\mu_n, \nu_n))$ should be large.

Therefore, we measure generalization as the gap between $SW^p_p(\mu, \nu; \rho)$ and $SW^p_p(\mu_n, \nu_n, \rho)$ for any $\rho \in P(S^{-1})$. We first derive a general bound on this gap, using PAC-Bayesian theory, then refine it to specific settings directed by conditions on the supports and the moments of $\mu$ and $\nu$.

#### 3.1. A Generic Generalization Bound

We establish a first generalization bound for adaptive SW, by combining statistical properties of adaptive SW and techniques from PAC-Bayesian theory.

**Theorem 2.** Let $p \in [1, +\infty)$ and $\mu, \nu \in P_p(\mathbb{R}^d)$. Assume there exists a constant $\varphi_{\mu, \nu, p}$ possibly depending on $\mu, \nu$ and $p$ such that: \( \forall \lambda > 0, \forall \theta \in \mathbb{S}^{d-1}, \)

$$E \left[ \exp \left( \lambda \left( W_p^p(\theta_p^* \mu_n, \theta_p^* \nu_n) - E[W_p^p(\theta_p^* \mu_n, \theta_p^* \nu_n)] \right) \right) \right] \leq \exp(\lambda^2 \varphi_{\mu, \nu, p} n^{-1}),$$

where $E$ is taken with respect to the support points of $\mu_n$ and $\nu_n$. Additionally, assume there exists $\psi_{\mu, \nu, p} : \mathbb{N}^* \rightarrow \mathbb{R}_+$, possibly depending on $\mu, \nu$ and $p$, such that, \( \forall \rho \in P(\mathbb{S}^{d-1}), \)

$$E[SW_p^p(\mu_n, \nu_n; \rho) - SW_p^p(\mu, \nu; \rho)] \leq \psi_{\mu, \nu, p}(n).$$

Let $\rho_0 \in P(\mathbb{S}^{d-1})$. Then, for any $\delta \in (0, 1)$, the following holds with probability at least $1 - \delta$: \( \forall \rho \in P(\mathbb{S}^{d-1}), \)

$$SW_p^p(\mu, \nu; \rho) \geq SW_p^p(\mu_n, \nu_n; \rho) - \frac{\lambda}{n} \varphi_{\mu, \nu, p} - \frac{1}{\lambda} \left( KL(\rho || \rho_0) + \log \left( \frac{1}{\delta} \right) \right) - \psi_{\mu, \nu, p}(n).$$

#### Link with PAC-Bayesian theory.** Theorem 2 can be interpreted as a novel PAC-Bayesian bound tailored to adaptive SW: the formal analogy between classical PAC-Bayesian framework and our work is summarized in Table 1. The key element is that $W_p^p(\theta_p^* \mu_n, \theta_p^* \nu_n)$ for some $\theta \in \mathbb{S}^{d-1}$

| PAC-Bayes framework | Our framework |
|---------------------|--------------|
| $\{ z_i \}_{i=1}^{n} \in \{ (x_i, y_i) \}_{i=1}^{n}$ | $\{ (x_i, y_i) \}_{i=1}^{n}$ |
| $\xi \in P(A)$ | $\mu \times \nu \in P(\mathbb{R}^d) \times P(\mathbb{R}^d)$ |
| $\omega \in \Omega$ | $\theta \in \mathbb{S}^{d-1}$ |
| $\hat{r}(\omega, \{ z_i \}_{i=1}^{n})$ | $W_p^p(\theta_p^* \mu_n, \theta_p^* \nu_n)$ |
| $E_{\omega \sim \rho}[\hat{r}(\omega, \{ z_i \}_{i=1}^{n})]$ | $SW_p^p(\mu_n, \nu_n; \rho)$ |
| $E_{\omega \sim \rho}[r(\omega)]$ | $E_{\omega \sim \rho}[r(\omega)]$ |

Table 1. Analogy between PAC-Bayes theory and our work.
We now clarify the role of each term involved in (12). Varadhan’s lemma, hence the KL divergence. As we elaborate on this in Appendix A2.1.

\[ \rho, \phi \]

Then, the quantities \( \frac{\partial D_{\text{KL}}(\mu, \nu)}{\partial \rho} \) equal-the dualization gap can be further illustrated with the examples introduced in Appendix A2.5. More precisely, the KL divergence results from a change of measure inequality known as Donsker-Varadhan’s lemma \( \text{(Donsker & Varadhan, 1975)} \). Previous work have applied other change of measure inequalities to derive PAC-Bayesian bounds \( \text{in (Alquier, 2021, Section 2.1.3)} \). More precisely, the KL divergence can be deduced, using \( \text{Lin et al., 2021, Section 2.1.3) to compute the explicit form of} \psi_{\mu, \nu, p} \text{in this setting.} \)

**3.2. Application to Measures with Bounded Support**

We first consider distributions supported on a bounded domain. We derive \( \varphi_{\mu, \nu, p} \) by applying similar arguments as in the proof of McDiarmid’s inequality \( \text{(McDiarmid, 1989)} \), similarly to \( \text{(Weed & Bach, 2019, Proposition 20)} \).

**Proposition 1.** Let \( X \subseteq \mathbb{R}^d \) such that \( X \) has a finite diameter \( \Delta \), i.e. \( \Delta \equiv \sup_{(x, x') \in X} \|x - x'\| < +\infty \). Let \( p \in [1, +\infty) \), \( \mu, \nu \in \mathcal{P}(X) \). Then, \( \mu, \nu \in \mathcal{P}(X) \) and \( \varphi_{\mu, \nu, p} = \Delta p/2 \).

Next, we adapt the proof of \( \text{(Manole et al., 2022, Lemma B.3)} \) to compute the explicit form of \( \psi_{\mu, \nu, p} \) in this setting.

**Proposition 2.** Let \( \mu, \nu \in \mathcal{P}(X) \), where \( X \subseteq \mathbb{R}^d \) has a finite diameter \( \Delta \). Let \( p \in [1, +\infty) \). Then, there exists a constant \( C \) such that, \( \psi_{\mu, \nu, p}(n) = C p \Delta n^{-1/2} \).

By combining Propositions 1 and 2, we refine Theorem 2 to distributions supported on a bounded domain: the resulting bound is given in Appendix A2.4.

**3.3. Application to Sub-Gaussian Measures**

Next, we apply Theorem 2 to distributions with unbounded supports. To handle this case, we assume specific constraints on the moments on \( \mu, \nu \), then derive \( \varphi_{\mu, \nu, p} \) by using generalizations of McDiarmid’s inequalities. More precisely, we assume that \( \mu, \nu \) are sub-Gaussian distributions.

**Definition 3 (Sub-Gaussian distribution).** Let \( \mu \in \mathcal{P}(\mathbb{R}^d) \) and \( \sigma > 0 \), \( \mu \) is a sub-Gaussian distribution with variance proxy \( \sigma^2 \) if the following holds: for any \( \theta \in \mathbb{S}^{d-1} \), for \( \lambda \in \mathbb{R} \), \( \int_{\mathbb{R}} \exp(\lambda t)\mathbb{d}(\theta^\top t \mu)(t) \leq \exp(\lambda^2 \sigma^2/2) \).

The next proposition results from applying the generalized McDiarmid’s inequality for unbounded spaces with finite sub-Gaussian diameter \( \text{(Kontorovich, 2014, Appendix A2.5)} \).

**Proposition 3.** Let \( \mu, \nu \in \mathcal{P}(\mathbb{R}^d) \) such that \( \mu, \nu \) are sub-Gaussian with variance proxy \( \sigma^2, \tau^2 \) respectively. Then, \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \) and \( \varphi_{\mu, \nu, 1} = \sigma^2 + \tau^2 \).

The last ingredient to specialize Theorem 2 is to derive \( \psi_{\mu, \nu, p} \) for \( \mu, \nu \) satisfying either Definition 3. To this end, we
leverage the rate recently established in (Manole et al., 2022, Theorem 2), which shows that \( \psi_{\mu,\nu,p} \) scales as \( n^{-1/2} \log(n) \) if \( \mu, \nu \) are sub-Gaussian distributions. Our final bound is obtained by plugging Proposition 3 and the explicit formula of \( \psi_{\mu,\nu,1} \) in Theorem 2. We present this result and its detailed proof in Appendix A2.7.

### 3.4. Bound for Measures with Bernstein moment conditions

We study a more general class of distributions: we consider sub-Gaussian distributions characterized by Definition 4. Consider \( \mu, \nu \) satisfying Definition 4. First, we leverage (Manole et al., 2022, Theorem 2) in that setting again, to show that \( \psi_{\mu,\nu,p} \) scales as \( n^{-1/2} \log(n) \) (Appendix A2.7). Then, we apply the Bernstein-type McDiarmid’s inequality given in (Lei, 2020, Theorem 5.1) to establish Proposition 4.

#### Proposition 4.
Let \( \mu, \nu \in \mathcal{P}(\mathbb{R}^d) \) be two distributions satisfying the Bernstein condition with parameters \( \sigma^2, b \) and \( (\tau^2, c) \), respectively. Let \( \sigma^2 = \max(\sigma^2, \tau^2) \), \( b_\lambda = \max(b, c) \). Then, \( \mu, \nu \in \mathcal{P}_1(\mathbb{R}^d) \) and, for any \( \lambda \in \mathbb{R}^*_+ \), \( \lambda < n/(2b_\lambda) \),

\[
E \left[ \exp \left( \lambda \left( \mathbb{W}_1(\theta^\star_\mu, \theta^\star_\nu) - \mathbb{W}_1(\theta^\star_\mu, \theta^\star_\nu) \right) \right) \right] 
\leq \exp(\lambda^2 \varphi_{\mu,\nu,1}(\lambda, n)^{-1}) ,
\]

(13)

where \( \varphi_{\mu,\nu,1}(\lambda, n) = 2\sigma^2 n^{-1}(1 - 2b_\lambda \lambda n)^{-1} \).

We emphasize the following difference between equations (13) and (11): \( \varphi_{\mu,\nu,1} \) is a function of \( \lambda \in \Lambda \subset \mathbb{R}_+ \) and \( n \in \mathbb{N}^* \), while in Theorem 2, \( \varphi_{\mu,\nu,p} \) is assumed to be a constant. Nevertheless, the proof of Theorem 2 can easily be adapted to derive a generic generalization bound assuming \( \varphi_{\mu,\nu,p} \) depends on \( \lambda, n \): we give the corresponding statement in Theorem A3. Hence, by plugging Proposition 4 and (Manole et al., 2022, Theorem 2) in Theorem A3, we derive the generalization bound for distributions under the Bernstein moment condition: see Appendix A2.7.

Note that for \( \mu, \nu \) satisfying Definition 3 or Definition 4, we derived \( \varphi_{\mu,\nu,p} \) for \( p = 1 \) only: the generalized McDiarmid’s inequalities used in the proofs of Propositions 3 and 4 can be applied if \( W^p \) is Lipschitz (Kontorovich, 2014; Lei, 2020). This property is easily verified for \( p = 1 \), but not for \( p > 1 \). Hence, the derivation of \( \varphi_{\mu,\nu,p} \) for \( p > 1 \) for such types of distributions with unbounded domains requires different proof techniques. We leave this problem for future work.

### 4. Optimization of Generalization Bounds for Adaptive SW

We develop a principled methodology to learn a highly discriminative Sliced-Wasserstein distance, by optimizing our PAC-Bayesian generalization bounds. The idea consists in making the lower bounds of \( SW^p_0(\mu, \nu; \rho) \) derived in Section 3 as tight as possible, in order to increase \( SW^p_0(\mu, \nu; \rho) \) while attaining a small generalization gap.

Given a training dataset \( \{(x_i, y_i)\}_{i=1}^n \) and a prior \( \rho_0 \in \mathcal{P}(\mathbb{S}^{d-1}) \), our objective is to find \( \rho^\star(\mu_n, \nu_n) \) such that,

\[
\rho^\star(\mu_n, \nu_n) = \arg \sup_{\rho \in \mathcal{F}} SW^p_0(\mu_n, \nu_n; \rho) - \frac{KL(\rho || \rho_0)}{\lambda} \tag{14}
\]

with \( \mathcal{F} \) a family of probability measures supported on \( \mathbb{S}^{d-1} \). The choice of \( \mathcal{F} \) manages the complexity of solving (14); it should allow simple optimization, while being flexible to make \( \rho^\star(\mu_n, \nu_n) \) expressive enough. We first propose to parameterize \( \mathcal{F} \) as the class of von Mises-Fisher distributions.

#### Definition 5.
The von Mises-Fisher distribution \( \text{vMF}(m, \kappa) \) with mean direction \( m \in \mathbb{S}^{d-1} \) and concentration parameter \( \kappa \in \mathbb{R}_+^* \) is a distribution on \( \mathbb{S}^{d-1} \) whose density is defined for \( \theta \in \mathbb{S}^{d-1} \) by \( \text{vMF}(\theta; m, \kappa) = C_{d/2}(\kappa) \exp(\kappa m^\top \theta), C_{d/2}(\kappa) = \kappa^{d/2-1}/\{(2\pi)^{d/2}I_{d/2-1}(\kappa)\}, \) with \( I_{d/2-1} \) the modified Bessel function of the first kind at order \( d/2 - 1 \).

Intuitively, the higher \( \kappa \), the more concentrated \( \text{vMF}(m, \kappa) \) is around \( m \). Our objective becomes finding \( (m^\star, \kappa^\star) \) such that \( \text{vMF}(m^\star, \kappa^\star) \) maximizes (14) over \( \mathcal{F} = \{ \text{vMF}(m, \kappa), m \in \mathbb{S}^{d-1}, \kappa \in \mathbb{R}_+^* \} \). Von Mises-Fisher distributions have been successfully deployed in several machine learning problems to effectively model spherical data (Hasnat et al., 2017; Kumar & Tsvetkov, 2018; Scott et al., 2021). Besides, one main advantage of using \( \text{vMF} \) is that both the KL divergence between \( \rho = \text{vMF}(m, \kappa) \) and

---

**Algorithm 1 PAC-SW: Adaptive SW via PAC-Bayes bound optimization.**

**Input:** dataset \( \{(x_i, y_i)\}_{i=1}^n \), parameter \( \lambda \), prior \( \rho_0 \), initialization \( \rho^{(0)} \), number of iterations \( T \), learning rate \( \eta \) for \( t = 1 \) to \( T \) do

\[
\begin{align*}
L_\rho(\rho^{(t-1)}) &= SW^p_0(\mu_n, \nu_n; \rho^{(t-1)}) - KL(\rho^{(t-1)} \mid || \rho_0) / \lambda \\
\rho^{(t)} &= \rho^{(t-1)} - \eta \nabla_{\rho} L_\rho(\rho^{(t-1)}) \\
\end{align*}
\]

end for

return \( \rho(T) \).
Shedding a PAC-Bayesian Light on Adaptive Sliced-Wasserstein Distances

We conduct an empirical analysis to confirm our theoretical contributions and illustrate their consequences in practice, on both synthetic and real data. More details on our experimental setup are given in Appendix A3, and the code is available at https://github.com/rubenohana/PAC-Bayesian_Sliced-Wasserstein.

Illustration of our bounds. Our first set of experiments aims at empirically validating the rates of convergence in Section 3. We sample two sets of \( n \) i.i.d. samples from \( \rho_0 = \mathcal{U}(S^{d-1}) \) and its gradient with respect to \((\mu, \kappa)\) admit an analytical formula (Davidson et al. 2018).

While the vMF parameterization is practical, as it yields an analytical objective, it may suffer from a lack of expressivity (e.g., vMF distributions are unimodal). To handle more complicated data, we also consider the parameterization proposed in Nguyen et al. 2021: we solve (14) over \( \mathcal{F} = \{ \rho = f \mathcal{U}(S^{d-1}), f \text{ a neural network} \} \). In that case, the KL penalty term is intractable and we approximate it with the methodology in Ohimire et al. 2021 — where approximation errors of the KL estimator are given in different scenarios.

We approximate the solution of (14) via gradient ascent: our methodology is depicted in Algorithm 1, and specialized in Algorithm A2 for the vMF parameterization.

Tuning \( \lambda \). In classical PAC-Bayesian theory, \( \lambda \) is usually set to \( n^{1/2} \) so that all terms in the bound that depend on \( \lambda \) converge at the same rate to 0, as \( n \) grows to \( + \infty \). Nevertheless, using \( \lambda = n^\alpha \) with \( \alpha \in (0, 1) \), \( \alpha \neq 1/2 \) can be more useful in some specific settings. For instance, a common issue when optimizing PAC-Bayesian bounds is that the objective can be dominated by the KL term (Chérif-Abdellatif et al. 2022). To overcome this, one can downweight the KL term by using \( \alpha > 1/2 \), or more sophisticated schemes (Blundell et al. 2015). On the other hand, as shown in Section 5.2, 5.3 and 5.4, \( \varphi_{\mu, \nu, p} \) depend on parameters related to the properties of \( \mu, \nu \), which cannot be easily controlled in practice. Choosing \( \lambda = n^\alpha \) with \( \alpha < 1/2 \) helps attenuate their influence on the objective (Haddouche et al. 2021).

5. Numerical Experiments

We conduct an empirical analysis to confirm our theoretical contributions and illustrate their consequences in practice, on both synthetic and real data. More details on our experimental setup are given in Appendix A3, and the code is available at https://github.com/rubenohana/PAC-Bayesian_Sliced-Wasserstein.

Figure 1. \( \text{SW}^p_{\rho}(\mu_n, \nu_n; \text{vMF}(m, \kappa)) \) vs. \( n \). Results are averaged over 30 runs, on log-log scale, with 10th-90th percentiles.

Figure 2. PAC-SW and DSW between \( \mu = \mathcal{N}(0, \Sigma_d) \) and \( \nu = \mathcal{N}(\gamma, \Sigma_d) \). The y-axis shows the distances or the associated objective functions (see legend). Results are averaged over 10 runs, and shown with 10th-90th percentiles.

the same distribution \( \mu \in \mathcal{P}(\mathbb{R}^d) \). To illustrate our bound on both bounded and unbounded supports, we choose \( \mu \) as a uniform or Gaussian distribution. We approximate \( \text{SW}^p_{\rho}(\mu_n, \nu_n; \text{vMF}(m, \kappa)) \) with \( m \sim \mathcal{U}(S^{d-1}) \) and \( \kappa > 0 \) by its Monte Carlo estimate (3) over 1000 projection directions. Figure 1 plots the approximation error (which reduces to \( \text{SW}^p_{\rho}(\mu_n, \nu_n; \text{vMF}(m, \kappa)) \), since the two datasets come from the same distribution) against \( n \), for different \( d \) and \( \kappa \). We observe that the error decays to 0 as \( n \) increases, and the convergence rate is slower as \( d \) and \( \kappa \) increase. This confirms our theoretical analysis: the higher \( d \), the larger the diameter (resp., the sub-Gaussian diameter) when \( \mu \) is uniform (resp., Gaussian), the larger \( \varphi_{\mu, \nu, p} \) (Proposition 1 and 3). Besides, the higher \( \kappa \), the larger \( \text{KL}(\text{vMF}(m, \kappa)||\mathcal{U}(S^{d-1})) \).

Generalization ability of PAC-SW. Next, we study the generalization properties of PAC-SW, i.e., whether the adaptive SW computed by Algorithm 1 is discriminative, even on unseen data. We compare \( \mu = \mathcal{N}(0, \Sigma_d) \) and \( \nu = \mathcal{N}(\gamma, \Sigma_d) \), with \( \gamma > 0, \Sigma_d \in \mathbb{R}^{d \times d} \) symmetric positive semi-definite set at random, and \( 0 \) (resp., 1) the vector whose components are all equal to 0 (resp., 1). The higher \( \gamma \), the more dissimilar \( \mu \) and \( \nu \). We sample \( n = 500 \) samples from \( \mu \) and \( \nu \) and optimize \( \rho^*(\mu_n, \nu_n) \): the optimization is performed on the space of vMF distributions, using Adam (Kingma & Ba 2015) with its default parameters. To analyze the generalization properties of \( \rho^*(\mu_n, \nu_n) \), we sample \( l = 2000 \) test points from \( \mu, \nu \) and compute \( \text{SW}^p_{\rho^*}(\mu_n, \nu_n; \rho^*(\mu_n, \nu_n)) \). We also compute the value of (14), to evaluate the tightness of our bound. Results for different values of \( d \) and \( \gamma \) are reported in Figure 2 and confirm the generalization ability of \( \rho^*(\mu_n, \nu_n) \).
We compute the Monte Carlo estimate with which consists in solving (Nguyen et al., 2021, Definition data (Deng, 2012), and we train a deep neural network that setup. We consider a generative modeling task on MNIST targets of a high generalization ability on a more complicated this encourages us to further explore the advantages of a high generalization ability on a more complicated experiments, we observed that DSW can generalize as well as PAC-SW. This encourages us to further explore the advantages of a high generalization ability on a more complicated tasks. We consider a generative modeling task on MNIST data (Deng, 2012), and we train a deep neural network that are able to better discriminate, even on test data. Note that max-SW and DSW share a common feature: they are able to better discriminate, even on test data. Next, we compare the generalization properties of PAC-SW and max-SW, with $\rho$ parameterized as a neural network. We also evaluate max-SW and SW (i.e., $\text{SW}_p^p(\mu_n, \nu_n; \rho)$) between 2 highly dissimilar classes of the Fashion-MNIST dataset (Xiao et al., 2017) (classes 4 (coats) and 5 (sandals)) for different number of training points. PAC-SW and DSW return higher values than max-SW and SW, illustrating they are able to better discriminate, even on test data.

Comparison to existing instances of SW. In our previous experiment, we also implement a variant of DSW, which consists in solving (Nguyen et al., 2021, Definition 2) based on our vMF parameterization. Figure 2 shows that the gap between $\text{SW}_p^p(\mu_n, \nu_n; \rho_{\text{DSW}}^p(\mu_n, \nu_n))$ and $\text{SW}_p^p(\mu_n, \nu_n; \rho_{\text{max-SW}}^p(\mu_n, \nu_n))$ is small, hence $\rho_{\text{DSW}}^p(\mu_n, \nu_n)$ generalizes well on that setup. DSW bound in Figure 2 corresponds to the associated objective function of (Nguyen et al., 2021, Definition 2).

For each minibatch of size 512, the distribution $\rho$ is learned by optimizing 100 projections over 100 iterations and the generative model is trained over 400 epochs. We also report results of a generative model trained with max-SW.

Figure 3 shows the evolution of the Wasserstein distance (WD) between generated data and the test set, with respect to training time. We use DSW as a loss, in the flavor of (Deshpande et al., 2018, Nguyen et al., 2021). Usually, the distribution $\rho$ is learned at each iteration, when the user receive new data. We conjecture that if the learned distribution generalizes well to unseen datasets, then gradients obtained from the distance between minibatches would still provide sufficient information to learn the generative model. As a consequence, we evaluate the robustness and generalization ability of the learned distribution using DSW updated only every 10 or 50 minibatches (denoted by $-10$ or $-50$ resp.). To train the model, we followed the same approach (architecture and optimizer) as the one described in (Nguyen et al., 2021). For each minibatch of size 512, the distribution $\rho$ is learned by optimizing 100 projections over 100 iterations and the generative model is trained over 400 epochs. We also report results of a generative model trained with max-SW.
leads to a very unstable learning and worst performances. Results for the PAC-SW loss and examples of generated digits can be found in Appendix \ref{app:additional}.

6. Conclusion

We introduced a specific notion of generalization for adaptive SW, related to discriminative power, and leveraged the PAC-Bayesian framework to derive generalization bounds. We then developed a principled methodology to learn \( \rho \) from the observed data so as SW\(^p(\cdot, \cdot; \rho) \) is discriminative with high probability, thus, generalizes well. Our work, which presents the first connection between PAC-Bayes and SW, paves the way to interesting research directions. First, we will study possible refinements of our bounds, using other PAC-Bayes bounds than Catoni’s. Then, we plan to further analyze why DSW generalizes well in our experiments, e.g. by investigating a potential connection between the optimization problem in \cite{Nguyen2021b} and ours. Finally, we would like to reduce the computational complexity of PAC-SW when \( \rho \) is parameterized as a neural network, since it suffers from slow execution times mainly because of the approximation of the KL term with \cite{Ghimire2021}.

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A1. Preliminaries

A1.1. Metric Properties of Sliced-Wasserstein Distances

Previous work has shown that for specific instances of \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \), \( \text{SW}_p(\cdot, \cdot; \rho) : \mathcal{P}_p(\mathbb{R}^d) \times \mathcal{P}_p(\mathbb{R}^d) \to \mathbb{R}_+ \) is a metric, as it satisfies all metric axioms (positivity, symmetry, triangle inequality, identity of indiscernibles) \cite{bonnotte2013, kolouri2019, nguyen2021, niles-weed2022}. However, to the best of our knowledge, the metric properties of \( \text{SW}_p(\cdot, \cdot; \rho) \) for any \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \) have not been established.

By adapting the proof techniques in \cite{bonnotte2013, kolouri2019}, and due to the metric properties of the Wasserstein distance, one can show that symmetry, positivity and triangle inequality hold for any \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \), and that for any \( \mu \in \mathcal{P}_p(\mathbb{R}^d) \), \( \text{SW}_p(\mu, \mu; \rho) = 0 \).

However, the reverse implication of the identity of indiscernibles, i.e.

\[
\forall \mu, \nu \in \mathcal{P}_p(\mathbb{R}^d), \quad \text{SW}_p(\mu, \nu; \rho) = 0 \implies \mu = \nu, \tag{A1}
\]

does not hold for any \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \). For example, consider \( \mu, \nu \in \mathcal{P}_p(X) \) with \( X \subset \mathbb{R}^d \), and \( \mu \) different from \( \nu \). Suppose that \( \rho \in \mathcal{P}(\Theta) \) with \( \Theta \in \mathbb{S}^{d-1} \) such that \( \forall (\theta, x) \in \Theta \times X, (\theta, x) = 0 \). In that case, for any \( \theta \sim \rho, \theta_0^*\mu = \theta_0^*\nu = \delta(0) \), and since \( W_p(\cdot, \cdot) \) is a metric, \( W_p(\theta_0^*\mu, \theta_0^*\nu) = 0 \). Therefore, \( \text{SW}_p(\mu, \nu; \rho) = \int_\Theta W_p^p(\theta_0^*\mu, \theta_0^*\nu)d\rho(\theta) = 0 \), but \( \mu \neq \nu \), so \( A1 \) is not satisfied.

We conclude that for any \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \), \( \text{SW}_p(\cdot, \cdot; \rho) \) is a pseudo-metric, and if \( A1 \) is satisfied, then it is a metric.

A1.2. Generalization Bounds for SW

We precise our argument in Section 1, which states that bounds on the generalization gap for SW distances can be established using existing results for max-SW.

Let \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \). By applying the triangle inequality for \( \text{SW}_p(\cdot, \cdot; \rho) \), then by the definition of max-SW, we obtain,

\[
\mathbb{E}[\text{SW}_p(\mu_n, \nu_n; \rho) - \text{SW}_p(\mu, \nu; \rho)] \leq \mathbb{E}[\text{SW}_p(\mu_n, \mu; \rho)] + \mathbb{E}[\text{SW}_p(\nu_n, \nu; \rho)] \leq \mathbb{E}[\lim\sup\text{SW}(\mu_n, \mu)] + \mathbb{E}[\lim\sup\text{SW}(\nu_n, \nu)], \tag{A2}
\]

where \( \mathbb{E} \) is taken with respect to \( \{x_i\}_{i=1}^n, \{y_i\}_{i=1}^n \) i.i.d. from \( \mu, \nu \) respectively. We can then bound from above \( A3 \) using the convergence rates established in \cite{lin2021, niles-weed2022} (Theorem 1). These rates vary depending on the properties of \( \mu, \nu \), for instance, \cite{lin2021} (Theorem 3.5) holds if \( \mu, \nu \) satisfy the Bernstein condition.

Nevertheless, we argue that the generalization bounds resulting from eq.\( A2 \)-\( A3 \) are not tight for an arbitrary \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \). For instance, since we bound \( A3 \) with \( \text{Lin et al., 2021, Niles-Weed & Rigollet, 2022} \), we obtain convergence rates that linearly depend on \( d \) for any \( \rho \), due to the properties of maximum SW. However, if we consider \( \rho = \mathcal{U}(\mathbb{S}^{d-1}) \), it is known that \( \mathbb{E}[\text{SW}_p(\mu_n, \nu_n; \rho) - \text{SW}_p(\mu, \nu; \rho)] \) converges to 0 at a dimension-free rate \cite{nadjah2020b}.

Another important drawback of such bounds is that the impact of \( \rho \) on the convergence rates is unclear. In Appendix A2.1, we will further explain why our generalization bounds derived from PAC-Bayesian theory are more flexible and informative for arbitrary \( \rho \).

A2. Postponed Proofs for Section 3

A2.1. Proof of Theorem 2

Theorem 2 is obtained by adapting the proof techniques of Catoni’s PAC-Bayesian bound \cite{catoni2003}. First, we recall Donsker and Varadhan’s variational formula, which plays a central role in the PAC-Bayesian framework.

**Lemma A1** \cite{donsker1975}. Let \( \Theta \) be a set equipped with a \( \sigma \)-algebra and \( \pi \in \mathcal{P}(\Theta) \). For any measurable, bounded function \( h : \Theta \to \mathbb{R} \),

\[
\log \mathbb{E}_{\theta \sim \pi} \left[ \exp(h(\theta)) \right] = \sup_{\rho \in \mathcal{P}(\Theta)} \left[ \mathbb{E}_{\theta \sim \rho} [h(\theta)] - KL(\rho \| \pi) \right].
\]
Proof of Theorem 2. Let $p \in [1, +\infty)$ and $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$. Assume there exists $\varphi_{\mu,\nu,p}$ such that for any $\theta \in \mathbb{S}^{d-1}$ and $\lambda > 0$,

$$
E_{\mu,\nu} \left[ \exp \left( \lambda \left\{ W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2) - E_{\mu,\nu}[W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2)] \right\} \right) \right] \leq \exp(\lambda^2 \varphi_{\mu,\nu,p} n^{-1}).
$$

(A4)

Let $\rho_0 \in \mathcal{P}(\mathbb{S}^{d-1})$. By taking the expectation of (A4) with respect to $\rho_0$, then using Fubini’s theorem to interchange the expectation over $\rho_0$ and the one over $\mu, \nu$, we obtain

$$
E_{\mu,\nu} E_{\theta \sim \rho_0} \left[ \exp \left( \lambda \left\{ W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2) - E_{\mu,\nu}[W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2)] \right\} \right) \right] \leq \exp(\lambda^2 \varphi_{\mu,\nu,p} n^{-1}).
$$

(A5)

By definition of the Wasserstein distance between empirical, univariate distributions of (1), one can prove that $\theta \mapsto \lambda \left\{ W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2) - E_{\mu,\nu}[W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2)] \right\}$ is a bounded real-valued function on $\mathbb{S}^{d-1}$. Therefore, we can apply Lemma 1 to rewrite (A5) as follows.

$$
E_{\mu,\nu} \left[ \exp \left( \sup_{\rho \in \mathcal{P}(\mathbb{S}^{d-1})} \left[ \lambda \left\{ W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2) - E_{\mu,\nu}[W_p^{\theta}(\theta^{*}_{1}\mu_1, \theta^{*}_{2}\nu_2)] \right\} \right) - KL(\rho||\rho_0) \right] \right] \leq \exp(\lambda^2 \varphi_{\mu,\nu,p} n^{-1}),
$$

which, using the linearity of the expectation along with the definition of SW (2), is equivalent to

$$
E_{\mu,\nu} \left[ \exp \left( \sup_{\rho \in \mathcal{P}(\mathbb{S}^{d-1})} \left[ \lambda \left\{ SW_p^{\theta}(\mu_1, \nu_2; \rho) - E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] \right\} \right) - KL(\rho||\rho_0) \right] \right] \leq \exp(\lambda^2 \varphi_{\mu,\nu,p} n^{-1}),
$$

or,

$$
E_{\mu,\nu} \left[ \exp \left( \sup_{\rho \in \mathcal{P}(\mathbb{S}^{d-1})} \left[ \lambda \left\{ SW_p^{\theta}(\mu_1, \nu_2; \rho) - E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] \right\} \right) - KL(\rho||\rho_0) \right] \right) \leq 1.
$$

(A6)

Let $s > 0$. By the Chernoff bound $\mathbb{P}(X > a) = \mathbb{P}(e^{sX} \geq e^{sa}) \leq \mathbb{E}[e^{tX}] e^{-ta}$

$$
\mathbb{P}_{\mu,\nu} \left( \sup_{\rho \in \mathcal{P}(\mathbb{S}^{d-1})} \left[ \lambda \left\{ SW_p^{\theta}(\mu_1, \nu_2; \rho) - E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] \right\} \right) - KL(\rho||\rho_0) \right] \leq s
$$

$$
\leq E_{\mu,\nu} \left[ \exp \left( \sup_{\rho \in \mathcal{P}(\mathbb{S}^{d-1})} \left[ \lambda \left\{ SW_p^{\theta}(\mu_1, \nu_2; \rho) - E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] \right\} \right) - KL(\rho||\rho_0) \right] \right) \exp(-s)
$$

$$
\leq 1 \cdot \exp(-s) = \exp(-s),
$$

where the last inequality follows from (A6).

Let $e^{-s} = \varepsilon$ such that $s = \log(1/\varepsilon)$. Then,

$$
\mathbb{P}_{\mu,\nu} \left( \exists \rho \in \mathcal{P}(\mathbb{S}^{d-1}), \lambda \left\{ SW_p^{\theta}(\mu_1, \nu_2; \rho) - E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] \right\} - KL(\rho||\rho_0) \right) \leq \varepsilon
$$

(A7)

Taking the complement of (A7) and rearranging the terms yields

$$
\mathbb{P}_{\mu,\nu} \left( \forall \rho \in \mathcal{P}(\mathbb{S}^{d-1}), SW_p^{\theta}(\mu_1, \nu_2; \rho) < E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho)] + \lambda^{-1} \left\{ KL(\rho||\rho_0) + \log(1/\varepsilon) \right\} + \lambda \varphi_{\mu,\nu,p} n^{-1} \right)
$$

$$
\geq 1 - \varepsilon.
$$

Our final bound results from assuming there exists $\psi_{\mu,\nu,p}(n)$ such that,

$$
E_{\mu,\nu}[SW_p^{\theta}(\mu_1, \nu_2; \rho) - SW_p^{\theta}(\mu_1, \nu_2; \rho)] \leq \psi_{\mu,\nu,p}(n).
$$
Comparison with Appendix A1.2 In our work, instead of bounding $SW^p_\rho(\cdot; \cdot; \rho)$ by maxSW, we apply PAC-Bayesian theory directly on $SW^p_\rho(\cdot; \cdot; \rho)$ for any $\rho$. As a result, our PAC-Bayes-inspired bounds are more flexible than bounds in Appendix A1.2 since their convergence rates adapt to the distribution $\rho$ (via the KL divergence). However, when $\rho$ is a Dirac measure, Theorem 2 become vacuous because of the KL term, as with most PAC-Bayesian bounds. In such cases, which include maxSW, the bounds in Appendix A1.2 are more informative.

As discussed in Section 3.4 in specific settings, $\varphi_{\mu,\nu,p}$ can be a function of $\lambda \in \mathbb{R}_+$ and $n \in \mathbb{N}^*$. In that case, a straightforward adaptation of the proof of Theorem 2 yields Theorem 3 which will be leveraged for distributions with Bernstein-type moment conditions (Definition 4).

**Theorem 3.** Let $p \in [1, +\infty)$ and $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$. Let $\Lambda \subset \mathbb{R}_+$ and assume there exists $\varphi_{\mu,\nu,p}: \Lambda \times n \rightarrow \mathbb{R}_+$, possibly depending on $\mu, \nu$ and $p$ such that: $\forall \lambda \in \Lambda, \forall \theta \in \mathbb{S}^{d-1}$,

$$
\mathbb{E} \left[ \exp \left( \lambda \left\{ W^p_\rho(\theta^*_\mu \mu_n, \theta^*_\nu \nu_n) - E[W^p_\rho(\theta^*_\mu \mu_n, \theta^*_\nu \nu_n)] \right\} \right) \right] \leq \exp(\lambda^2 \varphi_{\mu,\nu,p}(\lambda, n)^{-1})
$$

where $\mathbb{E}$ is taken with respect to the support points of $\mu_n$ and $\nu_n$. Additionally, assume there exists $\psi_{\mu,\nu,p} : \mathbb{N}^* \rightarrow \mathbb{R}_+$, possibly depending on $\mu, \nu$ and $p$, such that, $\forall p \in \mathcal{P}(\mathbb{S}^{d-1})$,

$$
\mathbb{E}[SW^p_\rho(\mu, \nu; p) - SW^p_\rho(\mu, \nu; p)] \leq \psi_{\mu,\nu,p}(n).
$$

Let $\rho_0 \in \mathcal{P}(\mathbb{S}^{d-1})$. Then, for any $\delta \in (0, 1)$, the following holds with probability at least $1 - \delta$: $\forall p \in \mathcal{P}(\mathbb{S}^{d-1})$,

$$
SW^p_\rho(\mu, \nu; p) \geq SW^p_\rho(\mu_n, \nu_n; p) - \frac{\lambda}{n} \varphi_{\mu,\nu,p}(\lambda, n)
$$

$$
- \frac{1}{\lambda} \left\{ KL(p|p_0) + \log \left( \frac{1}{\delta} \right) \right\} - \psi_{\mu,\nu,p}(n).
$$

**A2.2. Proof of Proposition 1**

To prove Proposition 1 we leverage a concentration result that appears in the proof of McDiarmid’s inequality (recalled in Theorem A4), and which relies on the bounded differences property (Definition A6).

**Definition A6 (Bounded differences property).** Let $X \subset \mathbb{R}^d$, $n \in \mathbb{N}^*$ and $c = \{c_i\}_{i=1}^n \in \mathbb{R}^n$. A mapping $f : X^n \rightarrow \mathbb{R}$ is said to satisfy the $c$-bounded differences property if for $i \in \{1, \ldots, n\}$, $\{x_i\}_{i=1}^n \in X^n$ and $x' \in X$,

$$
|f(x_1, \ldots, x_n) - f(x_1, \ldots, x_i, x', x_{i+1}, \ldots, x_n)| \leq c_i.
$$

**Theorem A4 (McDiarmid[1989]).** Let $(X_i)_{i=1}^n$ be a sequence of $n \in \mathbb{N}^*$ independent random variables with $X_i$ valued in $X \subset \mathbb{R}^d$ for $i \in \{1, \ldots, n\}$. Let $c = \{c_i\}_{i=1}^n \in \mathbb{R}^n$ and $f : X^n \rightarrow \mathbb{R}$ satisfying the c-bounded differences property. Then, for any $\lambda > 0$,

$$
\mathbb{E} \left[ \exp(\lambda \{ f - \mathbb{E}[f] \}) \right] \leq \exp(\lambda^2 ||c||^2/8).
$$

The proof of Proposition 1 consists in applying Theorem A4 to a specific choice of $f$. To this end, we first show that the Wasserstein distance between univariate distributions satisfies the bounded differences property, assuming bounded supports.

**Lemma A2.** Let $X \subset \mathbb{R}$ be a bounded set with diameter $\Delta = \sup_{x,x' \in X} ||x - x'|| < +\infty$. Then, the mapping $f : (X^2)^n \rightarrow \mathbb{R}_+$ defined for $w_{1:n} = \{(u_i, v_i)\}_{i=1}^n \in (X^2)^n$ as

$$
f(w_{1:n}) = W^p_\rho(\tilde{\mu}_n, \tilde{\nu}_n)
$$

where $\tilde{\mu}_n, \tilde{\nu}_n$ are the univariate empirical measures computed over $\{u_i\}_{i=1}^n, \{v_i\}_{i=1}^n$ respectively, satisfies the c-bounded differences property with $c_i = 2\Delta^p/n$ for $i \in \{1, \ldots, n\}$.

**Proof.** For clarity purposes, we start by introducing some notations. Let $n \in \mathbb{N}^*$ and $w_{1:n} = \{(u_j, v_j)\}_{j=1}^n \in (X^2)^n$. Denote by $\tilde{\mu}_n, \tilde{\nu}_n$ the empirical distributions supported over $(u_j)_{j=1}^n, (v_j)_{j=1}^n \in X^n$ respectively. Let $(u', v') \in X^2$ and $i \in \{1, \ldots, n\}$. Denote by $\tilde{\mu}'_n$ the empirical distribution supported on $(u'_j)_{j=1}^n$ where $u'_j = u'$ if $j = i$, $u'_j = u_j$ otherwise, and by $\tilde{\nu}'_n$ the empirical distribution over $(v'_j)_{j=1}^n$ where $v'_j = v'$ if $j = i$, $v'_j = v_j$ otherwise.
By definition of the Wasserstein distance between univariate distributions,  
\[
W_p(\tilde{\mu}_n, \tilde{\nu}_n) - W_p(\tilde{\mu}'_n, \tilde{\nu}'_n) = \frac{1}{n} \sum_{j=1}^{n} |u_{\sigma(j)} - v_{\tau(j)}|^p - \frac{1}{n} \sum_{j=1}^{n} |u'_{\sigma'(j)} - v'_{\tau'(j)}|^p
\]
where \( \sigma : \{1, \ldots, n\} \to \{1, \ldots, n\} \) (respectively, \( \sigma' : \{1, \ldots, n\} \to \{1, \ldots, n\} \)) is the permutation s.t. for \( j \in \{1, \ldots, n\}, u_{\sigma(j)} \) (resp., \( u'_{\sigma'(j)} \)) is the \( j \)-th smallest value of \( (u_j)_{j=1}^{n} \) (resp., \( (u'_j)_{j=1}^{n} \)). Let \( \tau : \{1, \ldots, n\} \to \{1, \ldots, n\} \) (respectively, \( \tau' : \{1, \ldots, n\} \to \{1, \ldots, n\} \)) s.t. for \( j \in \{1, \ldots, n\}, v_{\tau(j)} \) (resp., \( v'_{\tau'(j)} \)) is the \( j \)-th smallest value of \( (v_j)_{j=1}^{n} \) (resp., \( (v'_j)_{j=1}^{n} \)).

Therefore,
\[
W_p(\tilde{\mu}_n, \tilde{\nu}_n) - W_p(\tilde{\mu}'_n, \tilde{\nu}'_n) \leq \frac{1}{n} \sum_{j=1}^{n} |u_{\sigma(j)} - v_{\tau(j)}|^p - \frac{1}{n} \sum_{j=1}^{n} |u'_{\sigma'(j)} - v'_{\tau'(j)}|^p
\]
\[
= \frac{1}{n} \left( |u_i - v_{\tau(\sigma^{-1}(i))}|^p - |u'_{\sigma'(\tau^{-1}(i))} - v_{\tau(\sigma^{-1}(i))}|^p + |u_{\sigma^{-1}(\tau^{-1}(i))} - v_i|^p - |u'_{\sigma'(\tau^{-1}(i))} - v'|^p \right)
\]
\[
\leq \frac{2\Delta^p}{n}
\]
We can use the same arguments to prove that \( W_p(\tilde{\mu}'_n, \tilde{\nu}'_n) - W_p(\tilde{\mu}_n, \tilde{\nu}_n) \leq \frac{2\Delta^p}{n} \). We conclude that,
\[
|W_p(\tilde{\mu}_n, \tilde{\nu}_n) - W_p(\tilde{\mu}'_n, \tilde{\nu}'_n)| \leq \frac{2\Delta^p}{n}.
\]

\[\square\]

Remark 1. Lemma A2 is an extension of [Weed & Bach 2019 Proposition 20], which establishes a concentration bound for \( W_p(\mu, \mu_n) \) around its expectation on any finite-dimensional compact space by exploiting McDiarmid’s inequality along with the Kantorovich duality. We thus use similar arguments to prove Proposition 7, except that we leverage the closed-form expression of the one-dimensional Wasserstein distance instead of the dual formulation since we compare univariate (projected) distributions.

Proof of Proposition 7 Let \( \mu, \nu \in \mathcal{P}(X) \) where \( X \subset \mathbb{R}^d \) has a finite diameter \( \Delta \). Let \( \theta \in \mathbb{S}^{d-1} \). Then, \( \theta^* \mu, \theta^* \nu \) are both supported on a bounded domain \( \Omega_\theta \subset \mathbb{R}^d \) whose diameter is denoted by \( \Delta_\theta \) and satisfies \( \Delta_\theta \leq \Delta \). Consider the mapping \( f \) defined as in \( \lambda \). Given Lemma A2 we can apply Theorem A3 to bound the moments-generating function of \( f - Ef \) for any \( \lambda > 0 \),
\[
\mathbb{E} \left[ \exp(\lambda \{ f - \mathbb{E}[f] \}) \right] \leq \exp(\lambda^2 \sum_{i=1}^{n} (2\Delta^p_\theta/n)^2/8)
\]
\[
\leq \exp(\lambda^2 \Delta^p_\theta/(2n)) \leq \exp(\lambda^2 \Delta^p/(2n))
\]
where the expectation is computed over \( n \) samples \( w_{1:n} = \{(u_i, v_i)\}_{i=1}^{n} \in (X_\theta^n) \) i.i.d. from \( \theta^* \mu \times \theta^* \nu \). We conclude by using the property of push-forward measures, which gives
\[
\mathbb{E}_{w_{1:n} \sim (\theta^* \mu \times \theta^* \nu)^n} \left[ \exp(\lambda \{ f(w_{1:n}) - \mathbb{E}[f(w_{1:n})] \}) \right] = \mathbb{E}_{z_{1:n} \sim (\mu \times \nu)^n} \left[ \exp(\lambda \{ f(\theta^*(z'_{1:n})) - \mathbb{E}[f(\theta^*(z'_{1:n}))] \}) \right]
\]
\[\text{(A9)}\]
where \( z_{1:n} = \{(x_i, y_i)\}_{i=1}^{n} \in (X^2)^n, \theta^*(z_{1:n}) = \{(\theta, x_i), (\theta, y_i)\}_{i=1}^{n} \in (X_\theta^n) \).
Lemma A3. Let \( X \subset \mathbb{R} \) be a bounded set whose diameter is denoted by \( \Delta < +\infty \). Let \( \mu, \nu \in \mathcal{P}(X) \) and denote by \( \mu_n, \nu_n \) the empirical distributions supported over \( n \in \mathbb{N}^+ \) samples i.i.d. from \( \mu, \nu \) respectively. Let \( p \in [1, +\infty) \). Then, there exists a constant \( C \) such that,

\[
\mathbb{E}(W^p_p(\mu, \nu) - W^p_p(\mu_n, \nu_n)) \leq Cp\Delta^p n^{-1/2}.
\]

Proof. Lemma A.3 is obtained by adapting the techniques used in the proof of (Manole et al. 2022) Lemma 6, then applying (Fournier & Guillin 2015) Theorem 1. We provide the detailed proof for completeness.

Starting from the definition of \( W^p_p(\mu, \nu) \), then using a Taylor expansion of \((x, y) \mapsto |x - y|^p \) around \((x, y) = (F^{-1}_\mu(t), F^{-1}_\nu(t))\), we obtain

\[
W^p_p(\mu, \nu) = \int_0^1 |F^{-1}_\mu(t) - F^{-1}_\nu(t)|^p dt
\]

\[
= \int_0^1 |F^{-1}_\mu(t) - F^{-1}_\nu(t)|^p dt
\]

\[
= \int_0^1 \sum_{i=1}^n \left| \frac{\partial}{\partial t} F^{-1}_\mu(t) \right|^p dt
\]

\[
\leq p \sup_{t \in (0,1)} \left| \frac{\partial}{\partial t} F^{-1}_\mu(t) \right|^p \left( W_1(\mu, \nu) + W_1(\nu, \mu) \right)
\]

where \( \sup_{t \in (0,1)} \left| \frac{\partial}{\partial t} F^{-1}_\mu(t) \right|^p \) results from the definition of the Wasserstein distance of order 1 between univariate distributions.

We then bound \( \sup_{t \in (0,1)} |F^{-1}_\mu(t) - F^{-1}_\nu(t)|^{p-1} \) from above. By the definition of \( \tilde{F}^{-1}_\mu(t), \tilde{F}^{-1}_\nu(t) \) for \( t \in (0,1) \), we distinguish the following four cases:

(i) \( \tilde{F}^{-1}_\mu(t) \leq F^{-1}_\mu(t), \tilde{F}^{-1}_\nu(t) \leq F^{-1}_\nu(t) \)

(ii) \( \tilde{F}^{-1}_\mu(t) \leq F^{-1}_\mu(t), \tilde{F}^{-1}_\nu(t) \leq F^{-1}_\nu(t) \)

(iii) \( \tilde{F}^{-1}_\mu(t) \leq F^{-1}_\mu(t), \tilde{F}^{-1}_\nu(t) \leq F^{-1}_\nu(t) \)

(iv) \( \tilde{F}^{-1}_\mu(t) \leq F^{-1}_\mu(t), \tilde{F}^{-1}_\nu(t) \leq F^{-1}_\nu(t) \)

Hence, using the definition of quantile functions and the fact that the supports of \( \mu, \nu \) are assumed to be bounded, we obtain

\[
\sup_{t \in (0,1)} \left| \tilde{F}^{-1}_\mu(t) - \tilde{F}^{-1}_\nu(t) \right|^{p-1} \leq \Delta^{p-1}.
\]

We conclude that,

\[
|W^p_p(\mu_n, \nu_n) - W^p_p(\mu, \nu)| \leq p\Delta^{p-1}\left\{ W_1(\mu, \nu) + W_1(\nu, \mu) \right\}
\]

and by linearity of the expectation,

\[
\mathbb{E}(W^p_p(\mu_n, \nu_n) - W^p_p(\mu, \nu)) \leq p\Delta^{p-1}\left\{ \mathbb{E}[W_1(\mu_n, \mu)] + \mathbb{E}[W_1(\nu_n, \nu)] \right\}.
\]

(A.13)
Our final result follows from applying (Fournier & Guillin, 2015) Theorem 1. Since $\mu, \nu \in \mathcal{P}(X)$ where $X \subset \mathbb{R}$ is a bounded set with finite diameter $\Delta < \infty$, then for any $q \geq 1$, the moment of $\mu$ (or $\nu$) of order $q$ is bounded by $\Delta^q$. Therefore, the application of (Fournier & Guillin, 2015) Theorem 1 yields,

$$\mathbb{E}[W_1(\mu_n, \mu)] \leq C' \Delta n^{-1/2}, \quad \mathbb{E}[W_1(\nu_n, \nu)] \leq C' \Delta n^{-1/2}.$$ (A14)

where $C'$ is a constant. We conclude by plugging (A14) in (A13).

Proof of Proposition 2. Let $\theta \in \mathbb{S}^{d-1}$. Since we assume that $\mu, \nu \in \mathcal{P}(X)$ where $X \subset \mathbb{R}^d$ is a bounded subset with finite diameter $\Delta$, one can easily prove that $\theta^*_\mu, \theta^*_\nu$ are supported on a bounded domain with diameter $\Delta_\theta \leq \Delta < +\infty$. Therefore, by Lemma A3 there exists a constant $C$ such that,

$$\mathbb{E}|W_p^p(\theta^*_\mu, \mu, \theta^*_\nu, \nu) - W_p^p(\theta^*_\mu, \nu, \theta^*_\nu, \nu)| \leq C p \Delta p n^{-1/2}.$$ (A15)

Next, we adapt the proof techniques in (Nadjahi et al., 2020b) Theorem 4 to establish the following inequality: for any $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$,

$$\mathbb{E}[SW_p^p(\mu_n, \nu_n; \rho) - SW_p^p(\mu, \nu; \rho)] \leq \int_{\mathbb{S}^{d-1}} |W_p^p(\theta^*_\mu, \mu, \theta^*_\nu, \nu) - W_p^p(\theta^*_\mu, \nu, \theta^*_\nu, \nu)| d\rho(\theta).$$ (A16)

Hence, by plugging (A15) in (A16), we obtain

$$\mathbb{E}[SW_p^p(\mu_n, \nu_n; \rho) - SW_p^p(\mu, \nu; \rho)] \leq C p \Delta p n^{-1/2}.$$ □

A2.4. Final Bound for Bounded Supports

By incorporating Propositions 1 and 2 in Theorem 2, we obtain the following result. Corollary A1 corresponds to a specialization of our generic bound when considering distributions with bounded supports.

Corollary A1. Let $p \in [1, +\infty)$ and assume a bounded diameter $\Delta$. Let $\rho_0 \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\delta > 0$. Then, with probability at least $1 - \delta$, for all $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\lambda > 0$, there exists a constant $C$ such that,

$$SW_p^p(\mu_n, \nu_n; \rho) \leq SW_p^p(\mu, \nu; \rho) + \{KL(\rho||\rho_0) + \log(1/\delta)\}^{1/2} \lambda^{-1} + \lambda \Delta^{2p(2n)}^{-1} + C p \Delta p n^{-1/2}.$$ A2.5. Proof of Proposition 3

When the supports of the distributions are not bounded, Lemma A2 does not hold true, thus preventing the use of McDiarmid’s inequality. Hence, to compute $\varphi_{\mu,\nu,p}$, we may use extensions of McDiarmid’s inequality which replace the finite-diameter constraint by conditions on the moments of the distributions.

In particular, Proposition 3 follows from applying (Kontorovich, 2014) Theorem 1, a concentration result based on the notion of sub-Gaussian diameter.

Definition A7 (Sub-Gaussian diameter [Kontorovich, 2014]). Let $\eta$ be a distance function and $(X, \eta, \mu)$ be the associated metric probability space. Consider a sequence of $n \in \mathbb{N}$ independent random variables $(X_i)_{i=1}^n$ with $X_i$ distributed from $\mu$ for $i \in \{1, \ldots, n\}$. Let $\Xi(X)$ be the random variable defined by

$$\Xi(X) = \varepsilon \eta(X, X'),$$

where $X, X'$ are two independent realizations from $\mu$ and $\varepsilon$ is a random variable valued in $\{-1, 1\}$ s.t. $p(\varepsilon = 1) = 1/2$ and $\varepsilon$ is independent from $X, X'$. Additionally, suppose there exists $\sigma > 0$ s.t. for $\lambda \in \mathbb{R}$, $\mathbb{E}_\mu[\exp(\lambda X)] \leq \exp(\sigma^2\lambda^2/2)$. The sub-Gaussian diameter of $(X, \eta, \mu)$, denoted by $\Delta_{SG}(X)$, is defined as $\Delta_{SG}(X) = \sigma(\Xi(X))$.

Note that $\Delta_{SG} \leq \Delta$ (Kontorovich, 2014) Lemma 1. Since a set with infinite diameter may have a finite sub-Gaussian diameter, Theorem A3 relaxes the conditions of Theorem A4.
Theorem A5 (Theorem 1 (Kontorovich 2014)). Let $X \subseteq \mathbb{R}^d$ and $\eta : X \times X \to \mathbb{R}_+$ be a distance function. Consider the metric probability space $(X, \eta)$. For $n \in \mathbb{N}^*$, let $X^n$ be the product probability space equipped with the product measure $\mu^\otimes = \mu_1 \times \cdots \times \mu_n$, where $\mu_i = \mu$. Define the $L_1$ product metric $\eta^\otimes$ for any $(x, x') \in X^n \times X^n$ as,

$$\eta^\otimes(x, x') = \sum_{i=1}^n \eta(x_i, x'_i).$$

Let $f : X^n \to \mathbb{R}$ s.t. $f$ is 1-Lipschitz with respect to $\eta^\otimes$, i.e. for any $(x, x') \in X^n \times X^n$, $|f(x) - f(x')| \leq \eta(x, x')$. Then, $\mathbb{E}[f] < +\infty$ and for $\lambda > 0$,

$$\mathbb{E}[\exp(\lambda (f - \mathbb{E}[f]))] \leq \exp(\lambda^2 n \Delta_{SG}(X)^2 / 2).$$

As discussed in (Kontorovich 2014), the sub-Gaussian distributions on $\mathbb{R}$ are precisely those for which $\Delta_{SG}(\mathbb{R}) < +\infty$. Proposition 5 then results from applying Theorem A5 as explained below.

Proof of Proposition 5. First, we prove that for any $\mu \in \mathcal{P}(\mathbb{R}^d)$ such that $\mu$ is sub-Gaussian with parameter $\sigma^2$, then $\mu \in \mathcal{P}_1(\mathbb{R}^d)$. By definition, the first moment of $\mu$ is $m_1(\mu) = \int_{\mathbb{R}^d} \|x\| d\mu(x)$. For any $x \in \mathbb{R}^d$, we know that

$$\|x\| = \left( \sum_{k=1}^d |x_k|^2 \right)^{1/2} \leq \sum_{k=1}^d |x_k|$$

Therefore, $m_1(\mu)$ can be bounded from above as follows.

$$m_1(\mu) \leq \int_{\mathbb{R}^d} \sum_{k=1}^d |x_k| d\mu(x)$$

$$\leq \sum_{k=1}^d \int_{\mathbb{R}^d} |x_k| d\mu(x)$$

$$\leq \sum_{k=1}^d \int_{\mathbb{R}^d} |\langle \theta^k, x \rangle| d\mu(x)$$

$$\leq \sum_{k=1}^d \int_{\mathbb{R}^d} |t| d(\theta^k) \mu(t)$$

$$\leq d \sqrt{2 \pi \sigma^2}$$

(A19)

where for $k \in \{1, \ldots, d\}$, $\theta^k \in S^{d-1}$ is defined as $(\theta^k)_i = 1$ if $i = k$, $(\theta^k)_i = 0$ otherwise. (A17) results from the linearity of the expectation. (A18) is obtained by applying the property of pushforward measures. (A19) follows from the sub-Gaussian assumption on $\mu$ (Definition 5) and (Rivasplata 2012 Proposition 3.2). Since $m_1(\mu) < \infty$ (A19), we conclude that $\mu \in \mathcal{P}_1(\mathbb{R}^d)$.

Now, consider the product metric space $(\mathbb{R}^2, \eta)$ where $\eta : \mathbb{R}^2 \to \mathbb{R}_+$ is the distance function defined for $w \equiv (u, v) \in \mathbb{R}^2$, $w' \equiv (u', v') \in \mathbb{R}^2$ as,

$$\eta(w, w') \equiv \|u-u'\| + \|v-v'\| = |u-u'| + |v-v'|.$$

Let $n \in \mathbb{N}^*$ and define $f : (\mathbb{R}^2)^n \to \mathbb{R}_+$ as: for any $w_{1:n} \equiv (w_i)_{i=1}^n \in (\mathbb{R}^2)^n$ such that $\forall i \in \{1, \ldots, n\}, w_i = (u_i, v_i) \in \mathbb{R}^2$,

$$f(w_{1:n}) = n W_1(\tilde{\mu}_n, \tilde{\nu}_n),$$

(A20)

where $\tilde{\mu}_n, \tilde{\nu}_n$ are the empirical distributions computed over $(u_i)_{i=1}^n, (v_i)_{i=1}^n$ respectively, i.e., denoting by $\delta_x$ the Dirac measure at $x$,

$$\tilde{\mu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{u_i}, \quad \tilde{\nu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{v_i}.$$
We conclude from (A20) and (A22) that
\[ f = \tilde{\mu} \]
where \( u \) is defined in (A21).

By (A18), the first order moment of \( X \) is \( \mu \)-Lipschitz with respect to the product metric \( \eta \), as defined in (A21).

\[ \mathbb{P}(X) \]

Applying a generalized McDiarmid’s inequality, which we recall in Theorem A6.

Proposition 4 results from the same arguments as in the proof of (Lei, 2020, Corollary 5.2). The latter result is obtained by
A2.6. Proof of Proposition 4

As defined in (A20), then reformulating the expectation over \( f \) as defined in (A20), then reformulating the expectation over \( X \) and \( \mu \) using the property of push-forward measures (see (A9)).

We conclude from (A20) and (A22) that \( f \) is \( \mu \)-Lipschitz with respect to the product metric \( \eta \), as defined in (A21).

Next, let \( \theta \in \mathbb{S}^{d-1} \) and \( \mu, \nu \in \mathcal{P}(\mathbb{R}^d) \) such that \( \mu, \nu \) are sub-Gaussian with respective variance proxy \( \sigma^2, \tau^2 \). Consider the probability metric space \((\mathbb{R}^2, \eta, \theta^* \mu \times \theta^* \nu)\). By Definition A7 and the properties of the sum of independent sub-Gaussian random variables (Rivasplata, 2012 Theorem 2.7), the sub-Gaussian diameter of that space is \( \Delta_{SG}(\mathbb{R}^2) = \sqrt{2(\sigma^2 + \tau^2)} \). We conclude the proof by applying Theorem A5 to \( f \) as defined in (A20), then reformulating the expectation over \( \theta^* \mu \times \theta^* \nu \) as an expectation over \( \mu \times \nu \) using the property of push-forward measures (see (A9)).

\[ (A23) \]

\[ \mathbb{E}[|f(X) - f(X_{(i)})|^k | X_{-i}] \leq c^2 k! M^{k-2} / 2, \]

where \( X_{-i} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n) \). Then, for \( \lambda > 0 \) s.t. \( \lambda M < 1 \),

\[ \mathbb{E}[\exp\{\lambda(f - \mathbb{E}[f])\}] \leq \exp\left(\lambda^2 c^2 |\lambda|^2 / (2(1 - \lambda))\right) \].

Proof of Proposition 4 First, we justify why for any \( \mu \in \mathcal{P}(\mathbb{R}^d) \) s.t. \( \mu \) satisfies the \((\sigma^2, \beta)\)-Bernstein condition, \( \mu \in \mathcal{P}_1(\mathbb{R}^d) \).

By (A18), the first order moment of \( \mu \), \( m_1(\mu) \) can be bounded as,

\[ m_1(\mu) \leq \sum_{k=1}^d \int_{\mathbb{R}} |t| d(\theta^k)_\mu(t) \]

\[ \leq \sum_{k=1}^d \left\{ \int_{\mathbb{R}} |t|^2 d(\theta^k)_\mu(t) \right\}^{1/2} \]

\[ \leq da \]
where (A24) is obtained by applying Hölder’s inequality, and (A25) results from Definition 4. Hence, \( m_1(\mu) < \infty \) and \( \mu \in \mathcal{P}_1(\mathbb{R}^d) \).

The rest of the proof consists in applying Theorem A6 to \( f : (\mathbb{R}^2)^n \to \mathbb{R}_+ \), defined for any \( w_{1:n} \equiv \{(u_i, v_i)\}_{i=1}^n \in (\mathbb{R}^2)^n \) as,

\[
f(w_{1:n}) = W_1(\tilde{\mu}_n, \tilde{\nu}_n)
\]

(A26)

where \( \tilde{\mu}_n, \tilde{\nu}_n \) are the empirical distributions of \( (u_i)_{i=1}^n, (v_i)_{i=1}^n \), respectively.

For \( i \in \{1, \ldots, n\} \), let \( (u'_i, v'_i) \in \mathbb{R}^2 \). Denote by \( \tilde{\mu}'_n \) the empirical distribution supported on \( (u_1, \ldots, u_{i-1}, u'_i, u_{i+1}, \ldots, u_n) \in \mathbb{R}^n \), and by \( \tilde{\nu}'_n \) the empirical distribution supported on \( (v_1, \ldots, v_{i-1}, v'_i, v_{i+1}, \ldots, v_n) \in \mathbb{R}^n \). Then,

\[
W_1(\tilde{\mu}_n, \tilde{\nu}_n) - W_1(\tilde{\mu}'_n, \tilde{\nu}'_n) \leq W_1(\tilde{\mu}_n, \tilde{\mu}'_n) + W_1(\tilde{\mu}'_n, \tilde{\nu}'_n)
\]

(A27)

\[
\leq \frac{1}{n} \sum_{j=1}^n |u_j - u'_j| + \frac{1}{n} \sum_{j=1}^n |v_j - v'_j|
\]

(A28)

\[
\leq \frac{1}{n} \left( |u_i - u'_i| + |v_i - v'_i| \right)
\]

(A29)

where (A27) follows from the fact that \( W_1 \) satisfies the triangle inequality, and (A28) results from the definition of the Wasserstein distance between univariate empirical distributions (Peyré & Cuturi 2019 Remark 2.28).

Now, let \( \mu \in \mathcal{P}(\mathbb{R}^d) \) (respectively, \( \nu \in \mathcal{P}(\mathbb{R}^d) \)) satisfy the \((\sigma^2, b)\) (resp., \((\tau^2, c)\))-Bernstein condition (Definition 4). Let \( \theta \in \mathbb{S}^{d-1} \) and consider \( w_{1:n} = \{(u_i, v_i)\}_{i=1}^n \in (\mathbb{R}^2)^n \) i.i.d. from the product measure \( \theta_\mu \times \theta_\nu \). We justify why \( f \) satisfies the conditions of Theorem A6.

First, we show that \( \mathbb{E}[f] \) is finite, where the expectation \( \mathbb{E} \) is computed over \( n \) i.i.d. samples \( \{(u_i, v_i)\}_{i=1}^n \) from \( \theta_\mu \times \theta_\nu \).

\[
\mathbb{E}[f] \leq \frac{1}{n} \sum_{i=1}^n \mathbb{E}[|u_i - v_i|] \leq \frac{1}{n} \sum_{i=1}^n \{\mathbb{E}|u_i| + \mathbb{E}|v_i|\}
\]

(A30)

\[
\leq \frac{1}{n} \sum_{i=1}^n \left\{ \mathbb{E}[(|u_i|^2)^{1/2}] + \mathbb{E}[(|v_i|^2)^{1/2}] \right\}
\]

(A31)

where (A30) results from Hölder’s inequality, and (A31) directly follows from the definition of the Bernstein condition (Definition 4).

Besides, by using (A29) and the Bernstein condition Definition 4 one can show that

\[
\mathbb{E}[W_1(\tilde{\mu}_n, \tilde{\nu}_n) - W_1(\tilde{\mu}'_n, \tilde{\nu}'_n) | u_{-i}, v_{-i}] \leq n^{-k} 2^{2(k-1)} [\sigma^2 b^{k-2} + \tau^2 c^{k-2}] k!
\]

where the expectation is computed over \( \{(u_i, v_i)\}_{i=1}^n \) i.i.d. from \( \theta_\mu \times \theta_\nu \). In other words, \( f \) as defined in (A26) satisfies (A23) with, for \( i \in \{1, \ldots, 2n\}, c_i = 2\sigma n^{-1} \) and \( M = 4b n^{-1} \), where \( \sigma_* = \max(\sigma, \tau) \) and \( b_* = \max(b, c) \). Our final result follows from applying Theorem A6 to \( f \), then applying the property of push-forward measures to obtain the expectation with respect to \( \mu \times \nu \) (see (A9)).

A2.7. Final Bound for Unbounded Supports

Before deriving the specialization of Theorem 2 for distributions with unbounded supports, we recall a useful bound on \( \text{SW}_p^\mu(\nu; \pi) \) with \( \pi = \mathcal{U}(\mathbb{S}^{d-1}) \) (Theorem A7), which can be generalized for SW based on any \( \rho \in \mathcal{P}(\mathbb{S}^{d-1}) \) by adapting the proof techniques in (Manole et al. 2022, Theorem 2).

**Theorem A7** (Manole et al. 2022). Let \( p \geq 1, q \geq 2p, s \geq 1 \) and \( \pi = \mathcal{U}(\mathbb{S}^{d-1}) \). Denote \( \mathcal{P}_{p,q}(s) = \{\mu \in \mathcal{P}(\mathbb{R}^d) : \mathbb{E}_\mu[|\theta|^p]^{1/p} |\mathcal{D}_s(\theta) \leq s\} \). Let \( \mu, \nu \in \mathcal{P}_{p,q}(s) \). Then, there exists a constant \( C(p, q) > 0 \) depending on \( p, q \) such that,

\[
\mathbb{E}[\text{SW}_p^\mu(\mu, \nu; \pi) - \text{SW}_p^\mu(\mu, \nu; \pi)] \leq C(p, q) s \log(n)^{1/2} n^{-1/2}
\]
We show that under the sub-Gaussian or the Bernstein moment condition assumptions, the assumptions in Theorem A7 are satisfied, thus allowing its application in these two settings. This yields Corollaries A2 and A3 which we state and prove hereafter.

**Corollary A2.** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ and $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$. Assume that $\mu$ (respectively, $\nu$) is sub-Gaussian with variance proxy $\sigma^2$ (resp., $\tau^2$). Let $\sigma_*^2 = \max(\sigma^2, \tau^2)$. Then, there exists $C'(p) > 0$ such that,

$$\mathbb{E}|\text{SW}_p^\rho(\mu_n, \nu_n; \rho) - \text{SW}_p^\rho(\mu, \nu; \rho)| \leq C'(p)(4\sigma_*^2)^p \log(n)^{1/2}n^{-1/2}.$$ 

**Proof.** Under the sub-Gaussian assumption on $\mu$ and $\nu$, the moments of $\theta^2_\rho \mu, \theta^2_\rho \nu$ can be bounded for any $\theta \in \mathbb{S}^{d-1}$ as follows: for any $k \in \mathbb{N}^*$,

$$\mathbb{E}_\mu[|\langle \theta, x \rangle |^{2k}] \leq k!(4\sigma^2)^k, \quad \mathbb{E}_\nu[|\langle \theta, y \rangle |^{2k}] \leq k!(4\tau^2)^k.$$ 

We conclude that $\mu, \nu \in \mathcal{P}_{p,2(p+1)}(s)$ with $s = ((p+1)!/(2(p+1)!))(4\sigma_*^2)^p$ and $\sigma_*^2 = \max(\sigma^2, \tau^2)$. The final result follows from applying Theorem A7.

**Corollary A3.** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ and $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$. Assume that $\mu$ and $\nu$ satisfy the Bernstein condition, with parameters $(\sigma^2, b)$ and $(\tau^2, c)$ respectively. Let $\sigma_*^2 = \max(\sigma^2, \tau^2)$ and $b_* = \max(b, c)$. Then, there exists $C'(p, q) > 0$ such that

$$\mathbb{E}|\text{SW}_p^\rho(\mu_n, \nu_n; \rho) - \text{SW}_p^\rho(\mu, \nu; \rho)| \leq C'(p, q)\sigma_*^{2p/q}b_*^{p(q-2)/q} \log(n)^{1/2}n^{-1/2}.$$ 

**Proof.** Under the Bernstein condition on the moments of $\mu, \nu$, we can use the definition of the push-forward measures along with the Cauchy-Schwarz inequality and obtain for any $\theta \in \mathbb{S}^{d-1}$ and $k \in \mathbb{N}^*$,

$$\mathbb{E}_\mu[|\langle \theta, x \rangle |^{2k}] \leq \sigma^2 k!b^{k-2}/2, \quad \mathbb{E}_\nu[|\langle \theta, y \rangle |^{2k}] \leq \tau^2 k!c^{k-2}/2. \quad (A32)$$

Let $q > 2p$. By (A32), $\mu, \nu \in \mathcal{P}_{p,q}(s)$ with $s = (\sigma_*^2 q!/2)^{p/q}b_*^{(q-2)/q}$. The application of Theorem A7 concludes the proof.

We can finally provide the refined bounds, assuming the distributions are either sub-Gaussian or satisfy the Bernstein condition. On the one hand, incorporating Proposition 13 and Corollary A2 in Theorem 2 gives us the following corollary.

**Corollary A4.** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$. Assume $\mu$ (resp., $\nu$) is sub-Gaussian with variance proxy $\sigma^2$ (resp., $\tau^2$). Let $\sigma_*^2 = \max(\sigma^2, \tau^2)$. Let $\rho_0 \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\delta > 0$. Then, with probability at least $1 - \delta$, for all $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\lambda > 0$, there exists $C > 0$ such that

$$\text{SW}_1(\mu_n, \nu_n; \rho) \leq \text{SW}_1(\mu, \nu; \rho) + \{KL(\rho || \rho_0) + \log(1/\delta)\} \lambda^{-1} + \lambda(\sigma^2 + \tau^2)n^{-1} + C\sigma_*^2 \log(n)^{1/2}n^{-1/2}.$$ 

On the other hand, we leverage Proposition 4, Corollary A3 and Theorem A7 to derive the specified bound below.

**Corollary A5.** Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$. Assume that $\mu$ and $\nu$ satisfy the Bernstein condition, with parameters $(\sigma^2, b)$ and $(\tau^2, c)$ respectively. Let $\sigma_*^2 = \max(\sigma^2, \tau^2)$ and $b_* = \max(b, c)$. Let $\rho_0 \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\delta > 0$. Then, with probability at least $1 - \delta$, for all $\rho \in \mathcal{P}(\mathbb{S}^{d-1})$ and $\lambda > 0$ s.t. $\lambda < (2b_*)^{-1}n$, for $q > 2$, there exists $C(q) > 0$ such that

$$\text{SW}_1(\mu_n, \nu_n; \rho) \leq \text{SW}_1(\mu, \nu; \rho) + \{KL(\rho || \rho_0) + \log(1/\delta)\} \lambda^{-1} + 2\lambda(\sigma_*^2(1 - 2b_*\lambda n^{-1})^{-1}n^{-2} + C(q)\sigma_*^{2/q}b_*^{(q-2)/q} \log(n)^{1/2}n^{-1/2}.$$ 

**A3. Additional Experimental Details**

All our numerical experiments presented in Section 5 can be reproduced using the code we provided in https://github.com/rubenohana/PAC-Bayesian_Sliced-Wasserstein.
Algorithm A2 PAC-Bayes bound optimization for vMF-based SW

**Input:** Datasets: $x_{1:n} = (x_i)_{i=1}^n$, $y_{1:n} = (y_i)_{i=1}^n$
- SW order, number of slices: $p \in [1, +\infty)$, $n_S \in \mathbb{N}^*$
- Bound parameter: $\lambda \in \mathbb{R}_+^*$
- Number of iterations, learning rate: $T \in \mathbb{N}^*$, $\eta \in (0, 1)$
- Initialized parameters: $(m^{(0)}, \kappa^{(0)}) \in \mathbb{S}^{d-1} \times \mathbb{R}_+^*$

**Output:** Final parameters: $(m^{(T)}, \kappa^{(T)})$

for $t \leftarrow 0$ to $T - 1$
- $\rho^{(t)} \leftarrow \text{vMF}(m^{(t)}, \kappa^{(t)})$
  for $k \leftarrow 1$ to $n_S$
    $\theta^{(t)}_k \sim \rho^{(t)}$ (Davidson et al., 2018, Algorithm 1)
  end for
  $\rho^{(t)}_{n_S} \leftarrow n_S^{-1} \sum_{k=1}^{n_S} \delta_{\theta^{(t)}_k}$
  $L(x_{1:n}, y_{1:n}, \rho^{(t)}, \lambda) \leftarrow \text{SW}_p^p(\mu_n, \nu_n; \rho^{(t)}_n) - \lambda^{-1} \text{KL}(\rho^{(t)}||\rho^{(0)})$
  $[m^{(t+1)}, \kappa^{(t+1)}] \leftarrow [m^{(t)}, \kappa^{(t)}] + \eta \left[ \nabla_m L(x_{1:n}, y_{1:n}, \rho^{(t)}, \lambda) \right.$
  $\left. - \nabla_\kappa L(x_{1:n}, y_{1:n}, \rho^{(t)}, \lambda) \right]$
end for

Return $(m^{(T)}, \kappa^{(T)})$

---

**Figure A1.** Examples of generated MNIST digits. Left to right: DSW, DSW-10, maxSW, maxSW-10.

### A3.1. Details on the Algorithmic Procedure

For clarity, we specify Algorithm [1] when the optimization is performed over the space of von Mises-Fisher distributions (Definition 5). The procedure is detailed in Algorithm [2].

### A3.2. Additional Results

Figure [A1] displays additional qualitative results for the generative modeling experiment. We observe that the images generated by DSW have a better quality than the ones produced by maxSW, even if DSW is not optimized at every training iteration.

On Figure [A2] are shown the results obtained on the generative modeling experiment of Section [5] using the PAC-SW loss. PAC-SW can be competitive with DSW, but takes more time to execute as the computation of the KL cost is more costly than the regularization term of DSW. However, we observe that the distribution of slices that we learn generalizes well.
Figure A2. Generative modeling experiment when the slice distribution of PAC-SW is updated either at each iteration (PACSW), every 50 iterations (PACSW-50) or every 100 iterations (PACSW-100). Timing results of this experiment were obtained with a NVIDIA GPU A100 80 GB, compared to Figure 4 which was on a NVIDIA V100.