BAYESIAN LEARNING WITH WASSERSTEIN BARYCENTERS

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ABSTRACT. We introduce a novel paradigm for Bayesian learning based on optimal transport theory. Namely, we propose to use the Wasserstein barycenter of the posterior law on models as a predictive posterior, thus introducing an alternative to classical choices like the maximum a posteriori estimator and the Bayesian model average. We exhibit conditions granting the existence and statistical consistency of this estimator, discuss some of its basic and specific properties, and provide insight into its theoretical advantages. Finally, we introduce a novel numerical method which is ideally suited for the computation of our estimator, and we explicitly discuss its implementations for specific families of models. This method can be seen as a stochastic gradient descent algorithm in the Wasserstein space, and is of independent interest and applicability for the computation of Wasserstein barycenters. We also provide an illustrative numerical example for experimental validation of the proposed method.

Keywords: Bayesian learning, non-parametric estimation, Wasserstein distance, Wasserstein barycenter, Fréchet means, consistency, gradient descent, stochastic gradient descent.

1. Introduction

Consider samples $D = \{x_1, \ldots, x_n\}$ in a data space $X$ and a set of feasible models or probability measures $M$ on $X$. Learning a model $m \in M$ from $D$ consists in choosing an element $m \in M$ that best explains the data as generated by $m$, under some given criterion. We adopt the Bayesian viewpoint, which provides a probabilistic framework to deal with model uncertainty, in terms of a prior distribution $\Pi$ on the space $M$ of models; we refer the reader to [21, 32] and references therein for mathematical background on Bayesian statistics and methods. A critical challenge in the Bayesian perspective, is that of calculating a predictive law on $X$ from the posterior distribution on $M$, usually referred to as the predictive posterior. This shall be the learning task to which this work is devoted. Our motivation is to find an alternative, non-parametric learning strategy which can cope with some of the drawbacks of standard approaches such as maximum a posteriori (MAP) or Bayesian model average (BMA).

The first and main conceptual contribution of our work is the introduction of the Bayesian Wasserstein barycenter estimator (BWB) as a novel model-selection criterion based on optimal transport theory. This is our non-parametric model-selection alternative to MAP and BMA. In a nutshell, given a prior on models $\Pi$ and observations $D = \{x_1, \ldots, x_n\} \subseteq X$, a BWB estimator is any minimizer $\hat{m}_n \in M$ of the loss function

$$M \ni m \mapsto \int_{\mathcal{P}(X)} W_p(m, \bar{m})d\Pi_n(dm),$$

where $\mathcal{P}(X)$ denotes the set of probability measures on $X$, $\Pi_n$ is the posterior distribution on models given the data $D$, and $W_p$ is the celebrated $p$-Wasserstein distance ([38, 39]). In fact we shall consider in Section 2 a general framework for Bayesian estimation based on loss functions over probability measures. This allows us to cover both finitely-parametrized and parameter-free model spaces, and also to retrieve classical selection criteria including MAP, Bayesian model average estimators and generalizations thereof, as particular instances of Fréchet means ([41]) with respect to suitable metrics/divergences on the space of probability measures. Then, in Sections 3.1 and 3.2 we recall the notions of Wasserstein distances and, relying on the previously developed framework, we rigorously introduce the Bayesian Wasserstein barycenter estimator. We explore its existence, uniqueness, absolute continuity, and prove that our estimator has less variance than the Bayesian model average.
The second main contribution of our work, carried out in Section 3.3 and culminating in Theorem 3.11, refers to the statistical consistency for the BWB estimator $\hat{m}_n$. See [16, 21], and references therein, for a detailed treatment on posterior consistency. Assuming the observations are independent and identically distributed like $m_0$, we will provide sufficient conditions guaranteeing that

$$\lim_{n \to \infty} W_p(\hat{m}_n, m_0) = 0 \text{ (a.s.)}$$

This is a highly desirable feature of our estimator, both from a semi-frequentist perspective as well as from the “merging of opinions” point of view in the Bayesian framework (cf. [21, Chapter 6]). The main mathematical difficulty in our analysis comes from the fact that the data space $X$ is, in general, an unbounded metric space. The underlying tools that we employ are the celebrated Schwartz theorem ([37, 21, Proposition 6.16]) on one hand, and the concentration of measure phenomenon for averages of unbounded random variables (e.g., [31, Corollary 2.10]) on the other hand.

The minimization of functionals akin to (1.1) is an active field of current research. For instance, if the model space $M$ equals the set of all probability measures on $X$, then our estimator $\hat{m}_n$ coincides with the (population) Wasserstein barycenter of $\Pi_n$. The study of Wasserstein barycenters was introduced by [11], but see also [29, 9] for more recent developments and references to the literature, or our own Appendix B.

The third and final main contribution of our work pertains a new algorithm which is ideally suited for the computation of the BWB estimator, and more generally for Wasserstein barycenters. Current numerical methods allowing to compute minimizers of the functional (1.1), and therefore to compute the BWB estimator in particular, are mostly conceived for the case when the prior $\Pi$ (and hence the posteriors $\Pi_n$) has a finite support. Among these methods we stress the contributions [3, 41]. For obvious reasons this leads us to find a method which can directly deal with the general case when the support of $\Pi$ or $\Pi_n$ is infinite. Our contribution in this regard is the development of an algorithm which can be seen as a stochastic gradient descent method on Wasserstein space; see Sections 4.3 and 4.4.

Crucially, we will establish the almost sure convergence of our stochastic algorithm under given conditions in Theorem 4.7 and Proposition 4.11.

Our stochastic gradient descent method, just like all other algorithms for the computation of Wasserstein barycenters, takes for granted the availability of optimal transport maps between any two regular probability measures. For this reason we shall present in Section 5 examples of model-families for which these optimal maps are explicitly given. These families also serve to illustrate how the iterations of our stochastic descent algorithm simplify.

We close the article with a comprehensive numerical experiment. On the one hand, this serves to illustrate the advantages of the Bayesian Wasserstein barycenter estimator over the Bayesian model average. On the other hand, this experiment suggests as well that the stochastic gradient descent method is a superior alternative for the computation of the Bayesian Wasserstein barycenter estimator, when compared to the more conventional empirical barycenter estimator (cf. Section 4.1).

Let us establish the required notation and conventions. We assume throughout the whole article that

$$\mathcal{M} \subseteq \mathcal{P}_{ac}(X) \subseteq \mathcal{P}(X),$$

where $\mathcal{P}(X)$ denotes the set of probability measures on $X$, and $\mathcal{P}_{ac}(X)$ is the subset of absolutely continuous measures with respect to a common reference $\sigma$-finite measure $\lambda$ on $X$. As a convention, we shall use the same notation for an element $m(dx) \in \mathcal{M}$ and its density $m(x)$ with respect to $\lambda$. Finally, given a measurable map $T : Y \to Z$ and a measure $\nu$ on $Y$ we denote by $T(\nu)$ the image measure (or push-forward), which is the measure on $Z$ given by $T(\nu)(\cdot) = \nu(T^{-1}(\cdot))$. We denote by $\text{supp}(\nu)$ the support of a measure $\nu$ and by $|\text{supp}(\nu)|$ its cardinality.
2. Bayesian learning in the model space

Consider a fixed prior probability measure $\Pi$ on the model space $\mathcal{M}$, namely

$$\Pi \in \mathcal{P}(\mathcal{M}).$$

Assuming as customary that, conditionally on the choice of model $m$, the data $x_1, \ldots, x_n \in \mathcal{X}$ are distributed as i.i.d. observations from the common law $m$, we can write

$$\Pi(dx_1, \ldots, dx_n|m) = m(x_1) \cdots m(x_n) \lambda(dx_1) \cdots \lambda(dx_n). \tag{2.1}$$

By virtue of the Bayes rule, the posterior distribution $\Pi(dm|x_1, \ldots, x_n)$ on models given the data, which is denoted for simplicity $\Pi_m(dm)$, is given by

$$\Pi_m(dm) := \frac{\Pi(x_1, \ldots, x_n|m) \Pi(dm)}{\int_M \Pi(x_1, \ldots, x_n) \Pi(dm)} = \frac{m(x_1) \cdots m(x_n) \Pi(dm)}{\int_M \Pi(x_1, \ldots, x_n) \Pi(dm)}, \tag{2.2}$$

The density $\Lambda_m(m)$ of $\Pi_m(dm)$ with respect the prior $\Pi(dm)$ is called the likelihood function.

Given the model space $\mathcal{M}$, a loss function $L : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ is a non-negative functional. We interpret $L(m_0, \hat{m})$ as the cost of selecting model $\hat{m} \in \mathcal{M}$ when the true model is $m_0 \in \mathcal{M}$. With a loss function and the posterior distribution over models, we define the Bayes risk (or expected loss) $R(\hat{m}|D)$ and a Bayes estimator $\hat{m}_L$ as follows:

$$R_L(\hat{m}|D) := \int_M L(m, \hat{m}) \Pi_m(dm), \tag{2.3}$$

$$\hat{m}_L \in \arg\min_{m \in \mathcal{M}} R_L(\hat{m}|D). \tag{2.4}$$

Since both $L$ and $\Pi_m$ operate directly on the model space, model learning according to the above equations does not depend on geometric aspects of parameter spaces. Moreover, the above point of view allows us to define loss functions in terms of various metrics/divergences directly on the space $\mathcal{P}(\mathcal{X})$, and therefore to enhance the classical Bayesian estimation framework, by using in particular optimal transportation distances. Before further developing these ideas, we briefly describe how this general framework includes model spaces which are finitely parametrized, and discuss standard choices in that setting, together with their appealing features and drawbacks. This could be helpful for readers who are used to parametrically-defined models. The parametric setting is useful as well, since it helps to illustrate the drawbacks of maximum likelihood estimation (MLE). If the reader is already comfortable with the present non-parametric setup, and is aware of the drawbacks of MLE, he or she may skip Section 2.1 altogether.

2.1. Parametric setting. We say that $\mathcal{M}$ is finitely parametrized if there is integer $k$, a set $\Theta \subseteq \mathbb{R}^k$ termed parameter space, and a (measurable) function $\mathcal{T} : \Theta \mapsto \mathcal{P}_\text{fin}(\mathcal{X})$, called parametrization mapping, such that $\mathcal{M} = \mathcal{T}(\Theta)$; in such case we denote the model as $m_0 := \mathcal{T}(\theta)$. If the model space $\mathcal{M}$ is finitely parametrized, learning a model boils down to finding the best model parameters $\theta \in \Theta$. This is usually done in a frequentist fashion through the maximum likelihood estimator. We next illustrate the role of the above-introduced objects in a standard learning application.

Example 2.1. In linear regression, data consist of input $(z_i)$ and output $(y_i)$ pairs, that is, $x_i = (z_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ for $i = 1, \ldots, n$, and the model space is given by the set of joint distributions $p(z, y) = p(y|z)p(z)$ with linear relationship between $y$ and $z$. If we moreover assume that $y|z$ is normally distributed, then $p(y|z) = \mathcal{N}(y; z^\top \beta, \sigma^2)$ for some fixed $\beta \in \mathbb{R}^d$ and $\sigma^2 > 0$. In this setting we need to choose the parameters $\beta, \sigma^2$ and $p(z)$ to obtain the joint distribution $p(z, y)$, i.e. the generative model, though one often needs to deal with the conditional distribution $p(y|z)$, i.e. the discriminative model. Hence, for each fixed $p_0 \in \mathcal{P}_\text{fin}(\mathbb{R}^d)$, the parameter space $\Theta = \mathbb{R}^d \times \mathbb{R}^+$ induces a model space $\mathcal{M}$ through the mapping $\mathcal{T}(\beta, \sigma) \mapsto \mathcal{T}(\beta, \sigma)$, where $\mathcal{T}(\beta, \sigma)$ has the density $\mathcal{N}(y; z^\top \beta, \sigma^2)p_0(z)$, $(z, y) \in \mathbb{R}^d \times \mathbb{R}$. Conditioning this joint density $p(y, z)$ with respect to a new input $z_*$, we obtain the predictive distribution addressing the regression problem $p(y|z_*)$. In particular, denoting $y = (y_1, \ldots, y_n) \in \mathbb{R}^d$ and $Z = (z_1, \ldots, z_n) \in \mathbb{R}^{n \times d}$, the MLE parameters are then given by $\hat{\beta} = (Z^\top Z)^{-1}Z^\top y$ and $\hat{\sigma}^2 = \frac{1}{n}(y - Z\hat{\beta})^\top(y - Z\hat{\beta})$. 
Given \( p \in \mathcal{P}(\Theta) \) a prior distribution over a parametric space \( \Theta \), its push-forward through the map \( T \) is the probability measure \( \Pi = T(p) \) given by \( \Pi(A) = p(T^{-1}(A)) \). Expressing the likelihood function \( \Lambda_\ell(m) \) in terms of the parameter \( \theta \) such that \( T(\theta) = m \), we then easily recover from (2.2) the standard posterior distribution over the parameter space, \( p(d\theta|x_1, \ldots, x_n) \). Moreover, any loss function \( L \) induces a functional \( \ell \) defined on \( \Theta \times \Theta \) (and vice versa) by \( \ell(\theta_0, \hat{\theta}) = L(m_{\theta_0}, m_{\hat{\theta}}) \), interpreted as the cost of choosing parameter \( \hat{\theta} \) when the actual true parameter is \( \theta_0 \). The Bayes risk \( \mathcal{R}_\ell(\hat{\theta}|D) = \int_\Theta \ell(\theta, \hat{\theta}) p(d\theta|x_1, \ldots, x_n) = \int_\Theta L(m, \hat{m}) \Pi_\lambda(dm) \),

whence \( \Pi_\lambda(dm) = \Lambda_\ell(m) \Pi(dm) \), with the prior distribution \( \Pi = T(p) \). The associated Bayes estimator is of course given by \( \hat{\theta}_\ell \in \arg\min_{\theta \in \Theta} \mathcal{R}_\ell(\theta|D) \).

For illustration, consider the 0-1 loss defined as \( \ell_{0-1}(\theta, \hat{\theta}) = 1 - \delta(\theta, \hat{\theta}) \) yields \( \mathcal{R}_{0-1}(\hat{\theta}|D) = 1 - p(\hat{\theta}|D) \), that is, the corresponding Bayes estimator is the posterior mode, also referred to as Maximum a Posteriori Estimator (MAP), \( \hat{\theta}_{\text{MAP}} = \hat{\theta}_{\text{MAP}} \). For continuous-valued quantities the use of a quadratic loss \( \ell_2(\theta, \hat{\theta}) = \| \theta - \hat{\theta} \|^2 \) is often preferred. The corresponding Bayes estimator is the posterior mean \( \hat{\theta}_2 = \int \theta p(d\theta|D) \). In one dimensional parameter space, the absolute loss \( \ell_1(\theta, \hat{\theta}) = |\theta - \hat{\theta}| \) yields the posterior median estimator.

The MAP approach is computationally appealing as it reduces to an optimization problem in a finite dimensional space. The performance of this method might however be highly sensitive to the choice of the initial condition used in the optimization algorithm \([40]\). This is a critical drawback, since likelihood functions over parameters may be populated with numerous local optima. A second drawback of this method is that it fails to capture global information of the model space, which might result in an overfit of the predictive distribution. Indeed, the mode can often be a very poor summary or atypical choice of the posterior distribution (e.g. the mode of an exponential density is 0, irrespective of its parameter). Yet another serious failure of MAP estimation is its dependence on the parameterization. Indeed, for instance, in the case of a Bernoulli distribution on \([0, 1]\) with \( p(y = 1) = \mu \) and an uniform prior on \([0, 1]\) for \( \mu \), the mode can be anything in \([0, 1]\). On the other hand, parameterizing the model by \( \theta = \mu^{1/2} \) yields the mode 1, while parametrizing it by \( \theta = 1 - (1 - \mu)^{1/2} \) yields 0 as mode.

Using general Bayes estimators on parametrized models enables for a richer choice of criteria for model selection (by integrating global information of the parameter space) while providing a measure of uncertainty (through the Bayes risk value). However, this approach might also neglect parametrization related issues, such as overparametrization of the model space (we say that \( T \) overparametrizes \( M \) if it is not one-to-one). The latter might result in a multi-modal posterior distribution over parameters. For example, take \( X = \Theta = \mathbb{R} \), \( m_0 = N(\mu, 1) \) and \( T(\theta) = N(\theta^2, 1) \). If we choose a symmetric prior \( p(\theta) \), e.g. \( p(\theta) = N(\theta|0, 1) \), then with enough data, the posterior distribution is symmetric with modes near \( |\mu|, -|\mu| \), so both \( \ell_1 \) and \( \ell_2 \) estimators are close to 0.

By the above issues, we propose using free-parameter selection criteria via loss functions that compare directly distributions instead of their parameters.

### 2.2. Posterior average estimators

The next result, proved in Appendix \( \Box \) illustrates the fact that many Bayesian estimators, including the classic model average estimator, correspond to finding a so-called Fréchet mean or barycenter \( [41] \) under a suitable metric/divergence on probability measures.

**Proposition 2.2.** Let \( M = \mathcal{P}_\mathfrak{ac}(X) \) and consider the loss functions \( L(m, \hat{m}) \) given by:

1. The \( L_2 \)-distance: \( L_2(m, \hat{m}) = \frac{1}{2} \int_X (m(x) - \hat{m}(x))^2 \lambda(dx) \),
2. The reverse Kullback-Leibler divergence: \( D_{KL}(m||\hat{m}) = \int m(x) \ln \frac{m(x)}{\hat{m}(x)} \lambda(dx) \),
3. The forward Kullback-Leibler divergence \( D_{KL}(\hat{m}||m) = \int \hat{m}(x) \ln \frac{\hat{m}(x)}{m(x)} \lambda(dx) \),
4. The squared Hellinger distance \( H^2(m, \hat{m}) = \frac{1}{2} \int \left( \sqrt{m(x)} - \sqrt{\hat{m}(x)} \right)^2 \lambda(dx) \).
Then, in cases i) and ii) the corresponding Bayes estimators of Equation (2.4) coincide with the Bayesian model average:

$$\hat{m}(x) := E_{\Pi_n}[m] = \int_M m(x)\Pi_n(dm).$$  \hspace{1cm} (2.6)

Furthermore, with $Z_1$ and $Z_2$ denoting normalizing constants, the Bayes estimators corresponding to the cases iii) and iv) are given by the exponential model average and the square model average, respectively:

$$\hat{m}_{exp}(x) = \frac{1}{Z_{exp}} \exp \int_M m(x)\Pi_n(dm), \quad \hat{m}_{s}(x) = \frac{1}{Z} \left( \int_M \sqrt{m(x)\Pi_n(dm)} \right)^2.$$  \hspace{1cm} (2.7)

All the above-described Bayesian estimators (Eqs. (2.6) and (2.7)) share a common feature: their values at each point $x \in X$ are computed in terms of some posterior average of the values of certain functions evaluated at $x$. This is due to the fact that all the above distances are vertical [36], in the sense that computing the distance between $m$ and $\hat{m}$ involves the integral of vertical displacements between the graphs of these two densities. An undesirable fact about vertical averages is that they do not preserve properties of the original model space. For example, if the posterior distribution is equally concentrated on two different models $m_0 = N(\mu_0, 1)$ and $m_1 = N(\mu_1, 1)$ with $\mu_0 \neq \mu_1$, that is, both models are unimodal (Gaussian) with unit variance, the model average is in turn a bimodal (non-Gaussian) distribution with variance strictly greater than 1. More generally, model averages might yield intractable representations or be hardly interpretable in terms of the prior and parameters.

We shall next introduce the analogous objects in the case of Wasserstein distances, which are horizontal distances [36], in the sense that they involve integrating horizontal displacements between the graphs of the densities. We will further develop the theory of the corresponding Bayes estimators, which will correspond to Wasserstein barycenters arising in optimal transport theory (see [11, 35, 25, 29]). Going back to the Gaussian example, say for two models given by the univariate Gaussian distributions $m_0 = N(\mu_0, \sigma_0^2)$ and $m_1 = N(\mu_1, \sigma_1^2)$, it turns out that the so-called 2-Wasserstein barycenter distribution is given by $\hat{m} = m_{\bar{x}} = N(\frac{\mu_0 + \mu_1}{2}, \frac{\sigma_0^2 + \sigma_1^2}{2})$. In Fig. 1, we illustrate for the reader’s convenience a vertical and a horizontal interpolation between two Gaussian densities.

![Figure 1](image_url) Vertical interpolation (left) and horizontal interpolation (right) of two Gaussian densities.

3. The Bayesian Wasserstein Barycenter Estimator

We propose a novel Bayesian estimator obtained by using the Wasserstein distance as loss function. This estimator is therefore given by a Fréchet mean in the Wasserstein metric and, therefore, it is usually referred to as Wasserstein barycenter [1]. For a summary of the notion of Wasserstein barycenters we refer to Appendix [B]. We state conditions for the statistical consistency of our estimator, which is a basic desirable property: briefly put, this means that as more data becomes available, the estimator converges to the true model. The main result in this regard is Theorem [3.11]. We then illustrate the advantage of this estimator by comparing it to the Bayesian model average: it turns out that our estimator is less dispersed, and in particular, it has less variance than the model average.

From now until the end of the article, unless otherwise stated, we assume:

**Assumption 3.1.** $(X, d)$ is a separable locally-compact geodesic space and $p \geq 1$. 
Geodesic means that is complete and any pair of points admit a mid-point with respect to $d$. The reader can think of $X$ as a Euclidean space with $d$ the Euclidean distance. On the other hand $d^q$ will control the tail of the models to be considered. We now recall some elements of optimal transport theory.

3.1. Optimal transport and Wasserstein distances in a nutshell. A thorough introduction of optimal transport and some of its applications can be found in the books by Villani [38, 39]. It is difficult to overstate the impact that the field has had in mathematics as a whole. In particular, regarding statistical applications, we refer to the recent survey [33] and the many references therein. In parallel, optimal transport has become increasingly popular within the machine learning community [28], though most of the published works have focused on the discrete setting (e.g., comparing histograms in [15], classification in [20] and images in [13, 6], among others). Let us briefly review definitions and results needed to present our approach.

Given two measures $\mu, \nu$ over $X$ we denote by $\Gamma(\mu, \nu)$ the set of couplings with marginals $\mu$ and $\nu$, i.e. $\gamma \in \Gamma(\mu, \nu)$ if $\gamma \in \mathcal{P}(X \times X)$ and we have that $\gamma(dx, x) = \mu(dx)$ and $\gamma(X, dy) = \nu(dy)$. Given a real number $p \geq 1$ we define the $p$-Wasserstein space $\mathcal{W}_p(X)$ by

$$\mathcal{W}_p(X) := \{\eta \in \mathcal{P}(X) : \int_X d(x_0, x)^p \eta(dx) < \infty, \text{ some } x_0\}.$$ 

The $p$-Wasserstein between measures $\mu$ and $\nu$ is given by

$$\mathcal{W}_p(\mu, \nu) = \left(\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{X \times X} d(x, y)^p \gamma(dx, dy)\right)^{\frac{1}{p}}.$$ (3.1)

An optimizer of the right-hand side of (3.1) is called an optimal transport. The quantity $W_p$ defines a distance turning $\mathcal{W}_p(X)$ into a complete metric space. In the Euclidean case, there often exist explicit formulae for the optimal transport and the Wasserstein distance, e.g., for the generic one-dimensional case, and for the multivariate Gaussian case with $p = 2$ (see [13]). If in (3.1) we assume that $p = 2$, $X$ is Euclidean space, and $\mu$ is absolutely continuous, then Brenier’s theorem [38, Theorem 2.12(ii)] establishes the uniqueness of a minimizer. Furthermore, this optimizer is supported on the graph of the gradient of a convex function.

3.2. Wasserstein population barycenter. We start with the definition of Wasserstein population barycenter:

Definition 3.2. Given $\Gamma \in \mathcal{P}(\mathcal{P}(X))$, the $p$-Wasserstein risk of $\bar{m} \in \mathcal{P}(X)$ is

$$V_p(\bar{m}) := \int_{\mathcal{P}(X)} \mathcal{W}_p(m, \bar{m})^p \text{d}m.$$ 

Any measure $\mathring{m}_p \in \mathcal{M}$ which is a minimizer of the problem

$$\inf_{\bar{m} \in \mathcal{M}} V_p(\bar{m}),$$

is called a $p$-Wasserstein population barycenter of $\Gamma$ over $\mathcal{M}$.

In the case $\mathcal{M} = \mathcal{W}_p(X)$, the above is nothing but the $p$-Wasserstein population barycenter of $\Gamma$ introduced in [9]. The term population is used to emphasize that the support of $\Gamma$ might be infinite. Let us introduce some required notation. For $\Gamma \in \mathcal{P}(\mathcal{P}(X))$ we write $\Gamma \in \mathcal{P}(\mathcal{W}_p(X))$ if $\Gamma$ is concentrated on a set of measures with finite moments of order $p$, and $\Gamma \in \mathcal{W}_p(\mathcal{W}_p(X))$ if furthermore for some (and then all) $\bar{m} \in \mathcal{W}_p(X)$ it satisfies

$$\int_{\mathcal{P}(X)} \mathcal{W}_p(m, \bar{m})^p \text{d}m < \infty.$$ 

If $\Gamma$ is concentrated on measures with finite moments of order $p$ and with density with respect to $\lambda$, then we rather write $\Gamma \in \mathcal{P}(\mathcal{W}_{p, \text{ac}}(X))$, with the notation $\Gamma \in \mathcal{W}_p(\mathcal{W}_{p, \text{ac}}(X))$ if as before $\int_{\mathcal{P}(X)} \mathcal{W}_p(m, \bar{m})^p \text{d}m < \infty$ for some $\bar{m}$.

We come to the most important definition (and conceptual contribution) of the article. A Bayesian Wasserstein barycenter estimator is nothing but a $p$-Wasserstein population barycenter of the posteriors $\Pi_n$ over the model space $\mathcal{M}$:
Lemma 3.5. \( M \) which is relevant since the model space
In Appendix C we provide a su-
Wasserstein barycenter estimator
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\( \tilde{y} \)
\( \beta \)
\( \delta \)
\( \Lambda \)
\( \left( \frac{\delta}{\omega}, m \right) \)
\( \Gamma \)
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3.3. Statistical consistency.

A natural question is whether our estimator is consistent in the statistical sense (see [37, 16, 21]). In short, consistency corresponds to the convergence of opinions after a few computations. But, by Brenier’s theorem [38, Theorem 2.12(ii)] we know that

\[ \int W_2^2(\Phi(x,y) d\gamma) = \int W_2^2(\Phi(x,y) d\mu) \]

after a few computations. But, by Brenier’s theorem [38, Theorem 2.12(ii)] we know that

\[ \int W_2^2(\Phi(x,y) d\gamma) = \int W_2^2(\Phi(x,y) d\mu) \]

Bringing together these three observations, we deduce

\[ \int W_2^2(\Phi(x,y) d\gamma) = \int W_2^2(\Phi(x,y) d\mu) \]

and in particular \( \hat{m} \) cannot be the barycenter.

Definition 3.9. The prior \( \Pi \) is said to be \( p \)-Wasserstein strongly consistent at \( m_0 \) if for each open neighbourhood \( U \) of \( m_0 \) in the \( p \)-Wasserstein topology of \( W_p(X) \), we have \( \Pi_n(U^c) \to 0 \), \( m_0^{(\infty)} \) - a.s.

The celebrated Schwartz theorem provides sufficient conditions for strong consistency. See the original [37] or [21, Proposition 6.16] for a more modern treatment. A key ingredient in Schwartz’ approach is the notion of Kullback-Leibler support:

Definition 3.10. A measure \( m_0 \) belongs to the Kullback-Leibler support of \( \Pi \), denoted \( m_0 \in KL(\Pi) \), if \( \Pi m: D_{KL}(m_0||m) < \varepsilon > 0 \) for \( \forall \varepsilon > 0 \), where \( D_{KL}(m_0||m) = \int \log \frac{m_0}{m} d\gamma \).

We are mostly interested in the important question, of whether our Wasserstein barycenter estimator converges to the model \( m_0 \), i.e. we are after conditions which guarantee that

\[ W_p(\hat{m}_{m_0}, m_0) \to 0 \text{, } m_0^{(\infty)} \text{ a.s.} \]

This is evidently linked to the question of strong consistency of the prior. We assume throughout Section 3.3 that

\[ m_0 \in KL(\Pi) \text{ and } m_0 \in M. \]

This implies that the model is correct or well specified as discussed in [8, 23, 26, 27]. This setting could be slightly relaxed in the misspecified framework dealt with in those works by considering the reverse Kullback-Leibler projection on \( M \) instead of the true model \( m_0 \), i.e. the unique model \( \hat{m}_0 \in M \) that minimizes \( D_{KL}(m_0||\hat{m}_0) \) over \( M \).

We can now state our main result concerning consistency of the barycenter estimator:

Theorem 3.11. Suppose that \( \Pi \) fulfils the following conditions:

(a) \( \text{supp}(\Pi) \) is bounded, namely \( \text{diam}(\Pi) := \sup_{m \in \text{supp}(\Pi)} W_p(m, \hat{m}) < \infty, \)

Proof. The existence of a jointly measurable version of the unique optimal maps is proved in [19]. Now assume that the last assertion is not true, so in particular

\[ 0 < \int (x - \int T^m(x) \Pi(dm))^2 \hat{m}(dx) \]

On the other hand, we have

\[ \int W^2_2(H \Pi(dm)) \hat{m}(dx) \leq \int W^2_2(x - H \Pi(dm)) \hat{m}(dx) \]

where

\[ H \Pi(dm) = \int W^2_2(x - H \Pi(dm)) \hat{m}(dx) \]

In the setting that concerns us, the correct notion of consistency at the level of the prior is given by:
(b) there is $\lambda_0 > 0$ and $x_0 \in X$ such that

$$\sup_{m \in \text{supp}(\Pi)} \int_X e^{\lambda_0 d^p(x, x_0)} dm(x) < +\infty.$$ 

Then under our standing assumptions (in particular, $m_0 \in KL(\Pi)$) we have that $\Pi$ is $p$-Wasserstein strongly consistent at $m_0$, $W_p(\Pi_n, \delta_{m_0}) \to 0$ ($m_0^{(0)}$-a.s.), and the barycenter estimator is consistent in the sense that

$$W_p(\hat{m}_p^n, m_0) \to 0, \quad m_0^{(0)} - a.s.$$ 

A typical example where the boundedness of the support of $\Pi$ holds is in the finitely parametrized case, when the parameter space is compact and the parametrization function continuous. We stress that $X$ may be unbounded and still $\text{diam}(\Pi)$ may be finite. The proof of Theorem 3.11 is given at the end of this part. Towards this goal, we start with a rather direct sufficient condition for the convergence of $\hat{m}_p^n$ to $m_0$. We use $W_p$ to denote throughout the Wasserstein distance both on $\mathcal{W}_p(\mathcal{M}(\mathcal{X}))$ and on $\mathcal{W}_p(X)$, not to make the notation heavier.

**Proposition 3.12.** If $W_p(\Pi_n, \delta_{m_0}) \to 0$ ($m_0^{(0)}$-a.s.) then $W_p(\hat{m}_p^n, m_0) \to 0$ ($m_0^{(0)}$-a.s.).

**Proof.** We have, by minimality of the barycenter

$$W_p(\Pi_n, \delta_{m_0})^p = \int_M W_p(m, m_0)^p \Pi_n(dm) \geq \int_M W_p(m, \hat{m}_p^n)^p \Pi_n(dm).$$

On the other hand,

$$W_p(m_0, \hat{m}_p^n)^p \leq c W_p(m, \hat{m}_p^n)^p + c W_p(m, m_0)^p, \quad \forall m,$$

where the constant $c$ only depends on $p$. We conclude by

$$W_p(m_0, \hat{m}_p^n)^p \leq c \int_M W_p(m, \hat{m}_p^n)^p \Pi_n(dm) + c \int_M W_p(m, m_0)^p \Pi_n(dm)$$

$$\leq c \int_M W_p(m, \hat{m}_p^n)^p \Pi_n(dm) + c W_p(\Pi_n, \delta_{m_0})^p$$

$$\leq 2c W_p(\Pi_n, \delta_{m_0})^p.$$ 

\[ \square \]

**Proposition 3.13.** If $\Pi$ is $p$-Wasserstein strongly consistent at $m_0$ and supp$(\Pi)$ is bounded, then $W_p(\Pi_n, \delta_{m_0}) \to 0$ and in particular $W_p(\hat{m}_p^n, m_0) \to 0$ ($m_0^{(0)}$ - a.s.).

**Proof.** Let $B = \{m : W_p(m, m_0) < \varepsilon\}$ and $\varepsilon$ arbitrary, then

$$W_p(\Pi_n, \delta_{m_0})^p = \int_B W_p(m, m_0)^p \Pi_n(dm)$$

$$\leq \int_B W_p(m, m_0)^p \Pi_n(dm) + \int_B W_p(m, m_0)^p \Pi_n(dm)$$

$$\leq \varepsilon^p + \int_B W_p(m, m_0)^p \Pi_n(dm).$$

Since $\varepsilon$ is arbitrary, we only need to check that the second term goes to zero. Strong consistency implies $\Pi_n(B^c) \to 0$ ($m_0^{(0)}$-a.s.), and since supp$(\Pi_n) \subseteq$ supp$(\Pi)$, we have

$$\int_B W_p(m, m_0)^p \Pi_n(dm) \leq \text{diam}(\Pi) \varepsilon^p \Pi_n(B^c) \to 0 (m_0^{(0)} - a.s.).$$ 

\[ \square \]

We now provide the proof of Theorem 3.11. If the Wasserstein metric was bounded, the argument would be as in [21, Example 6.20], where the main tool is Hoeffding’s inequality. In general Wasserstein metrics are unbounded if $X$ is itself unbounded, and this forces us to assume Conditions (a) and (b) in Theorem 3.11. The argument still rests on the concentration of measure phenomenon:

**Proof of Theorem 3.11.** We aim to apply Proposition 3.13. First we show that if $U$ is any $\mathcal{W}_p(\mathcal{X})$-neighbourhood of $m_0$ then $m_0^{(0)}$-a.s. we have $\liminf_n \Pi_n(U) \geq 1$. According to Schwartz Theorem (in the form of [21, Theorem 6.17]), under the assumption that $m_0 \in KL(\Pi)$, it is enough to find for each such $U$ a sequence of measurable functions $\varphi_n : X \to [0, 1]$ such that
These sets form a subbase for the Proposition 3.13 thanks to our Assumption (a).

we have established that \( \Pi \epsilon > 0 \) we define the open set neighborhoods.

We may apply Bernstein’s inequality in the form of [31, Corollary 2.10] to the random variables where \( v \).

Since all the moments of \( Z \) are non-negative, we can bound all the \( k \)-moments by

Thanks to the above bound, we have

We may apply Bernstein’s inequality in the form of [31] Corollary 2.10 to the random variables \( \{-\psi(x)\} \) under the measure \( m^{(\infty)} \) on \( X^\Omega \), obtaining for any \( \alpha < 0 \) that

where \( v := 2m \丽\( m^t \丽\) t^{-2}, \( c := t^{-1} \), and \( 0 < t \leq \Lambda_0 \).

Going back to the tests \( \phi_n \) and using the definition of \( U^r \) we deduce

Under our assumption (b) we conclude as desired that

Now, a general neighborhood \( U \) contains a finite intersection of \( N \in \mathbb{N} \) neighborhoods from the subbase, i.e. \( \bigcap_{n=1}^{N} U_{\psi_i, \epsilon} \subseteq U \), so

and therefore we may conclude as in the subbase case that Point 2 is verified. All in all we have established that \( \Pi \) is \( p \)-Wasserstein strongly consistent at \( m_0 \), so we conclude by Proposition 3.13 thanks to our Assumption (a).
3.4. **Bayesian Wasserstein barycenter versus Bayesian model average.** It is illustrative to compare the Bayesian model average with our barycenter estimators. First we show that if the Bayesian model converges, then our estimator converges too. We even have the stronger condition that the posterior distribution converges in $\mathcal{W}_p$. Recall that the model average is given by $\bar{m}(dx) = \mathbb{E}_{\Pi_n}[m](dx)$.

**Lemma 3.14.** If $m_0^{(\omega)}$-a.s. the $p$-moments of the model average converge to those of $m_0 \in KL(\Pi)$, then $W_p(\Pi_n, \delta_{m_0}) \to 0$ ($m^{(\omega)}_0$-a.s.). In particular, also $W_p(\bar{m}, m_0) \to 0$ ($m^{(\omega)}_0$-a.s.).

**Proof.** By [21, Example 6.20] we already know that the prior is strongly consistent at $m_0$ with respect to the weak topology (rather than the $p$-Wasserstein topology). Notice that

$$\int W_p(m, \delta_{z})(\Pi_n(dm)) = \int \int d(x, z)^p m(dz) \Pi_n(dm) = \int d(x, z)^p \bar{m}(dz),$$

so a.s. $\Pi_n \to \delta_{m_0}$, not only weakly but in $W_p$. Conclude by Proposition 3.12.

We now briefly consider the case of $\Pi \in \mathcal{W}_2(W_2, \text{Lebesgue})$, $M = \mathcal{W}_2, \lambda = \text{Lebesgue}$, and $d = \text{Euclidean}$ distance. Let $\hat{m}$ be its unique population barycenter, and denote by $(m, x) \mapsto T^n(x)$ a measurable function equal $\lambda(dx)\Pi(dm)$ a.e. to the unique optimal transport map from $\hat{m}$ to $m \in \mathcal{W}_2(X)$. As a consequence of Lemma 3.14 we have

$$\hat{m} = (\int T^n(\Pi)(dm))(\hat{m}).$$

Thanks to this fixed-point property, for all convex functions $\varphi$ with at most quadratic growth, we have

$$\mathbb{E}[\varphi(x)] = \int_X \varphi(x)\hat{m}(dx) = \int_X \varphi\left(\int_M T^n(x)\Pi(dm)\right)\hat{m}(dx) \geq \int_X \varphi\left(\int_M T^n(x)\Pi(dm)\right)\hat{m}(dx) \int_X \varphi(x) \int_M T^n(x)\Pi(dm) = \mathbb{E}[\varphi(x)],$$

where $\bar{m} = \mathbb{E}[m]$ is the Bayesian model average. We have used here Jensen’s inequality and Fubini. Since we can replace $\Pi$ by $\Pi_n$ in this discussion, we have established that the 2-Wasserstein barycenter estimator is less dispersed than the Bayesian model average: namely, in the convex-order sense. In particular we have established:

**Lemma 3.15.** Let $\bar{m}$ be the Bayesian model average and $\hat{m}$ the 2-Wasserstein barycenter of the posterior $\Pi_n$. Then we have $\mathbb{E}[\varphi]\{x\} \geq \mathbb{E}_m[\varphi\{x\}] \geq \mathbb{E}_n[\varphi\{x\}]$, so the 2-Wasserstein barycenter estimator has less variance than the model average estimator.

4. **On the computation of the population Wasserstein barycenter.**

In this part we discuss possible ways to compute/approximate the population Wasserstein barycenter. This is a crucial step in constructing our Bayesian Wasserstein estimator (see Section 4.3). To this effect, we introduce a novel algorithm for computation of barycenters in Section 4.4, which can be seen as a stochastic gradient descent on Wasserstein space. This is the main contribution of this part of the article, followed by Section 4.4 where we present a generalization of this method (batch stochastic gradient descent). We begin this development in Section 4.1 with a straightforward Monte-Carlo method, which has an illustrative purpose and therefore is not studied in depth. This method motivates us to summarize in Section 4.2 the essentials of the gradient descent method in Wasserstein space, developed in [21, 31], where we can fix important notation and ideas for our main contribution in Sections 4.3 and 4.4.

For our results, we assume we are capable of generating independent models $m$ from the posteriors $\Pi_n$ and the prior $\Pi$. In the parametric setting, we can use efficient Markov Chain Monte Carlo (MCMC) techniques [22] or transport sampling procedures [17, 34, 24, 30] to generate models $m_i$ sampled from $\Pi_n$ or $\Pi$.

4.1. **Empirical Wasserstein barycenter.** In practice, except in special cases, we cannot calculate integrals over the entire model space $M$. Thus we must approximate such integrals by e.g., Monte Carlo methods. For this reason, we now discuss the empirical Wasserstein barycenter and its usefulness as an estimator. For a related statement when $\text{supp}(\Pi) < \infty$ see [10, Theorem 3.1].
Lemma 4.3. Given \( m_i \sim \Pi_n \) for \( i = 1, \ldots, k \), the empirical measure \( \Pi_n^{(k)} \) over models is

\[
\Pi_n^{(k)} := \frac{1}{k} \sum_{i=1}^{k} \delta_{m_i} \in \mathcal{P}(M).
\]

Note that if a.s. \( \Pi_n \in \mathcal{W}_p'(\mathcal{W}_p,\mathcal{X}) \) then a.s. \( \Pi_n^{(k)} \in \mathcal{W}_p'(\mathcal{W}_p,\mathcal{X}) \), so all hypothesis about \( \Pi_n \) stand on \( \Pi_n^{(k)} \). Using \( \Pi_n^{(k)} \) instead of \( \Pi_n \), we define the \( p \)-Wasserstein empirical Bayes risk \( V_p^{\Pi_n^{(k)}}(\hat{m}D) \), as well as a corresponding empirical Bayes estimator \( \hat{m}^{(k)}_n \), which in the case \( M = \mathcal{W}_p \) is referred to as a \( p \)-Wasserstein empirical barycenter of \( \Pi_n \) (see [9]).

### Remark 4.2.

It is known that a.s. \( \Pi_n^{(k)} \) converges weakly to \( \Pi_n \) as \( k \to \infty \). If \( \Pi_n \) has finite \( p \)-th moments, by the strong law of large numbers we have convergence of \( p \)-th moments:

\[
\int W_p(m, m_0)^p \Pi_n^{(k)}(dm) = \frac{1}{k} \sum_{i=1}^{k} W_p(m_i, m_0)^p \to \int W_p(m, m_0)^p \Pi_n(dm) \text{ a.s.}
\]

Thus we have that a.s. \( \Pi_n^{(k)} \to \Pi_n \) in \( \mathcal{W}_p \) as \( k \to \infty \). Thanks to [29, Theorem 3], any sequence of empirical barycenters \( (\hat{m}^{(k)}_n)_{k \geq 1} \) of \( (\Pi_n^{(k)})_{k \geq 1} \) converges (up to selection of a subsequence) in \( p \)-Wasserstein distance to a (population) barycenter \( \hat{m}_n \) of \( \Pi_n \). Combining these facts, the following result is immediate:

### Lemma 4.3.

If \( W_p(\Pi_n, \delta_{m_0}) \to 0 \), \( m_0^{(\infty)} \)-a.s., there exists a data-dependent sequence \( k_n := k_0(x_1, \ldots, x_n) \) such that \( (\hat{m}^{(k_n)}_m)_{k \geq 1} \) satisfy \( W_p(\hat{m}^{(k_n)}_m, m_0) \to 0 \), \( m_0^{(\infty)} \)-a.s..

**Proof.** Since \( W_p \) is a metric we have that \( W_p(\hat{m}^{(k_n)}_m, m_0) \leq W_p(\hat{m}^{(k_n)}_n, \hat{m}_n) + W_p(\hat{m}_n, m_0) \) for all \( k, n \geq 0 \), and thanks to Proposition 3.12 the last term tends to zero \( m_0^{(\infty)} \)-a.s. as \( n \to \infty \). Using a diagonal argument, for each \( \hat{m}_n \) exists \( k_n \) (determined by the data-dependent \( \Pi_n \)) s.t. the empirical barycenter \( \hat{m}^{(k_n)}_n \) satisfies \( W_p(\hat{m}^{(k_n)}_n, \hat{m}_n) \leq \frac{1}{k} \), thus obtaining the convergence.

### 4.2. Gradient descent on Wasserstein space.

We first survey the gradient descent method for the computation of 2-Wasserstein empirical barycenters. This will serve as a motivation for the subsequent development of the stochastic gradient descent in Sections 4.3 and 4.4.

From now until the end of the article we strengthen Assumption [3.6] by further assuming (cf. Remark [3.7]) that

### Assumption 4.4.

\( \mathcal{X} = \mathbb{R}^d \), \( d = \text{Euclidean metric}, \lambda = \text{Lebesgue measure}, p = 2 \).

Let us consider \( m_1, \ldots, m_k \in \mathcal{W}_{2,\infty}(\mathbb{R}^d) \), weights \( \lambda_1, \ldots, \lambda_k \in \mathbb{R}^+ \), \( \sum_{i=1}^{k} \lambda_i = 1 \) and the respective discrete measure \( \Pi^{(k)} = \sum_{i=1}^{k} \lambda_i \delta_{m_i} \). Given some measure \( m \in \mathcal{W}_{2,\infty}(\mathbb{R}^d) \), we denote the optimal transport map from \( m \) to \( m_i \) as \( T_m^{m_i} \) for \( i = 1, \ldots, k \). The uniqueness and existence of this map is guaranteed by Brenier’s Theorem. With this notation one can define the operator \( G_k : \mathcal{W}_{2,\infty}(\mathbb{R}^d) \to \mathcal{W}_{2,\infty}(\mathbb{R}^d) \) as

\[
G_k(m) := \left( \sum_{i=1}^{k} \lambda_i T_m^{m_i} \right)(m).
\]

(4.1)

Owing to [3] the operator \( G_k \) is continuous for the \( W_2 \) distance. Also, if at least one of the \( m_i \) has a bounded density, then the unique Wasserstein barycenter \( m \) of \( \Pi^{(k)} \) has a bounded density and satisfies \( G_k(m) = m \). Thanks to this, starting from \( m_0 \in \mathcal{W}_{2,\infty}(\mathbb{R}^d) \) one can define the sequence

\[
\mu_{n+1} := G_k(\mu_n), \quad \text{for } n \geq 0.
\]

(4.2)

The following result was established by Álvarez-Esteban, del Barrio, Cuesta-Albertos and Matrán in [3] Theorem 3.6], as well as independently by Zemel and Panaretos in [21, Theorem 3,Corollary 2]:

The sequence \( \{\mu_n\}_{n \geq 0} \) defined in (4.2) is tight and every weakly convergent subsequence of \( \{\mu_n\}_{n \geq 0} \) must converge in \( W_2 \) distance to a measure in \( \mathcal{W}_{2,\infty}(\mathbb{R}^d) \) which is a fixed point of \( G_k \). If some \( m \) has a bounded density, and if \( G_k \) has a unique fixed point \( m \), then \( m \) is the

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1One can think of \( \Pi^{(k)} \) as an empirical approximation of the posterior \( \Pi \) or the prior \( \Pi \).
Wasserstein barycenter of $\Pi^{(k)}$ and we have that $W_2(\mu, \hat{m}) \to 0$.

The previous result allows one to estimate the barycenter of any discrete measure (i.e. any prior/posterior with a finite support), as long as one is able to construct the optimal transports $T^m_m$. Thanks to the almost Riemannian geometry of the Wasserstein space $W_2(\mathbb{R}^d)$ (see [5], Chapter 8) one can reinterpret the iterations defined in (4.2) as a gradient descent iteration. This was discovered by Panaretos and Zemel in [41, 33]. In fact, in [41] Theorem 1] the authors prove the following: Letting $\Pi^{(k)} = \sum_{i=1}^{I_k} \lambda_i \delta_{m_i}$ as above, then the (half) Wasserstein Bayes risk of $m \in \mathcal{W}_{2,\infty}(\mathbb{R}^d)$ and its Fréchet derivative are given respectively by

$$F_k(m) := \frac{1}{2} \sum_{i=1}^{I_k} \lambda_i W_2^2(m_i, m),$$

$$F'_k(m) = - \sum_{i=1}^{I_k} \lambda_i (T^m_{m_i} - I) = I - \sum_{i=1}^{I_k} \lambda_i T^m_{m_i},$$

where $I$ is the identity map on $\mathbb{R}^d$. It follows by Brenier’s theorem [38, Theorem 2.12(ii)] that $\hat{m}$ is a fixed point of $G_k$ defined in (4.1) if and only if $F'_k(\hat{m}) = 0$ (one says that $\hat{m}$ is a Karcher mean of $\Pi^{(k)}$). The gradient descent sequence with step $\gamma \in [0, 1]$ starting from $\mu_0 \in \mathcal{W}_{2,\infty}(\mathbb{R}^d)$ is defined as

$$\mu_{n+1} := G_{k,n}(\mu_n), \text{ for } n \geq 0,$$

where

$$G_{k,n}(m) := \left[ I + \gamma F'_k(m) \right](m) = \left[ (1 - \gamma)I + \gamma \sum_{i=1}^{I_k} \lambda_i T_{m_i}^m \right](m).$$

These ideas by Zemel and Panaretos serve us as an inspiration for the stochastic gradient descent iteration in the next part. Let us finally remark that if $\gamma = 1$ the aforementioned gradient descent sequence equals the sequence in (4.2), i.e. $G_{k,1} = G_k$. In fact in [41] the authors prove that the choice $\gamma = 1$ is optimal.

4.3. Stochastic gradient descent for population barycenters. The method in Section 4.2 works perfectly well for calculating the empirical barycenter. For the estimation of a population barycenter (i.e. when the prior does not have a finite support) we would need to construct a convergent sequence of empirical barycenters, as in Section 4.1 and then apply the method in Section 4.2. Altogether this can be computationally expensive. To remedy this, we follow the ideas in [12] and define a stochastic version of the gradient descent sequence for the barycenter of $\Pi \in \mathcal{W}_2(\mathcal{W}_{2,\infty}(\mathbb{R}^d))$. Needless to say, $\Pi$ could represent the posterior or prior distribution.

**Definition 4.5.** Let $\mu_0 \in \mathcal{W}_{2,\infty}(\mathbb{R}^d)$, $m_k \overset{iid}{\sim} \Pi$, and $\gamma_k > 0$ for $k \geq 0$. Then we define the stochastic gradient descent sequence as

$$\mu_{k+1} := \left[ (1 - \gamma_k)I + \gamma_k T_{\mu_k}^m \right](\mu_k), \text{ for } k \geq 0.$$  

By Remark 3.7 and an induction argument, we clearly have

$$\{\mu_k\} \subseteq \mathcal{W}_{2,\infty}(\mathbb{R}^d), \text{ a.s.}$$

Let us introduce the key ingredients for the convergence analysis of the stochastic gradient iterations:

$$F(\mu) := \frac{1}{2} \int_{\mathcal{W}_{2,\infty}(\mathbb{R}^d)} W_2^2(\mu, m) \Pi(dm)$$

$$F'(\mu) := - \int_{\mathcal{W}_{2,\infty}(\mathbb{R}^d)} (T_{\mu}^m - I) \Pi(dm).$$

Observe that the population barycenter $\hat{\mu}$ is the minimizer of $F$ and that by Lemma 3.8 also $\|F'(\hat{\mu})\|_{L^2(\Pi)} = 0$. The next proposition (cf. [41] Lemma 2) indicates us that, in expectation, the sequence $\{F(\mu_k)\}$ is essentially decreasing for a sufficiently small step $\gamma_k$. This is a first indication of the behaviour of the sequence $\{\mu_k\}$. We denote by $\{\mathcal{F}_k\}$ the filtration of the i.i.d. sample $m_k \sim \Pi$, namely $\mathcal{F}_{-1}$ is the trivial sigma-algebra and $\mathcal{F}_{k+1}$ is the sigma-algebra generated by $m_0, \ldots, m_k$. In this way $\mu_k$ is $\mathcal{F}_k$-measurable.
Proposition 4.6. For the stochastic gradient descent sequence in (4.6), we have

\[ \mathbb{E}[F(\mu_{k+1}) - F(\mu_k)|\mathcal{F}_k] \leq \gamma_k^2 F(\mu_k) - \gamma_k \|F'(\mu_k)\|_{L^2(\mu_k)}, \]  

(4.10)

Proof. Let \( \nu \in \text{supp}(\Pi) \). By (4.7) we know that

\[ (1 - \gamma_k)I + \gamma_k T_{\mu_k}^m \]  

is a feasible (not necessarily optimal) coupling with first and second marginals \( \mu_{k+1} \) and \( \nu \) respectively. Denoting \( O_m = T_{\mu_k} - I \), we have

\[
W_2^2(\mu_{k+1}, \nu) \leq \| (1 - \gamma_k)I + \gamma_k T_{\mu_k}^m - T_{\mu_k}^m \|^2_{L^2(\mu_k)}
= \| -O_m + \gamma_k O_m \|^2_{L^2(\mu_k)}
= \| O_m \|^2_{L^2(\mu_k)} - 2\gamma_k \langle O_m, O_m \rangle_{L^2(\mu_k)} + \gamma_k^2 \| O_m \|^2_{L^2(\mu_k)}.
\]

Evaluating \( \mu_{k+1} \) on the functional \( F \) and thanks to the previous inequality, we have

\[
F(\mu_{k+1}) = \frac{1}{2} \int W_2^2(\mu_{k+1}, \nu) \Pi(d\nu)
\leq \frac{1}{2} \int \|O_m\|^2_{L^2(\mu_k)} \Pi(d\nu) - \gamma_k \left( \int O_m \Pi(d\nu), O_m \right)_{L^2(\mu_k)} + \frac{\gamma_k^2}{2} \|O_m\|^2_{L^2(\mu_k)}
= F(\mu_k) + \gamma_k \left( F'(\mu_k), O_m \right)_{L^2(\mu_k)} + \frac{\gamma_k^2}{2} \|O_m\|^2_{L^2(\mu_k)}.
\]

Taking conditional expectation with respect to \( \mathcal{F}_k \), and as \( m_k \) is independently sampled from this sigma-algebra, we conclude

\[
\mathbb{E}[F(\mu_{k+1})|\mathcal{F}_k] \leq F(\mu_k) + \gamma_k \left( F'(\mu_k), \int O_m \Pi(dm) \right)_{L^2(\mu_k)} + \frac{\gamma_k^2}{2} \int \|O_m\|^2_{L^2(\mu_k)} \Pi(dm)
= (1 + \gamma_k^2) F(\mu_k) - \gamma_k \|F'(\mu_k)\|^2_{L^2(\mu_k)}.
\]

\( \square \)

Now we will show that under reasonable assumptions the sequence \( \{F(\mu_k)\}_k \) converges a.s. to the unique minimizer of \( F \). As mentioned above, this minimizer is the 2-Wasserstein population barycenter of \( \Pi \), which we denote \( \hat{\mu} \). We will need the following convergence result recalled in [11]:

(Quasi-martingale convergence theorem) Given a random sequence \( \{h_i\}_{i \geq 0} \) adapted to the filtration \( \{\mathcal{F}_i\} \), define \( \delta_i := 1 \) if \( \mathbb{E}[h_{i+1} - h_i|\mathcal{F}_i] > 0 \) and \( \delta_i := 0 \) otherwise. If \( h_i \geq 0 \) for all \( i \geq 0 \), and the infinite sum of the positive expected variations is finite \( (\sum_{i=1}^{\infty} \mathbb{E}[\delta_i(h_{i+1} - h_i)] < \infty) \) then the sequence \( \{h_i\} \) converges almost surely to some \( h_\infty \geq 0 \).

We will assume the following conditions over the steps \( \gamma_i \) appearing in (4.6):

\[
\sum_{i=1}^{\infty} \gamma_i^2 < \infty \quad \text{and} \quad \sum_{i=1}^{\infty} \gamma_i = \infty.
\]

(4.11)  
(4.12)

Additionally the following conditions will be useful to finish the arguments:

* \( W_{2,q}(\mathbb{X}) \ni \mu \mapsto \|F'(\mu)\|_{L^2(\mu)}^2 \) is lower semicontinuous w.r.t. \( W_q \) for some \( q < 2 \),
* \( W_{2,q}(\mathbb{X}) \ni \mu \mapsto \|F'(\mu)\|_{L^2(\mu)}^2 \) has a unique zero.

We shall examine these conditions in Remark 4.8. Now the main result of this part:

Theorem 4.7. Under conditions (4.11) and (4.12), the stochastic gradient descent sequence \( \{\mu_k\}_k \) is a.s. relatively compact in \( W_q \) for all \( q < 2 \) (in particular it is tight). If furthermore (4.13) and (4.14) hold, then a.s. \( \{\mu_k\}_k \) converges to the \( W_2 \)-population barycenter \( \hat{\mu} \) of \( \Pi \) in the \( W_q \) topology (in particular it weakly converges).

Proof. Denote \( \hat{F} := F(\hat{\mu}) \) and introduce the sequences

\[ h_t := F(\mu_t) - \hat{F}, \quad \alpha_t := \prod_{i=1}^{t-1} \frac{1}{1 + \gamma_i}. \]
Observe that \( h_t \geq 0 \) for all \( t \). Thanks to condition (4.11), the sequence \( \alpha_t \) converges to some \( \alpha_\infty > 0 \), as can be checked by taking logarithm. By Proposition 4.6 we have

\[
\mathbb{E} \left[ h_{t+1} - (1 + \gamma_t) h_t \bigg| F_t \right] \leq \gamma_t^2 \hat{F} - \gamma_t \| F'(\mu_t) \|_{L^2(\mu_t)}^2 \leq \gamma_t^2 \hat{F},
\]

so after multiplying by \( \alpha_{t+1} \) we derive the bound

\[
\mathbb{E} \left[ \alpha_{t+1} h_{t+1} - \alpha_t h_t \bigg| F_t \right] \leq \alpha_{t+1} \gamma_t^2 \hat{F} - \alpha_t \gamma_t \| F'(\mu_t) \|_{L^2(\mu_t)}^2 \leq \alpha_t \gamma_t^2 \hat{F}.
\]

(4.15)

We define \( \delta_t := 1 \) if \( \mathbb{E} [\alpha_{t+1} h_{t+1} - \alpha_t h_t | F_t] > 0 \) and \( \delta_t := 0 \) otherwise. Then

\[
\sum_{t=1}^{\infty} \mathbb{E} [\delta_t (\alpha_{t+1} h_{t+1} - \alpha_t h_t)] = \sum_{t=1}^{\infty} \mathbb{E} [\delta_t \mathbb{E} [\alpha_{t+1} h_{t+1} - \alpha_t h_t | F_t]]
\]

\[
\leq \hat{F} \sum_{t=1}^{\infty} \alpha_t \gamma_t^2 \leq \hat{F} \sum_{t=1}^{\infty} \gamma_t^2 < \infty.
\]

(4.16)

Since \( \alpha_t h_t \geq 0 \), by the quasi-martingale convergence theorem \( \{\alpha_t h_t\} \) converges almost surely, but as \( \alpha_t \) converges to \( \alpha_\infty > 0 \), then \( h_t \) also converges almost surely to some \( h_\infty \geq 0 \).

Taking expectations is (4.16), summing in \( t \) so that a telescopic sum forms, we have

\[
\mathbb{E} [\alpha_{t+1} h_{t+1}] \leq \alpha_0 h_0 + \hat{F} \sum_{s=1}^{\infty} \alpha_s \gamma_s^2 \leq C.
\]

(4.17)

Taking limit inferior, applying Fatou’s lemma, and since \( \alpha_\infty > 0 \), we conclude \( \mathbb{E} [h_\infty] < \infty \).

In particular \( h_\infty \) is a.s. finite. This means that \( F(\mu_t) \) has a finite a.s. limit, which we call \( L \).

By convexity of transport costs ([52] Theorem 4.8) we have

\[
\frac{1}{q} W_q^2 (\mu, \int m \Pi (dm)) \leq F(\mu_t) \leq L + 1,
\]

for \( t \) eventually large enough. Since \( \Pi \in \mathcal{W}_q(W_2(\mathbb{R}^q)) \) we have \( \int m \Pi (dm) \in \mathcal{W}_q(\mathbb{R}^q) \), so it follows that the second moments of \( \{\mu_t\} \) are a.s. bounded by some finite (random) constant \( M \).

An application of Markov’s inequality proves that the sequence \( \{\mu_t\} \) is a.s. tight, since closed balls in \( \mathbb{R}^q \) are compact. Further, for \( q < 2 \), by Hölder and Chebyshev inequalities we have that

\[
\int_{|x| > K} |x|^q d\mu_t \leq \frac{1}{K^{q-2}} \int |x|^q d\mu_t \leq \frac{M}{K^{q-2}},
\]

so \( \mu_{t_K} \) is a.s. relatively compact in \( \mathcal{W}_q \) thanks to [38] Theorem 7.12 and

\[
\lim_{K \to \infty} \sup_{t \to \infty} \int_{|x| > K} |x|^q d\mu_t \leq \lim_{K \to \infty} \limsup_{t \to \infty} \frac{M}{K^{q-2}} = 0.
\]

Back to (4.16), taking expectations, summing in \( t \) to obtain a telescopic sum, we get

\[
\mathbb{E} [\alpha_{t+1} h_{t+1}] - h_0 \alpha_0 = \hat{F} \sum_{s=1}^{\infty} \alpha_s \gamma_s^2 - \sum_{s=1}^{\infty} \alpha_s \gamma_s \| F'(\mu_s) \|_{L^2(\mu_s)}^2.
\]

Taking limit inferior, by Fatou on the l.h.s. and monotone convergence on the r.h.s. we get

\[
-\infty < \mathbb{E} [\alpha_{t_K} h_{t_K}] - h_0 \alpha_0 \leq C - \mathbb{E} \left[ \sum_{s=1}^{\infty} \alpha_s \gamma_s \| F'(\mu_s) \|_{L^2(\mu_s)}^2 \right].
\]

(4.17)

In particular, we have

\[
\sum_{s=1}^{\infty} \gamma_s \| F'(\mu_s) \|_{L^2(\mu_s)}^2 < \infty, \quad \text{a.s.}
\]

Observe that \( \liminf \| F'(\mu_t) \|_{L^2(\mu_t)}^2 > 0 \) would be at odds with (4.17) and (4.12), so further

\[
\liminf \| F'(\mu_t) \|_{L^2(\mu_t)}^2 = 0, \quad \text{a.s.}
\]

We now assume Conditions (4.13) and (4.14). If some subsequence of \( \{\mu_t\} \), \( W_q \)-converges to some \( \mu \neq \hat{\mu} \), then along this subsequence we must have \( \liminf \| F'(\mu_t) \|_{L^2(\mu_t)}^2 > 0 \); indeed, otherwise by (4.13) we would have \( \| F'(\mu) \|_{L^2(\mu)}^2 = 0 \), contradicting (4.14) since already \( \| F'(\hat{\mu}) \|_{L^2(\hat{\mu})}^2 = 0 \). Since we do know that \( \liminf \| F'(\mu_t) \|_{L^2(\mu_t)}^2 = 0 \) a.s., it follows that realizations where \( \{\mu_t\} \) accumulates into a limit different than \( \hat{\mu} \) have zero measure. Thus a.s. the only possible accumulation point of \( \{\mu_t\} \) is \( \hat{\mu} \). In particular, by a.s. relative compactness of \( \{\mu_t\} \), this sequence must \( W_q \)-converge a.s. to the population barycenter \( \hat{\mu} \), concluding the proof.

\[ \square \]
Remark 4.8. The validity of (4.14) is equivalent to the uniqueness of an (absolutely continuous) fixed point for the functional
\[ \tilde{m} \mapsto \left( \int T_m^a \Pi(dm) \right)(\tilde{m}), \]
which is in general unsettled. In the finite-support case [1] Remark 3.9] and specially [41] Theorem 2) provide reasonable sufficient conditions. For the infinite-support case the uniqueness of fixed-points, as far as we know, has only been explored in [9, Theorem 5.1] under strong assumptions. It is imaginable that the arguments in [41] can be generalized to the infinite-support case, but we do not explore this in the present work.

On the other hand it seems plausible that (4.13) holds in full generality. In this direction we refer to [41] Proposition 3) for a continuity statement when, again, II has finite support. We give next a sufficient/alternative condition for (4.13) of our own, which does work for the infinite-support case.

**Proposition 4.9.** Assumption (4.13) is fulfilled if

(i) \( X = \mathbb{R} \)

Alternatively, assume that

(ii) \( \mu_0 \in \text{supp}(\Pi) \subseteq \mathcal{H} \subseteq W_{2,ac}(\mathbb{R}^d) \), where \( \mathcal{H} \) is geodesically closed and closed under composition of optimal maps, meaning respectively,\(^2\)

\[ \forall m, \tilde{m} \in \mathcal{H}, \forall \alpha \in [0, 1] : \left( (1 - \alpha)I + \alpha T_m^a \right)(m) \in \mathcal{H}, \]

\[ \forall m, \tilde{m} \in \mathcal{H} : T_m^0 = T_{\tilde{m}}^0 \circ \left( T_m^a \right)^{-1}. \]

Then for the stochastic gradient descent sequence we have a.s. \( \mu_1 \subseteq \mathcal{H} \). Further the functional \( \mathcal{H} \ni \mu \mapsto \|F(\mu)\|^2_{L^2(\mu)} \) is \( W_2 \)-continuous and weakly lower semicontinuous, and the conclusions of Theorem 4.7 remain valid if Condition (4.13) is dropped.

**Proof.** We first settle the case of Condition (ii). It is immediate from (4.19) that \( \mu_1 \in \mathcal{H} \), and by induction it follows similarly that a.s. \( \mu_k \subseteq \mathcal{H} \). We now establish the continuity statement, decomposing the functional as follows

\[ \|F(\mu)\|^2_{L^2(\mu)} = \int_X \left[ \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) - y \right]^2 \mu(dy) \]

\[ = \int_X \left[ \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) \right]^2 \mu(dy) - 2 \int_X y \cdot \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) \mu(dy) + \int_X \|y\|^2 \mu(dy). \]

The term \( \mu \mapsto \int_X \|y\|^2 \mu(dy) \) is continuous in \( W_2 \) and weakly lower semicontinuous. As Brenier maps are optimal, we have

\[ \int_X y \cdot T_m^a(\cdot) \mu(dy) = \sup_{y - \mu, \tilde{z} - \tilde{m}} \mathbb{E} [y \cdot z] := \rho(\mu, m). \]

Thus \( \rho(\cdot, m) \) is continuous in \( W_2 \) and weakly upper semicontinuous, so under the standing assumption that \( \Pi \in W_2(\mathcal{W}_{2,ac}) \) the term \( \int \rho(\mu, m) \Pi(dm) \) is continuous in \( W_2 \) and weakly upper semicontinuous too. Finally we only have to check that the first term is continuous:

\[ \int_X \left[ \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) \right]^2 \mu(dy) = \int_X \left[ \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) - \mu(dy) \right] \Pi(dm) \]

\[ = \int \left[ \left( \int T_m^a(\cdot) \Pi(dm) \right)(\cdot) \right] \Pi(dm) \]

\[ = \int G(\mu, m, \tilde{m}) \Pi(dm), \]

where \( G(\mu, m, \tilde{m}) = \int_X T_m^a(y) \cdot T_{\tilde{m}}(\cdot) \mu(dy) \). For \( \mu, m, \tilde{m} \in \mathcal{H} \) we have that

\[ G(\mu, m, \tilde{m}) = \int_X T_m^a(y) \cdot T_{\tilde{m}}(\cdot) \mu(dy) \]

\[ = \int \left[ T_m^a(y) \cdot \left( T_{\tilde{m}} \circ \left( T_m^a \right)^{-1} \right)(\cdot) \right] \mu(dy) \]

\[ = \int z \cdot \left[ T_m^a \circ \left( T_{\tilde{m}} \right)^{-1}(z) \right] m(dz) \]

\[ = \int z \cdot T_m^a(z) m(dz). \]

\(^2\)Since \( \mu, m \) are absolutely continuous we have by [35] Theorem 2.12(iv) \( \left( T_m^a \right)^{-1} = T_{\tilde{m}}(\cdot - \text{a.s.}) \)
thanks to the Condition (4.20). Since $G(\mu, m, \tilde{m})$ is independent of $\mu$, we conclude that the functional $\mu \mapsto ||F(\mu)||_{L^2(\mu)}^2$ is $W_2$-continuous and weakly lower semicontinuous on $\mathcal{H}$ as desired. With this at hand we can go back to the arguments in the proof of Theorem 4.7 checking their validity without Condition (4.13).

Finally let us consider Condition (i). In this case (4.20) is true for all $\mu, m, \tilde{m}$ absolutely continuous, since the composition of increasing functions on the line is increasing. The above arguments verbatim prove the validity of (4.13). □

Examples where Condition (4.20) are fulfilled are explained in [10] Proposition 4.1, and include the case of radial transformations and component-wise transformations of a base measure. In general (4.20) is rather restrictive, since the composition of gradients of convex functions need not be a gradient of some convex function.

4.4. Batch stochastic gradient descent on Wasserstein space. To generate the sequence (4.6) in the $k$-step, we sampled $m_k \overset{iid}{\sim} \Pi$, chose a suitable $\gamma_k > 0$ and then updated $\mu_k$ via the transport map $T_k := I + \gamma_k (T^m_\mu - I)$. The expected transport map is

$\mathbb{E}[T_k] = I + \gamma_k \int (T^m_\mu - I) \Pi(dm_k) = I - \gamma_k F'(\mu_k)$.

Notice that $-(T^m_\mu - I)$ is an unbiased estimator for $F'(\mu)$, but in many cases it can have a high variance so the learning rates $\gamma$ must be very small for convergence. This motivates us to propose alternative estimators for $F'(\mu)$ with less variance:

**Definition 4.10.** Let $\mu_0 \in \mathcal{W}_{2,\mu}(\mathbb{R}^q)$, $m_k \overset{iid}{\sim} \Pi$, and $\gamma_k > 0$ for $k \geq 0$ and $i = 1, \ldots, S_k$. The *batch stochastic gradient descent sequence* is given by

$$\mu_{k+1} := \left(1 - \gamma_k\right) I + \gamma_k \sum_{i=1}^{S_k} T^{m_i}_{\mu_k} \left(\mu_k\right). \tag{4.21}$$

Denote this time $\mathcal{F}_{k+1}$ the sigma-algebra generated by $\{m_i : \ell \leq k, i \leq S_k\}$. Notice that

$W := \frac{1}{\sqrt{2}} \sum_{i=1}^{S_k} T^{m_i}_{\mu_k} - I$ is an unbiased estimator of $-F'(\mu_k)$. Then, much as in Proposition 4.6 we have

$$\mathbb{E}[F(\mu_{k+1})]\mathcal{F}_k$$

$$= F(\mu_k) + \gamma_k (FW'(\mu_k), \int W \Pi(dm_1 \cdots dm_{S_k}) L^2(\mu_k)) + \frac{\gamma_k^2}{2} \int ||W||^2 L^2(\mu_k) \Pi(dm_1 \cdots dm_{S_k})$$

$$\leq F(\mu_k) - \gamma_k ||FW'(\mu_k)||^2 L^2(\mu_k) + \frac{\gamma_k^2}{2} \sum_{i=1}^{S_k} ||T^{m_i}_{\mu_k} - I||^2 L^2(\mu_k) \Pi(dm_k)$$

$$= \left(1 + \gamma_k^2\right) F(\mu_k) - \gamma_k ||FW'(\mu_k)||^2 L^2(\mu_k).$$

From here on it is routine to follow the arguments in the proof of Theorem 4.7 obtaining the following result:

**Proposition 4.11.** Under conditions (4.11) and (4.12) the batch stochastic gradient descent sequence $(\mu_i)$ is a.s. relatively compact in $\mathcal{W}_q$ for all $q < 2$. If furthermore (4.13) and (4.14) hold, then a.s. $(\mu_i)_{i \geq 0}$ converges to the $\mathcal{W}_2$-population barycenter $\hat{\mu}$ of $\Pi$ in the $\mathcal{W}_q$-topology.

The main idea of using mini-batch is *noise reduction* for the estimator of $F'(\mu)$. The variance of the one-sample estimator where $m \sim \Pi$ is

$$\forall [-(T^m_\mu - I)] = \mathbb{E} \left[ ||-(T^m_\mu - I)||^2_{L^2(\mu)} \right] - \mathbb{E} \left[ ||-(T^m_\mu - I)||^2_{L^2(\mu)} \right]$$

$$= \mathbb{E} \left[ W^2(\mu, m) - ||F'(\mu)||^2_{L^2(\mu)} \right]$$

$$= 2F(\mu) - ||F'(\mu)||^2_{L^2(\mu)};$$
On the other hand, the variance of the mini-batch estimator where \( m_i \sim \Pi \) for \( i \leq S \) is

\[
\forall \left[ -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right] = \mathbb{E} \left[ \left\| -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right\|_{L^2(\mu)}^2 \right] - \mathbb{E} \left[ \left\| -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right\|_{L^2(\mu)}^2 \right]
\]

For the first term we can expand it as

\[
\left\| -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right\|_{L^2(\mu)}^2 = \frac{1}{S^2} \left( \sum_{i=1}^{S} (T_{\mu_i}^m - I), \sum_{j=1}^{S} (T_{\mu_j}^m - I) \right)_{L^2(\mu)}
\]

so if we take expectation, as the samples \( m_i \sim \Pi \) are independent, we have

\[
\mathbb{E} \left[ \left\| -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right\|_{L^2(\mu)}^2 \right] = \frac{1}{S^2} \sum_{i=1}^{S} \mathbb{E} \left[ W_2^2(\mu, m_i) \right] + \frac{1}{S^2} \sum_{i=1}^{S} \mathbb{E} \left[ \left( T_{\mu_i}^m - I \right) \right]_{L^2(\mu)}
\]

Finally the variance of the mini-bath estimator is given by

\[
\forall \left[ -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right] = \frac{1}{S} \left[ 2F(\mu) - \|F'(\mu)\|_{L^2(\mu)}^2 \right].
\]

Thus we have established:

**Proposition 4.12.** The variance of the mini batch estimator \( -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \) for \( F'(\mu) \) decreases linearly as the sample size \( S \) grows, ergo \( \forall \left[ -\frac{1}{S} \sum_{i=1}^{S} (T_{\mu_i}^m - I) \right] = O(\frac{1}{S}). \)

5. **On families with closed-form gradient descent step and their barycenters**

In Section 4, we presented some methods to compute the population Wasserstein barycenter, which assume that we are capable of getting samples from the distributions \( \Pi \) and \( \Pi_\mu \), and that we can calculate the optimal transports between measures. While sampling is solved by techniques like MCMC, computing optimal transports is not achievable in a general way. For this reason we exhibit in this section some families of distributions for which it is possible to calculate these optimal transports. Furthermore we will examine their barycenter, establishing some properties which are conserved under the operation of taking barycenter.

5.1. **Univariate distributions.** For a continuous distribution \( m \) in \( \mathbb{R} \) we denote its cumulative distribution function by \( F_m(x) \) and its right-continuous quantile function by \( Q_m(\cdot) = F_m'(\cdot) \). The \( \rho \)-Wasserstein optimal transport map from some continuous \( m_0 \) to \( m \) is independent of \( p \) and given by the monotone rearrangement (see [38, Remark 2.19(iv)]):

\[
T_0^\rho(x) = Q_m(F_{m_0}(x)).
\]

Note that this class of functions is closed under composition, convex combination, and contains the identity. Given \( \Pi \) the barycenter \( \hat{m} \) is also independent of \( p \) and characterized by the averaged quantile function, i.e.

\[
Q_\hat{m}(\cdot) = \int Q_m(\cdot) \Pi(dm).
\]

A stochastic gradient descent iteration, starting from a distribution function \( F_\mu(x) \), sampling some \( m \sim \Pi \), and with step \( \gamma \), produces the measure

\[
v = ((1 - \gamma)I + \gamma T_\mu^m(m),
\]

which is characterized by its quantile function

\[
Q_v(\cdot) = (1 - \gamma)Q_\mu(\cdot) + \gamma Q_m(\cdot).
\]

A general batch stochastic gradient descent iteration is described by

\[
Q_v(\cdot) = (1 - \gamma)Q_\mu(\cdot) + \frac{\gamma}{S} \sum_{i=1}^{S} Q_m(\cdot).
\]
It is interesting to note that the model average \( \hat{m} \) is characterized by the \textit{averaged cumulative distribution function}, i.e. \( F_m(\cdot) = \int F_m(\cdot) \Pi(dm) \). As we mentioned earlier, the model average does not preserve intrinsic \textit{shape} properties from the distributions such as symmetry or unimodality. For example if \( \Pi = 0.3 \cdot \delta_{m_1} + 0.7 \cdot \delta_{m_2} \) with \( m_1 = N(1, 1) \) and \( m_2 = N(3, 1) \), the \textit{model average} is an asymmetric bimodal distribution with modes on 1 and 3.

A continuous distribution \( m \) on \( \mathbb{R} \) is called unimodal with a mode on \( \hat{x} \in \mathbb{R} \) if its cumulative distribution function \( F(x) \) is convex for \( x < \hat{x} \) and concave for \( x > \hat{x} \). One says that \( m \) is symmetric around \( x_\text{m} \in \mathbb{R} \) if \( F(x_{\text{m}} + x) = 1 - F(x_{\text{m}} - x) \) for \( x \in \mathbb{R} \). One can also characterize unimodality and symmetry by quantile function. A continuous distribution \( m \) on \( \mathbb{R} \) is unimodal with a mode on \( \hat{x} \) if its quantile function \( Q(y) \) is concave for \( y < \hat{y} \) and convex for \( y > \hat{y} \), where \( Q(\hat{y}) = \hat{x} \). Likewise, \( m \) is symmetric around \( x_\text{m} \in \mathbb{R} \) if \( Q(\hat{x} + y) = 2x_\text{m} - Q(\hat{x} - y) \) for \( y \in [0, \frac{1}{2}] \). Thanks to this characterization we conclude that the barycenter preserves unimodality/symmetry:

**Lemma 5.1.** If \( \Pi \in \mathcal{W}_p(\mathcal{P}_m(\mathbb{R})) \) is concentrated on symmetric (resp. symmetric unimodal) univariate distributions, then the barycenter \( \hat{m} \) is symmetric (resp. symmetric unimodal).

**Proof.** Using the quantile function characterization, we have that

\[
Q_{\hat{m}}(\frac{1}{2} + y) = \int Q_m(\frac{1}{2} + y) \Pi(dm) = \int \left[ 2x_m - Q_m(\frac{1}{2} - y) \right] \Pi(dm) = 2x_{\hat{m}} - Q_{\hat{m}}(\frac{1}{2} - y),
\]

where \( x_{\hat{m}} := \int x_m \Pi(dm) \) is the symmetric point, that coincides with the median and the mean of the barycenter. If a symmetric distribution is unimodal, then the mode coincides with the median and mean, i.e. \( Q_m(\frac{1}{2}) = x_m \). Since the average of convex (concave) functions is convex (concave), it is clear that the barycenter of symmetric unimodal distributions is also symmetric unimodal.

Although the unimodality is not preserved in general non-symmetric cases, there are still many families of distributions in which the unimodality is preserved after taking barycenter, as we show in the next result.

**Lemma 5.2.** If \( \Pi \in \mathcal{W}_p(\mathcal{P}_m(\mathbb{R})) \) is concentrated on log-concave univariate distributions, then the barycenter \( \hat{m} \) is unimodal.

**Proof.** Let \( f(x) \) be a log-concave density, then \( -\log(f(x)) \) is convex so \( \exp(-\log(f(x))) = \frac{1}{f(x)} \) is convex. Necessarily \( f \) must be unimodal for some \( \hat{x} \in \mathbb{R} \), so quantile function \( Q(y) \) is concave for \( y < \hat{y} \) and convex for \( y > \hat{y} \) where \( Q(\hat{y}) = \hat{x} \). Since \( \frac{1}{f(x)} \) is convex decreasing for \( x < \hat{x} \) and convex increasing for \( x > \hat{x} \), then \( \frac{1}{f(Q(y))} \) is convex. Hence \( \frac{\partial}{\partial y} Q(y) = \frac{1}{f(Q(y))} \) is convex positive with minima on \( \hat{y} \). Given \( \Pi \), its barycenter \( \hat{m} \) satisfies

\[
\frac{\partial Q_{\hat{m}}}{\partial y} = \int \frac{\partial Q_m}{\partial y} \Pi(dm),
\]

so if all \( \frac{\partial Q_m}{\partial y} \) are convex, then \( \frac{\partial Q_{\hat{m}}}{\partial y} \) is convex positive with minima on some \( \hat{y} \) so \( Q_{\hat{m}}(y) \) is concave for \( y < \hat{y} \) and convex for \( y > \hat{y} \) and \( \hat{m} \) is unimodal with a mode on \( \hat{x} = Q_{\hat{m}}(\hat{y}) \).

There are many useful common log-concave distribution families like the normal one, the exponential, logistic, Gumbel, chi-squared, chi and Laplace. Other examples include the Weibull, power, gamma and beta families, when the shape parameters are equal or greater than 1. It is interesting to note that some of these families are closed under taking barycenter. For example, the barycenter of normal distributions is normal, and this remains true for the exponential, logistic, Gumbel and Laplace families.

### 5.2. Distributions sharing a common copula

If two multivariate distributions \( P \) and \( Q \) over \( \mathbb{R}^q \) share the same copula, then their \( \mathcal{W}_p(\mathbb{R}^q) \) distance to the \( p \)-th power is the sum of the \( \mathcal{W}_p(\mathbb{R}) \) distances between their marginals raised to the \( p \)-power. Furthermore, if the marginals of \( P \) are continuous, then an optimal map is given by the coordinate-wise transformation \( T(x) = (T^1(x_1), \ldots, T^q(x_q)) \) where \( T^i(x_i) \) is the monotone rearrangement between the marginals \( P^i \) and \( Q^i \) for \( i = 1, \ldots, q \). Note that these kind of transports are
closed under composition, convex combination, and contain the identity. This setting allows us to easily extend the results from the univariate case to the multidimensional case.

**Lemma 5.3.** If $\Pi \in \mathcal{W}_p(P_{\alpha}(\mathbb{R}^d))$ is concentrated on a set of measures sharing the same copula $C$, then the $p$-Wasserstein barycenter $\hat{\mu}$ of $\Pi$ has copula $C$ as well, and its $i$-th marginal $\hat{\mu}_i$ is the barycenter of the $i$-th marginal measures of $\Pi$. In particular the barycenter does not depend on $p$.

**Proof.** It is known [13][2] that for two distributions $m$ and $\mu$ with $i$-th marginals $m_i$ and $\mu_i$ for $i = 1, \ldots, q$ respectively, the $p$-Wasserstein metric satisfies

$$W_p^p(m,\mu) \geq \sum_{i=1}^n W_p^p(m_i,\mu_i),$$

where equality is reached if $m$ and $\mu$ share the same copula $C$. (We abuse notation denoting $W_p$ the $p$-Wasserstein distance on $\mathbb{R}^d$ as well as on $\mathbb{R}$.)

Thus

$$\int W_p^p(m,\mu)\Pi(dm) \geq \sum_{i=1}^q \int W_p^p(m_i,\mu_i)\Pi(dm) = \sum_{i=1}^q \int W_p^p(\nu,\mu_i)\Pi'(dv),$$

where $\Pi'$ is defined via the identity $\int_{\mathcal{P}(\mathbb{R})} f(\nu)\Pi'(dv) = \int_{\mathcal{P}(\mathbb{R}^d)} f(m_i,\mu_i)\Pi(dm)$. The infimum for the lower bound is reached on the univariate measures $\hat{m}_1,\ldots,\hat{m}_q$ where $\hat{m}_i$ is the $p$-barycenter of $\Pi'$, i.e. $\hat{m}_i = \arg\min_{\nu} \int W_p^p(\nu,\mu_i)\Pi'(dv)$. It is plain that the infimum is reached on the distribution $\hat{m}$ with copula $C$ and $i$-th marginal $\hat{m}_i$ for $i = 1, \ldots, q$, which then has to be the barycenter of $\Pi$ and is independent of $p$. □

A stochastic gradient descent iteration, starting from a distribution $\mu$, sampling some $m \sim \Pi$, and with step $\gamma$, both $\mu$ and $m$ having copula $C$, produces the measure $\nu = (1 - \gamma)\mu + \gamma T_{\mu}(\mu)$ characterized by having copula $C$ and the $i$-th marginal quantile functions

$$Q_i(\cdot) = (1 - \gamma)Q_{\mu_i}(\cdot) + \gamma Q_{\nu_i}(\cdot),$$

for $i = 1, \ldots, q$. The batch stochastic gradient descent iteration works analogously. Alternatively, one can perform (batch) stochastic gradient descent componentwise (with respect to the marginals $\Pi'$ of $\Pi$) and then make use of the copula $C$.

### 5.3. Spherically equivalent distributions.

Following [13], another useful multidimensional case is constructed as follows: Given a fixed measure $\hat{m} \in \mathcal{W}_{2,\infty}(\mathbb{R}^d)$, its associated family of spherically equivalent distributions is

$$S_0 := \{m \mid m \sim \Pi \} \subset \mathcal{N}_0(\mathbb{R}^d),$$

where $\| \|_1$ is the Euclidean norm and $\mathcal{N}_0(\mathbb{R})$ is the set of non-decreasing non-negative functions of $\mathbb{R}_+$. These type of distributions include the simplicially contoured distributions, and also elliptical distributions with the same correlation structure. Here and in the sequel we denote by $L(\cdot)$ the law of a random vector, so $m = L(x)$ and $x \sim m$ are synonyms.

If $y \sim m \in S_0$, then we have that $\alpha(r) = Q_{\|r\|_1}(F_{\|r\|_1}(r))$, where $Q_{\|\|}$ is the quantile function of the norm of $y$, $F_{\|\|}$ is the distribution function of the norm of $\hat{x}$, and $y \sim m \sim \hat{x}$. More generally, if $m_1 = L_{\|\|_1}(\alpha_1^{-1}(r))$ and $m_2 = L_{\|\|_1}(\alpha_2^{-1}(r))$, then the optimal transport from $m_1$ to $m_2$ is given by $T_{m_1}^{m_2}(x) = \frac{\alpha_1^{-1}(r)}{\alpha_2^{-1}(r)} x$ where $\alpha(r) = Q_{\|r\|_1}(F_{\|r\|_1}(r))$. Since $F_{\|\|_1}(r) = \frac{\alpha(r)}{\alpha_2^{-1}(r)}$ and $Q_{\|\|_1}(r) = \alpha_2(Q_{\|\|_1}(\alpha_1^{-1}(r))) = \alpha_2(\alpha_1^{-1}(r))$, so finally

$$T_{m_1}^{m_2}(x) = \frac{\alpha_2(\alpha_1^{-1}(r))}{\alpha_2^{-1}(r)} x.$$

Note that these kind of transports are closed under composition, convex combination, and contain the identity.

A stochastic gradient descent iteration, starting from a distribution $\mu = L_{\|\|_1}(\alpha_0^{-1}(r))$, sampling some $m = L_{\|\|_1}(\alpha_1^{-1}(r)) \sim \Pi$, with step $\gamma$, produces the distribution $m_1 = T_0^{m_1}(\mu) = ((1 - \gamma)\mu + \gamma T_{\mu}(\mu))$. Since $T_0^{m_1}(x) = \frac{(1 - \gamma)\alpha_0 + \gamma \alpha_1}{1 + \gamma} x$, we have that $m_1 = L_{\|\|_1}(\alpha_2^{-1}(r))$ with $\alpha_1 = (1 - \gamma)\alpha_0 + \frac{\gamma}{1 - \gamma} \sum_{i=1}^q \alpha_{m_i}$. Analogously, the batch stochastic gradient descent iteration produces

$$\alpha_1 = (1 - \gamma)\alpha_0 + \frac{\gamma}{1 - \gamma} \sum_{i=1}^q \alpha_{m_i}.$$
Note that these iterations live in $S_0$, thus, so does the barycenter $\hat{m} \in S_0$.

For the barycenter $\hat{m} = \mathcal{L}(\hat{\theta}(\parallel x \parallel^1), \hat{x})$, the equation $\int T^m_\mu(x)\Pi(dm) = x$ can be expressed as $\hat{\theta}(r) = \int \theta_i(r)\Pi(dm)$, or equivalently, $Q^m_\Pi(p) = \int Q^m_\Pi(p)\Pi(dm)$, where $Q^m_\Pi$ is the quantile function of the norm of $y \sim m$. Note the similarity with the univariate case.

5.4. Scatter-location family. We borrow here the setting of [4], where another useful multidimensional case is defined as follows: Given a fixed distribution $\tilde{m} \in \mathcal{W}_{2,m}(\mathbb{R}^q)$, referred to as a generator, the generated scatter-location family is given by

$$T_0 := T_m = \{L(Ax + b) | A \in M_{n,q}^m, b \in \mathbb{R}^q, x \sim \tilde{m}\},$$

where $M_{n,q}^m$ is the set of symmetric positive definite matrices of size $n \times q$. Without loss of generality we can assume that $\tilde{m}$ has zero mean and identity covariance. Note that if $\tilde{m}$ is the standard multivariate normal distribution, then $T_0$ is the multivariate normal distribution family.

The optimal map between two members of $T_0$ is explicit. If $m_1 = L(A_1\tilde{x} + b_1)$ and $m_2 = L(A_2\tilde{x} + b_2)$ then the optimal map from $m_1$ to $m_2$ is given by $T_{m_1}^{m_2}(x) = A(x - b_1) + b_2$

where $A = A_1^{-1}(A_1A_2A_1)^{1/2}A_1^{-1} \in M_{n,q}^m$. Observe that this family of optimal transports contains the identity map and is closed under convex combination.

If $\Pi$ is supported on $T_0$, then its 2-Wasserstein barycenter $\hat{m}$ belongs to $T_0$. In fact call its mean $\hat{b}$ and its covariance matrix $\hat{\Sigma}$. Since the optimal map from $\tilde{m}$ to $m$ is $T_{\tilde{m}}^m(x) = A_{\tilde{m}}^{-1}(x - \tilde{b}) + b_m$ where $A_{\tilde{m}} = \Sigma^{-1/2}(\Sigma^{1/2} \Sigma \Sigma^{1/2} \Sigma^{-1/2})$ and we know that $\int T_{\tilde{m}}^m(x)\Pi(dm) = x$, $\hat{m}$-almost surely. Then we must have that $\int A_{m}^\mu \Pi(dm) = 1$, since clearly $b_\mu = \int b_m \Pi(dm)$, and as a consequence $\hat{\Sigma} = \int (\Sigma^{1/2} \Sigma^{1/2})/2 \Pi(dm)$.

A stochastic gradient descent iteration, starting from a distribution $\mu = L(A_0\tilde{x} + b_0)$, sampling some $m = L(A_m\tilde{x} + b_m) \sim \Pi$, and with step $\gamma$, produces the measure $\nu = T_{\tilde{m}}^m(\mu) := ((1 - \gamma)I + \gamma T_{\tilde{m}}^m(\mu))$. If $\tilde{x}$ has a multivariate distribution $F(x)$, then $\mu$ has distribution $F_0(x) = F(A_0^{-1}(x - b_0))$ with mean $b_0$ and covariance $\Sigma_0 = A_0^2$. We have that $T_{\tilde{m}}^m(x) = ((1 - \gamma)I + \gamma A_{\tilde{m}}^n(x - b_0)) + \gamma b_m + (1 - \gamma)b_0$ with $A_{\tilde{m}}^n = A_0^{-1}(A_0A_{\tilde{m}}A_0)^{1/2}A_0^{-1}$. Then $\nu$ has distribution

$$F_1(x) = F_0([T_{\tilde{m}}^m]^{-1}(x)) = F((1 - \gamma)A_0 + \gamma A_{\tilde{m}}^n A_0^{-1}(x - \gamma b_m - (1 - \gamma)b_0)),$$

with mean $b_1 = (1 - \gamma)b_0 + \gamma b_m$ and covariance

$$\Sigma_1 = A_1^2 = [(1 - \gamma)A_0 + \gamma A_{\tilde{m}}^n (A_0A_{\tilde{m}}A_0)^{1/2}][(1 - \gamma)A_0 + \gamma (A_0A_{\tilde{m}}A_0)^{1/2}A_0^{-1}]$$

$$= A_0^{-1}[(1 - \gamma)A_0 + \gamma (A_0A_{\tilde{m}}A_0)^{1/2}][(1 - \gamma)A_0 + \gamma (A_0A_{\tilde{m}}A_0)^{1/2}A_0^{-1}]$$

$$= A_0^{-1}[(1 - \gamma)A_0 + \gamma (A_0A_{\tilde{m}}A_0)^{1/2}]^2A_0^{-1}.$$

The batch stochastic gradient descent iteration is characterized by

$$b_1 = (1 - \gamma)b_0 + \frac{\gamma}{\frac{S}{i=1} b_{mi}}$$

$$A_1^2 = A_0^{-1}[(1 - \gamma)A_0^2 + \frac{\gamma}{\frac{S}{i=1} (A_0A_{\tilde{m}}A_0)^{1/2}A_0^{-1}]$$

6. Numerical experiments

We next present experimental validation for our theoretical contribution. The aim of this simulation experiment is to provide practical evidence for the implementation of the proposed approach to Wasserstein Bayesian learning and its relationship to the true model. Specifically, the following experiment consists in: i) defining a true model, ii) sampling from such model to yield a set of data points, iii) sampling from the posterior measures, iv) computing the proposed Bayesian 2-Wasserstein barycenter via empirical approximation, v) analysing our estimator with respect to both the true model and the standard Bayesian model average, and lastly, vi) comparing the empirical approximation versus the proposed stochastic gradient methods for computing population barycenters.
6.1. Choice of the true model, prior and posterior samples. Following the discussion in Sec. 5.4, we considered models within the location-scatter family (LS), since optimal transports between members of the LS can be computed in closed form but are not reduced to the well-known univariate case. We chose the generator of the LS family, denoted \( \tilde{m} \), as a distribution on \( \mathbb{R}^{15} \) with independent coordinates, where:

- coordinates 1 to 5 are standard Normal distributions
- coordinates 6 to 10 are standard Laplace distributions, and
- coordinates 11 to 15 are standard Student’s \( t \)-distributions (3 degrees of freedom).

Fig. 2 shows uni- and bi-variate marginals for 6 coordinates of \( \tilde{m} \).

![Figure 2](image)

**Figure 2.** Univariate (diagonal) and bivariate (off-diagonal) marginals for 6 coordinates from the generator distribution \( \tilde{m} \). The diagonal and lower triangular plots are smoothed histograms, whereas the upper-diagonal ones are collections of samples.

Within the LS family constructed upon \( \tilde{m} \), we chose the true model \( m_0 \) to be generated by the location vector \( b \in \mathbb{R}^{15} \) defined as \( b_i = i - 1 \) for \( i = 1, \ldots, 15 \), and the scatter matrix \( A = \Sigma^{1/2} \). The covariance matrix \( \Sigma \) was defined as \( \Sigma_{i,j} = K \left( \left( \frac{i-1}{14} \right)^{1.1}, \left( \frac{j-1}{14} \right)^{1.1} \right) \) for \( i, j = 1, \ldots, 15 \) with the kernel function \( K(i, j) = \epsilon \delta_{ij} + \sigma \cos(\omega(i - j)) \). Given the parameters \( \epsilon, \sigma \) and \( \omega \), the so constructed covariance matrix will be denoted \( \Sigma_{\epsilon,\sigma,\omega} \). We chose the parameters \( \epsilon = 0.01 \), \( \sigma = 1 \) and \( \omega = 5.652 \approx 1.8\pi \) for \( m_0 \). Therefore, under the true model \( m_0 \) the coordinates can be negatively/positively correlated due to the cosine term and there is also a coordinate-independent noise component due to the Kronecker delta \( \delta_{ij} \). Fig. 3 shows the covariance matrix and three coordinates of the generated true model \( m_0 \).

The model prior \( \Pi \) is the push-forward induced by the chosen prior over the mean vector \( b \) and the parameters of the covariance \( \Sigma_{\epsilon,\sigma,\omega} \). We chose all these priors to be independent and given by

\[
p(b, \Sigma_{\epsilon,\sigma,\omega}) = N(b|0, I) \text{Exp}(\epsilon|20) \text{Exp}(\sigma|1) \text{Exp}(\omega^{-1}|15),
\]

\( 6.1 \)

\( ^3 \)We chose \( \left( \frac{i-1}{14} \right)^{1.1} \) for \( j = 1, \ldots, 15 \) because this defines a non-uniform grid over \([0, 1]\).
where $\text{Exp} (\cdot | \lambda)$ is a exponential distribution with rate $\lambda$. Given $n$ samples from the true model $m_0$ (also referred to as observations or data points), we generated $k$ samples from the posterior measure $\Pi_n$ using Markov chain Monte Carlo (MCMC), all to obtain the empirical measure $\Pi^{(k)}_{n}$. The remaining part of our numerical analysis focuses on the behavior of the Bayesian Wasserstein barycenter as a function of both the number of samples $k$ and the number of data points $n$.

### 6.2. Numerical consistency of the empirical posterior under the Wasserstein distance.

We first validated the empirical measure $\Pi^{(k)}_{n}$, as a consistent sample version of the true posterior under the $W^2$ distance, that is, we would like to confirm that $W^2(\Pi^{(k)}_{n}, \delta_{m_0}) \to W^2(\Pi_n, \delta_{m_0})$ for large $k$. In this sense, we estimated $W^2(\Pi^{(k)}_{n}, \delta_{m_0})$ 10 times for each combination of (number of) observations $n$ and samples $k$ in the following sets

- $k \in \{1, 5, 10, 20, 50, 100, 200, 500, 1000\}$
- $n \in \{10, 20, 50, 100, 200, 500, 1000, 2000, 5000, 10000\}$

Fig. 4 shows the 10 estimates of $W^2(\Pi^{(k)}_{n}, \delta_{m_0})$ for different values of $k$ (in the x-axis) and of $n$ (color coded). Notice how the estimates become more concentrated for larger $k$ and that the Wasserstein distance between the empirical measure $\Pi^{(k)}_{n}$ and the true model $m_0$ decreases for larger $n$. Additionally, Table 1 shows that the standard deviation of the 10 estimates of $W^2(\Pi^{(k)}_{n}, \delta_{m_0})$ decreases as either $n$ or $k$ increases.

### 6.3. Distance between the empirical barycenter and the true model.

For each empirical posterior $\Pi^{(k)}_{n}$ we intend to compute their Wasserstein barycenter $\hat{m}^{(k)}_{n}$ as suggested in Section 4.1. We call $\hat{m}^{(k)}_{n}$ the empirical barycenter. For this purpose, we use the iterative procedure defined in (4.2), namely the (deterministic) gradient descent method, and repeated this calculation 10 times. As a stopping criterion for the gradient descent method, we considered the relative variation of the $W^2$ cost, terminating the computation if this quantity was less than $10^{-4}$. Fig. 5 shows all the $W^2$ distances between the so computed barycenters and the true model, while Table 2 shows the average across all these distances for each pair $(n, k)$. Notice that, in general, both the average and standard deviation of the barycenters decrease as either $n$ or $k$ increases, yet for large values (e.g., $n = 2000, 5000$) numerical issues appear.
6.4. Distance between the empirical barycenter and the Bayesian model average. Our aim was then to compare the computed empirical Wasserstein barycenters $\hat{m}_n^{(k)}$ to the standard Bayesian model averages $\bar{m}_n^{(k)}$, in terms of their distance to the true model $m_0$, for $n = 1000$ observations. In order to do so, we estimated the $W_2$ distances via empirical approximations with 1000 samples for each model based on [18]. We simulated this procedure 10 times for $k \in \{10, 20, 50, 100, 200, 500, 1000\}$. Fig. 6 shows the sample average and variance of the $W_2$ distances of the Wasserstein barycenters and Bayesian model averages, where it can be seen that the empirical barycenter is closer to the true model than the model average regardless of the number of MCMC samples $k$.

6.5. Computation of the barycenter using batches. Lastly, we compared the empirical barycenters $\hat{m}_n^{(k)}$ against the barycenter obtained by our batch stochastic gradient descent method $\hat{m}_{n,s}$. Fig. 7 shows the evolution of the $W_2^2$ distance between the stochastic gradient descent sequences and the true model $m_0$ for $n \in \{10, 20, 50, 100, 200, 500, 1000\}$ observations and batches of sizes $s \in \{1, 15\}$, with step-size $\gamma_t = \frac{1}{t}$ for $t = 1, \ldots, 200$. This means...
Figure 5. $W_2$ distance between the empirical barycenters $\hat{m}_n^{(k)}$ and the true model $m_0$ in logarithmic scale for different number of observations $n$ (color coded) and samples $k$ (x-axis). For each pair $(n, k)$, 10 estimates of $W_2(\hat{m}_n^{(k)}, m_0)$ are shown.

Table 2. Sample average of $W_2^2(\hat{m}_n^{(k)}, m_0)$, using 10 simulations, for different values of observations $n$ and samples $k$.

| n / k | 10   | 20   | 50   | 100  | 200  | 500  | 1000  | 2000  |
|-------|------|------|------|------|------|------|-------|-------|
| 10    | 2.1294 | 2.0139 | 2.0384 | 1.9396 | 1.9608 | 1.9411 | 1.9699 | 1.9548 |
| 20    | 1.4382 | 1.4498 | 1.4826 | 1.4973 | 1.4785 | 1.4953 | 1.4955 | 1.4914 |
| 50    | 0.2455 | 0.2759 | 0.2639 | 0.2468 | 0.2499 | 0.2483 | 0.2443 | 0.2454 |
| 100   | 0.1211 | 0.1387 | 0.1509 | 0.1458 | 0.1379 | 0.1328 | 0.1318 | 0.1349 |
| 200   | 0.1116 | 0.0922 | 0.0859 | 0.0817 | 0.0777 | 0.0824 | 0.0820 | 0.0819 |
| 500   | 0.0094 | 0.0077 | 0.0043 | 0.0047 | 0.0041 | 0.0038 | 0.0037 | 0.0039 |
| 1000  | 0.0068 | 0.0039 | 0.0031 | 0.0025 | 0.0023 | 0.0022 | 0.0021 | 0.0021 |
| 2000  | 0.0072 | 0.0066 | 0.0063 | 0.0062 | 0.0063 | 0.0060 | 0.0062 | 0.0062 |
| 5000  | 0.0037 | 0.0037 | 0.0028 | 0.0029 | 0.0031 | 0.0031 | 0.0028 | 0.0030 |
| 10000 | 0.0023 | 0.0017 | 0.0017 | 0.0015 | 0.0016 | 0.0017 | 0.0016 | 0.0017 |

that, for batch size $s$ and a number of observations equal to $n$, we carry out 200 iterations of the batch stochastic gradient method (4.21) with these explicit step-sizes $\{\gamma_t\}$: the resulting estimator is $\hat{m}_{n,s}$. Notice from Fig. 7 that the larger the batch, the more concentrated the trajectories of $\hat{m}_{n,s}$ become, and that the estimates exhibit random fluctuations when the batch size is small. Additionally, Table 3 summarizes the means of the distance $W_2^2$ to the true model $m_0$, using the sequences after $t = 100$ against the empirical estimator using all the simulations with $k \geq 100$. Finally, Table 4 shows the standard deviation of the distance $W_2^2$ to the true model $m_0$, where we can notice that the standard deviation decreases as the batch size grows. Critically, observe that for batch sizes $s \geq 5$ the stochastic estimation is better than its empirical counterpart, i.e. it has lower variance with similar (or less) bias. This is noteworthy given the fact that computing our Wasserstein barycenter estimator via the batch stochastic gradient descent method is computationally less demanding than computing it via the empirical method.

Based on this illustrative numerical example, we can conclude that:
• the empirical posterior constructed using MCMC sampling is consistent under the $W_2$ distance and therefore can be relied upon to compute Wasserstein barycenters,
• the empirical Wasserstein barycenter estimator tends to converge faster (and with lower variance) to the true model than the empirical Bayesian model average,
• computing the population Wasserstein barycenter estimator via batch stochastic gradient descent seems to be a superior alternative to computing the empirical barycenter (i.e., to applying the deterministic gradient descent method to a finitely sampled posterior).

![Figure 6. Averages (bars) and standard deviations (vertical lines) of $W_2(\hat{\theta}_n^{(k)}, m_0)$ denoted as WB in orange, and $W_2(\bar{\theta}_n^{(k)}, m_0)$ denoted as MA in blue, for $n = 1000$ and different numbers of samples $k$. We considered 10 simulations for each $k$.]

| $n$ | $s$ | 1   | 2   | 5   | 10  | 15  | 20  | empirical |
|-----|-----|-----|-----|-----|-----|-----|-----|-----------|
| 10  | 1   | 2.0421 | 2.0091 | 1.9549 | 1.9721 | 1.9732 | 1.9712 | 1.9532   |
|     | 2   | 1.4819 | 1.4868 | 1.5100 | 1.4852 | 1.4840 | 1.4891 | 1.4916   |
|     | 5   | 0.2406 | 0.2512 | 0.2465 | 0.2427 | 0.2444 | 0.2460 | 0.2469   |
|     | 10  | 0.1340 | 0.1392 | 0.1340 | 0.1349 | 0.1334 | 0.1338 | 0.1366   |
|     | 20  | 0.0843 | 0.0811 | 0.0819 | 0.0807 | 0.0820 | 0.0819 | 0.0811   |
|     | 50  | 0.0044 | 0.0042 | 0.0039 | 0.0039 | 0.0041 | 0.0040 | 0.0041   |

Table 3. Means of $W_2^2$ of the stochastic gradient estimations (using the sequences with $t \geq 100$) and that of the empirical estimator (using the simulations with $k \geq 100$), across different combinations of observations $n$ and batch size $s$.

| $n$ | $s$ | 1   | 2   | 5   | 10  | 15  | 20  | empirical |
|-----|-----|-----|-----|-----|-----|-----|-----|-----------|
| 10  | 1   | 0.1836 | 0.1071 | 0.0526 | 0.0474 | 0.0397 | 0.0232 | 0.0916   |
|     | 2   | 0.0751 | 0.0565 | 0.0553 | 0.0189 | 0.0253 | 0.0186 | 0.0790   |
|     | 5   | 0.0210 | 0.0174 | 0.0072 | 0.0084 | 0.0050 | 0.0039 | 0.0138   |
|     | 10  | 0.0102 | 0.0076 | 0.0049 | 0.0048 | 0.0035 | 0.0023 | 0.0112   |
|     | 20  | 0.0074 | 0.0045 | 0.0021 | 0.0035 | 0.0013 | 0.0017 | 0.0047   |
|     | 50  | 0.0016 | 0.0007 | 0.0005 | 0.0004 | 0.0004 | 0.0004 | 0.0009   |
|     | 100 | 0.0005 | 0.0006 | 0.0004 | 0.0004 | 0.0003 | 0.0003 | 0.0005   |

Table 4. Std. deviations of $W_2^2$ of the stochastic gradient estimations (using the sequences with $t \geq 100$) and that of empirical estimator (using the simulations with $k \geq 100$), across different combinations of observations $n$ and batch size $s$. 

| $n$ | $s$ | 1   | 2   | 5   | 10  | 15  | 20  | empirical |
|-----|-----|-----|-----|-----|-----|-----|-----|-----------|
| 10  | 1   | 0.1836 | 0.1071 | 0.0526 | 0.0474 | 0.0397 | 0.0232 | 0.0916   |
|     | 2   | 0.0751 | 0.0565 | 0.0553 | 0.0189 | 0.0253 | 0.0186 | 0.0790   |
|     | 5   | 0.0210 | 0.0174 | 0.0072 | 0.0084 | 0.0050 | 0.0039 | 0.0138   |
|     | 10  | 0.0102 | 0.0076 | 0.0049 | 0.0048 | 0.0035 | 0.0023 | 0.0112   |
|     | 20  | 0.0074 | 0.0045 | 0.0021 | 0.0035 | 0.0013 | 0.0017 | 0.0047   |
|     | 50  | 0.0016 | 0.0007 | 0.0005 | 0.0004 | 0.0004 | 0.0004 | 0.0009   |
|     | 100 | 0.0005 | 0.0006 | 0.0004 | 0.0004 | 0.0003 | 0.0003 | 0.0005   |
Figure 7. Evolution of the $W_2^2$ cost for 10 realizations of the stochastic barycenter and their mean (blue) versus an empirical barycenter estimator (red), for $n = 10, 20, 50, 100, 200, 500, 1000$ and batches sizes $s = 1, 15$.

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APPENDIX A. BAYES ESTIMATORS AS GENERALIZED MODEL AVERAGES

We prove Proposition 2.2. Consider the squared $L_2$-distance between densities:

$$L_2(m, \tilde{m}) = \frac{1}{2} \int_X (m(x) - \tilde{m}(x))^2 \lambda(dx).$$

By Fubini’s theorem we have that

$$RKL(\tilde{m}|D) = \frac{1}{2} \int_X \int_M (m(x) - \tilde{m}(x))^2 \Pi(dm|D) \lambda(dx).$$

By the fundamental lemma of calculus of variations, denoting

$$\mathcal{L}(x, \tilde{m}, \tilde{m}^\prime) = \frac{1}{2} \int_M (m(x) - \tilde{m}(x))^2 \Pi(dm|D)$$

the extrema of $RKL(\tilde{m}|D)$ are weak solutions of the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}(x, \tilde{m}, \tilde{m}^\prime)}{\partial \tilde{m}} = \frac{d}{dx} \frac{\partial \mathcal{L}(x, \tilde{m}, \tilde{m}^\prime)}{\partial \tilde{m}^\prime}$$

$$\int_M (m(x) - \tilde{m}(x)) \Pi(dm|D) = 0,$$

so we have that the optimal is reached on the Bayesian model average

$$\int_M m(x) \Pi(dm|D).$$

If we take the loss function as the reverse Kullback-Leibler divergence

$$D_{KL}(m|\tilde{m}) = \int_X m(x) \ln \frac{m(x)}{\tilde{m}(x)} \lambda(dx),$$

we have that the associate Bayes risk can be written as

$$R_{D_{KL}}(\tilde{m}|D) = \int_X \int_M m(x) \ln \frac{m(x)}{\tilde{m}(x)} \lambda(dx) \Pi(dm|D)$$

$$= \int_X \int_M m(x) \ln m(x) \Pi(dm|D) \lambda(dx) - \int_X \int_M m(x) \Pi(dm|D) \ln \tilde{m}(x) \lambda(dx)$$

$$= C - \int_X \mathbb{E}[m(x)] \ln \tilde{m}(x) \lambda(dx)$$

and changing the constant $C$ by the entropy of $\mathbb{E}[m]$ we have that

$$R_{D_{KL}}(\tilde{m}|D) = C' + \int_X \mathbb{E}[m(x)] \ln \mathbb{E}[m(x)] \lambda(dx) - \int_X \mathbb{E}[m(x)] \ln \tilde{m}(x) \lambda(dx)$$

$$= C' + D_{KL}(\mathbb{E}[m], \tilde{m}),$$

so the extremum of $R_{D_{KL}}(\tilde{m}|D)$ is given by the Bayesian model average. Instead if we take the forward Kullback-Leibler divergence as loss function

$$D_{KL}(\tilde{m}|m) = \int_X \tilde{m}(x) \ln \frac{\tilde{m}(x)}{m(x)} \lambda(dx),$$

we have

$$R_{D_{KL}}(\tilde{m}|D) = \int_X \int_M \tilde{m}(x) \ln \frac{\tilde{m}(x)}{m(x)} \lambda(dx) \Pi(dm|x_1, \ldots, x_n)$$

$$= \int_X \tilde{m}(x) \ln \tilde{m}(x) \lambda(dx) - \int_X \tilde{m}(x) \int_M \ln m(x) \Pi(dm|x_1, \ldots, x_n) \lambda(dx)$$

$$= \int_X \tilde{m}(x) \ln \tilde{m}(x) \lambda(dx) - \int_X \tilde{m}(x) \ln \exp \mathbb{E}[\mathbb{E}[m]] \lambda(dx)$$

$$= \int_X \tilde{m}(x) \ln \frac{\tilde{m}(x)}{\exp \mathbb{E}[\mathbb{E}[m]]} \lambda(dx).$$
Denote by $Z$ the normalization constant so that \( \frac{1}{2} \int_X \exp \left[ \ln m(x) \right] \lambda(dx) = 1 \), thus
\[
R_{D_{kl}}(\bar{m}|D) + \ln Z = \int_X \bar{m}(x) \ln \frac{\bar{m}(x)}{\exp[\ln m]} \lambda(dx) + \int_X \bar{m}(x) \ln Z \lambda(dx) = \int_X \bar{m}(x) \ln \frac{\bar{m}(x)}{\exp[\ln m]} \lambda(dx) = D_{KL} \left( \frac{1}{2} \exp[\ln m], \bar{m} \right).
\]
So the extremum of $R_{D_{kl}}(\bar{m}|D)$ is the Bayesian exponential model average given by
\[
\hat{m}(x) = \frac{1}{2} \exp \int_M \ln m(x) \Pi(dm).
\]
Finally, if we take the squared Hellinger distance as loss function
\[
H^2(m, \hat{m}) = \frac{1}{2} \int_X \left( \sqrt{m(x)} - \sqrt{\hat{m}(x)} \right)^2 \lambda(dx) = 1 - \int_X \sqrt{m(x) \hat{m}(x)} \lambda(dx),
\]
we easily check that the extremum of $R_{H^2}(\bar{m}|D)$ is the Bayesian square model average:
\[
\hat{m}(x) = \frac{1}{2} \left( \int_M \sqrt{m(x)} \Pi(dm|x_1, \ldots, x_n) \right)^2 Z = \int_X \left( \int_M \sqrt{m(x)} \Pi(dm|x_1, \ldots, x_n) \right)^2 \lambda(dx).
\]

**Appendix B. Wasserstein barycenters**

We start following the presentation in [29]. Let $X$ be a locally compact separable geodesic space with associated metric $d$. As before $W_p(\cdot, \cdot)$ denotes the Wasserstein distance of order $p$ based on $d$; see (3.1). This distance is defined on $\mathcal{W}_p(X)$, the set of probability measures which integrate $d(x, y)^p$ for some $x \in X$.

We can now consider $\mathcal{W}_p(X)$ with the complete metric $W_p$ as a base Polish space, and define $\mathcal{W}_p(\mathcal{W}_p(X))$ analogously, with an associated Wasserstein distance of order $p$ which for simplicity we still call $W_p$.

Let $\Pi \in \mathcal{W}_p(\mathcal{W}_p(X))$. By definition, its model-average belongs to $\mathcal{W}_p(X)$, since
\[
\int W_p(m, \delta_x)^p \Pi(dm) = \int \int d(x, y)^p m(dy) \Pi(dm) = \int d(x, y)^p \int m(dy) \Pi(dm).
\]
A $p$-Wasserstein population barycenter of $\Pi \in \mathcal{W}_p(\mathcal{W}_p(X))$ is an optimizer of
\[
V(\Pi) := \inf \left\{ \int_{\mathcal{W}_p(X)} W_p(v, m)^p \Pi(dm) : v \in \mathcal{W}_p(X) \right\},
\]
as in Definition (12) in the main text. We state an existence result first obtained in [29] Theorem 2; our argument here seems more elementary.

**Lemma B.1.** There exists a minimizer for $V(\Pi)$, i.e. a $p$-Wasserstein barycenter.

**Proof.** Taking $v = \delta_x$ we get that $V(\Pi)$ is finite. Now, let $\{v_n\} \subseteq \mathcal{W}_p(X)$ such that
\[
\int_{\mathcal{W}_p(X)} W_p(v_n, m)^p \Pi(dm) \to V(\Pi).
\]
For $n$ large enough we have
\[
W_p \left( v_n, \int \mathcal{W}_p(X) m \Pi(dm) \right)^p \leq \int_{\mathcal{W}_p(X)} W_p(v_n, m)^p \Pi(dm) \leq V(\Pi) + 1 =: K,
\]
by convexity of optimal transport costs. From this we derive that (for every $x$)
\[
\sup_n \int_X d(x, y)^p v_n(dy) < \infty.
\]
By Markov inequality this shows, for each $\varepsilon > 0$, that there is $\ell$ large enough such that \( \sup_n v_n(y \in X : d(x, y) > \ell) \leq \varepsilon \). As explained in [29], the assumptions made on $X$ imply that $y \in X : d(x, y) \leq \ell$ is compact (Hopf-Rinow theorem), and so we deduce the tightness of $\{v_n\}$. By Prokhorov theorem, up to selection of a subsequence, there exists $v \in \mathcal{W}_p(X)$ which is its weak limit. We can conclude by Fatou’s lemma:
\[
V(\Pi) = \lim \int W_p(v_n, m)^p \Pi(dm) \geq \liminf \int W_p(v_n, m)^p \Pi(dm) \geq \int W_p(v, m)^p \Pi(dm).
\]
\[\Box\]
It is plain from the above proof that if \( M \subseteq \mathcal{W}_p(\mathcal{X}) \) is weakly closed, then there also exists a minimizer in \( M \) of
\[
\inf \left\{ \int_{W_\mu,\nu} W_p^p(v,m)\Pi(dm) : v \in M \right\}.
\]

Let us now consider the relevant case of \( \mathcal{X} = \mathbb{R}^d \) with \( d \) the Euclidean distance and \( p = 2 \). We take
\[
\Pi \in \mathcal{W}_2(\mathcal{W}_2(\mathbb{R}^d)),
\]
observing that in such situation the previous lemma applies. We recall now the uniqueness result stated in [29, Proposition 6]:

**Lemma B.2.** Assume that there exists a set \( A \subseteq \mathcal{W}_2(\mathbb{R}^d) \) of measures with
\[
\mu \in A, \ B \in \mathcal{B}(\mathbb{R}^d), \ \dim(B) \leq q - 1 \implies \mu(B) = 0,
\]
and \( \Pi(A) > 0 \). Then \( \Pi \) admits a unique \( 2 \)-Wasserstein population barycenter.

**Appendix C. A condition for existence of barycenters of Bayesian posteriors**

We last provide a general condition on the prior \( \Pi \) ensuring that
\[
\Pi_n \in \mathcal{W}_p(\mathcal{W}_p(\mathcal{X})) \quad \text{for all } n,
\]
and therefore the existence of a barycenter estimator.

**Definition C.1.** We say that \( \Pi \in \mathcal{P}(\mathcal{P}(\mathcal{X})) \) is integrable after updates if it satisfies the conditions

1. For all \( x \in \mathcal{X}, \ell > 1 \):
   \[
   \int_{\mathcal{M}} m(x)^\ell \Pi(dm) < \infty.
   \]
2. For some \( y \in \mathcal{X}, \varepsilon > 0 \):
   \[
   \int_{\mathcal{M}} \left( \int_{\mathcal{X}} d(y,z)^p m(dz) \right)^{1+\varepsilon} \Pi(dm) < \infty.
   \]

Condition (2) above could be intuitively summarized with the notation \( \Pi \in \mathcal{W}_{p,\varepsilon}(\mathcal{W}_p(\mathcal{X})) \).

**Remark C.2.** If \( \Pi \in \mathcal{P}(\mathcal{W}_{p,\varepsilon}(\mathcal{X})) \) has finite support, then Conditions (1) and (2) are satisfied. On the other hand, if \( \Pi \) is supported on a scatter-location family (see Section 5.4) containing one element with a bounded density and a finite \( p \)-moment, then Conditions (1) and (2) are fulfilled if for example \( \text{supp}(\Pi) \) is tight.

**Lemma C.3.** Suppose that \( \Pi \) is integrable after updates. Then, for each \( x \in \mathcal{X} \), the measure
\[
\tilde{\Pi}(dm) := \frac{m(x|\Pi(dm))}{\int_{\mathcal{M}} m(x|\Pi(dm))}.
\]
is also integrable after updates.

**Proof.** We verify Property (1) first. Let \( \ell > 1 \) and \( \bar{x} \in \mathcal{X} \) given. Then
\[
\int_{\mathcal{M}} m(\bar{x})^\ell m(x)\Pi(dm) \leq \left( \int_{\mathcal{M}} m(x)^s \Pi(dm) \right)^{\ell/s} \left( \int_{\mathcal{M}} m(\bar{x})^t \Pi(dm) \right)^{1/t},
\]
with \( s, t \) conjugate Hölder exponents. This is finite since \( \Pi \) fulfills Property (1).

We now establish Property (2). Let \( y \in \mathcal{X}, \varepsilon > 0 \). Then
\[
\int_{\mathcal{M}} \left( \int_{\mathcal{X}} d(y,z)^p m(dz) \right)^{1+\varepsilon} m(x)\Pi(dm) \leq \left( \int_{\mathcal{M}} m(x)^s \Pi(dm) \right)^{1/s} \left( \int_{\mathcal{M}} \left( \int_{\mathcal{X}} d(y,z)^p m(dz) \right)^{(1+\varepsilon)y} \Pi(dm) \right)^{1/t}.
\]
The first term in the r.h.s. is finite by Property (1). The second term in the r.h.s. is finite by Property (2), if we take \( \varepsilon \) small enough and \( t \) close enough to 1. We conclude. \( \square \)

**Lemma C.4.** Suppose that \( \Pi \) is integrable after updates. Then for all \( n \in \mathbb{N} \) and \( \{x_1, \ldots, x_n\} \subseteq \mathcal{X} \), the posterior \( \Pi_n \) is also integrable after updates.
Proof. By Lemma C.3 we obtain that $\Pi_1$ is integrable after updates. By induction, suppose $\Pi_{n-1}$ has this property. Then as

$$\Pi_n(dm) = \frac{\mu(x_n, d\Pi_{n-1})(dm)}{\int_M \mu(x_n, d\Pi_{n-1})(dm)},$$

we likewise conclude that $\Pi_n$ is integrable after updates. \qed