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# Bayesian Kantorovich Deconvolution in Finite Mixture Models

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# Bayesian Kantorovich Deconvolution in Finite Mixture Models

Catia Scricciolo

**Abstract** This chapter addresses the Bayesian approach to the problem of recovering the latent or mixing distribution in finite general kernel mixture models, when the number of components is unknown, yet bounded above by a fixed number. Taking a step back to the historical development of the analysis of this problem within the Bayesian paradigm and making use of the current methodology for the study of the posterior contraction phenomenon, we show that, for general prior laws supported over the space of mixing distributions with at most a fixed number of components, under replicated observations from the mixed density, the mixing distribution is estimable in the Kantorovich or  $L^1$ -Wasserstein metric at the optimal frequentist rate  $n^{-1/4}$  (up to a logarithmic factor),  $n$  being the sample size.

**Key words:** Dirichlet distribution, Kantorovich metric, Kolmogorov metric, mixing distribution, mixture model, posterior distribution, rate of convergence, sieve prior, Wasserstein metric

## 1 Introduction

The Bayesian analysis of the problem of recovering the unknown mixing distribution in mixture models has recently attracted much attention and stimulated an active discussion encouraging new ideas. Several papers—including [Efron (4), Gao and van der Vaart (5), Ishwaran *et al.* (10), Nguyen (13), Scricciolo (17)]—have been devoted to the investigation of this topic, with extensive comparisons with the classical approaches. In order to introduce the problem, suppose that  $x \mapsto k(x | y)$  is a probability density for every  $y \in \mathcal{Y} \subseteq \mathbb{R}$  for a measurable space  $(\mathcal{Y}, \mathcal{B})$ . If the map

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$(x, y) \rightarrow k(x | y)$  is jointly measurable, then

$$p_G(x) := \int_{\mathcal{Y}} k(x | y) dG(y), \quad x \in \mathbb{R}, \quad (1)$$

defines a probability density on  $\mathbb{R}$  for every probability measure  $G$  on  $(\mathcal{Y}, \mathcal{B})$ , whose collection is denoted by  $\mathcal{G}$ . The cumulative distribution function of the mixed density in (1) is denoted by

$$F_G(x) = \int_{-\infty}^x p_G(u) du, \quad x \in \mathbb{R}.$$

Suppose we observe  $n$  independent random variables  $X_1, \dots, X_n$  identically distributed according to the mixed density

$$p_0(x) \equiv p_{G_0}(x) = \int_{\mathcal{Y}} k(x | y) dG_0(y), \quad x \in \mathbb{R}.$$

We denote by  $F_0$  the cumulative distribution function of the density  $p_0$ , namely,

$$F_0(x) \equiv F_{G_0}(x) = \int_{-\infty}^x p_0(u) du, \quad x \in \mathbb{R}.$$

The interest is in recovering the unknown mixing distribution  $G_0 \in \mathcal{G}$  from observations of the random sample  $X^{(n)} := (X_1, \dots, X_n)$ . The formulation of the problem applies to both finite and infinite mixtures, but the focus of this chapter is primarily on the case when the sampling density is a mixture with an unknown, but bounded number of components.

The problem has been initially studied from the frequentist perspective by Chen (1), who established that when  $p_0$  has an unknown number of components  $d_0$  such that  $1 \leq d_0 \leq N$ , for some fixed integer  $N$ , then the optimal rate for estimating the mixing distribution  $G_0$  is only  $n^{-1/4}$  and that this rate is achievable by some minimum distance estimator. The first Bayesian analysis of the problem we are aware of traces back to Ishwaran *et al.* (10), who define a prior law over the space of all mixing distributions with at most  $N$  components, the mixture weights being assigned an  $N$ -dimensional Dirichlet distribution with a non-informative choice for the shape parameters that are all set equal to  $\alpha/N$  for a positive constant  $\alpha$ . Under conditions similar to those postulated by Chen (1), which, in particular, employ the notion of strong identifiability in mixture models, they prove that Bayesian estimation of the mixing distribution in the Kantorovich metric is possible at the optimal frequentist rate  $n^{-1/4}$ , up to a  $\log n$ -factor. More recently, posterior convergence rates for estimating the mixing distribution in the  $L^2$ -Wasserstein metric for finite mixtures of multivariate distributions, have been discussed by Nguyen (13) following a completely different line of reasoning. In this chapter, we show that, by combining the approach of Ishwaran *et al.* (10), which instrumentally use posterior contraction rates in the sup-norm for the distribution function and strong identifiability to shift to the Kantorovich distance between mixing distributions, with the current methodology for the study of posterior contraction rates, which can by now count upon

many refined results for small ball prior probability estimates, the mixing distribution is estimable in the Kantorovich or  $L^1$ -Wasserstein metric at the optimal rate  $n^{-1/4}$  (up to a logarithmic factor), for a large class of prior laws over the space of mixing distributions with at most  $N$  components, under less stringent conditions than those used in Ishwaran *et al.* (10) or in Nguyen (13). Many aspects of this important statistical problem still remain unclear and we hope to contribute to a better understanding in a follow-up contribution.

Before presenting the notation, a note on the use of the phrase ‘‘Bayesian deconvolution’’. This term has been recently introduced by Efron (4) to describe a maximum likelihood procedure for estimating the mixing distribution in general mixture models of the form in (1). Even if the mixtures herein considered are not necessarily convolution kernel mixtures, we liked the evocative power of the expression to recall the general inverse problem of estimating the unknown mixing distribution.

*Notation.* In this paragraph, we set out the notation and recall some definitions used throughout the chapter.

- The symbols ‘‘ $\lesssim$ ’’ and ‘‘ $\gtrsim$ ’’ indicate inequalities valid up to a constant multiple that is universal or fixed within the context, but anyway inessential for our purposes.
- All probability density functions are meant to be with respect to Lebesgue measure on  $\mathbb{R}$  or on some subset thereof.
- The same symbol,  $G$  (say), is used to denote a probability measure on  $(\mathcal{Y}, \mathcal{B})$  as well as the corresponding cumulative distribution function.
- The degenerate probability distribution putting mass one at a point  $y \in \mathbb{R}$  is denoted by  $\delta_y$ .
- The notation  $Pf$  stands for the expected value  $\int f dP$ , where the integral is understood to extend over the entire natural domain when, here and elsewhere, the domain of integration is omitted. With this convention, for the empirical measure  $\mathbb{P}_n := n^{-1} \sum_{i=1}^n \delta_{X_i}$  associated with the random sample  $X_1, \dots, X_n$ , namely, the discrete uniform distribution on the sample values that puts mass  $1/n$  on each one of the observations, the notation  $\mathbb{P}_n f$  abbreviates  $n^{-1} \sum_{i=1}^n f(X_i)$ .
- For every pair  $\mathbf{x}_N, \mathbf{y}_N \in \mathbb{R}^N$ ,  $\|\mathbf{x}_N - \mathbf{y}_N\|_{\ell_1}$  stands for the  $\ell_1$ -distance  $\sum_{j=1}^N |x_j - y_j|$ .
- For a probability measure  $Q$  on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ , let  $q$  denote its density. For any  $\varepsilon > 0$ ,

$$B_{\text{KL}}(P_0; \varepsilon^2) := \left\{ Q : P_0 \left( \log \frac{p_0}{q} \right) \leq \varepsilon^2, P_0 \left( \log \frac{p_0}{q} \right)^2 \leq \varepsilon^2 \right\}$$

denotes the *Kullback-Leibler* type neighborhood of  $P_0$  of radius  $\varepsilon^2$ . Defined for every  $\alpha \in (0, 1]$ , the divergence  $\rho_\alpha(P_0 \| Q) := (1/\alpha)[P_0(p_0/q)^\alpha - 1]$ , see Wong and Shen (20), pp. 351–352,

$$B_{\rho_\alpha}(P_0; \varepsilon^2) := \{ Q : \rho_\alpha(P_0 \| Q) \leq \varepsilon^2 \}$$

denotes the  $\rho_\alpha$ -neighborhood of  $P_0$  of radius  $\varepsilon^2$ . The definition of  $\rho_\alpha$  extends to negatives values of  $\alpha \in (-1, 0)$ . In particular, for  $\alpha = -1/2$ , the divergence  $\rho_{-1/2}(P_0 \| Q) = -2 \int p_0 [(q/p_0)^{1/2} - 1] = \int (p_0^{1/2} - q^{1/2})^2$  is the squared

Hellinger distance. We can then define the following *Hellinger* type neighborhood of  $P_0$  of radius  $\varepsilon^2$ :

$$B_{\rho_{-1/2}\|\cdot\|_\infty}(P_0; \varepsilon^2) := \left\{ Q : \rho_{-1/2}(P_0\|Q) \left\| \frac{P_0}{Q} \right\|_\infty \leq \varepsilon^2 \right\}.$$

- For any real number  $p \geq 1$  and any pair of probability measures  $G_1, G_2 \in \mathcal{G}$  with finite  $p$ th absolute moments, the  $L^p$ -Wasserstein distance between  $G_1$  and  $G_2$  is defined as

$$W_p(G_1, G_2) := \left( \inf_{\gamma \in \Gamma(G_1, G_2)} \int_{\mathcal{Y} \times \mathcal{Y}} |y_1 - y_2|^p \gamma(dy_1, dy_2) \right)^{1/p},$$

where  $\Gamma(G_1, G_2)$  is the set of all joint probability measures on  $(\mathcal{Y} \times \mathcal{Y}) \subseteq \mathbb{R}^2$ , with marginal distributions  $G_1$  and  $G_2$  on the first and second arguments, respectively.

## 2 Main Results

This section is devoted to expose the main results of the chapter and is split into two parts. In the first one, preliminary results on Bayesian estimation of distribution functions in the Kolmogorov metric, which are compatible with a wide class of prior laws, are presented and some issues are highlighted. In the second part, arguably the most relevant, attention is restricted to finite mixtures with an unknown, but bounded number of components, and Bayesian estimation of the mixing distribution in the Kantorovich metric at the optimal frequentist rate  $n^{-1/4}$  (up to a logarithmic factor) is discussed.

### *Posterior Concentration of Kernel Mixtures in the Kolmogorov Metric*

The following assumption will be hereafter in force.

*Assumption A.* Let

$$\varepsilon_n := \left( \frac{\log n}{n} \right)^{1/2} L_n, \quad n \in \mathbb{N}, \quad (2)$$

where, depending on the prior concentration rate on small balls around  $P_0$ , the sequence of positive real numbers  $(L_n)$  can be either slowly varying at  $+\infty$  or degenerate at an appropriate constant  $L_0$ .

Comments on the two possible specifications of  $(L_n)$  in connection with the prior concentration rate are postponed to Lemma 1, which provides sufficient conditions on the distribution function  $F_0$  and the prior concentration rate  $\varepsilon_n$  for the posterior

to contract at a nearly  $\sqrt{n}$ -rate on Kolmogorov neighborhoods of  $F_0$ . We warn the reader that, unless otherwise specified, in all stochastic order symbols used hereafter, the probability measure  $\mathbf{P}$  is understood to be  $P_0^n$ , the joint law of the first  $n$  coordinate projections of the infinite product probability measure  $P_0^\infty$ . Also,  $\Pi_n$  stands for a prior law, possibly depending on the sample size, over the space of probability measures  $\{P_G, G \in \mathcal{G}\}$ , with density  $p_G$  as defined in (1).

**Lemma 1.** *Let  $F_0$  be a continuous distribution function. If, for a constant  $C > 0$  and a sequence  $\varepsilon_n$  as defined in (2), we have*

$$\Pi_n(B_{\text{KL}}(P_0; \varepsilon_n^2)) \gtrsim \exp(-Cn\varepsilon_n^2), \quad (3)$$

then, for  $M_n \gtrsim \sqrt{(C+1/2)L_n}$ ,

$$\Pi_n\left(\sqrt{n} \sup_x |(F_G - F_0)(x)| > M_n(\log n)^{1/2} \mid X^{(n)}\right) = o_{\mathbf{P}}(1). \quad (4)$$

*Proof.* The posterior probability of the event

$$A_n^c := \left\{ G : \sqrt{n} \sup_x |(F_G - F_0)(x)| > M_n(\log n)^{1/2} \right\}$$

is given by

$$\Pi_n(A_n^c \mid X^{(n)}) = \frac{\int_{A_n^c} \prod_{i=1}^n p_G(X_i) \Pi_n(dG)}{\int_{\mathcal{G}} \prod_{i=1}^n p_G(X_i) \Pi_n(dG)}.$$

We construct (a sequence of) tests  $(\phi_n)$  for testing the hypothesis

$$H_0 : P = P_0 \quad \text{versus} \quad H_1 : P = P_G, G \in A_n^c,$$

where  $\phi_n \equiv \phi_n(X^{(n)}; P_0) : \mathcal{X}^n \rightarrow \{0, 1\}$  is the indicator function of the rejection region of  $H_0$ , such that

$$P_0^n \phi_n \rightarrow 0 \quad \text{as } n \rightarrow +\infty$$

$$\text{and } \sup_{G \in A_n^c} P_G^n(1 - \phi_n) \leq 2 \exp(-2(M_n - K)^2 \log n) \quad \text{for sufficiently large } n,$$

with  $M_n > K > 0$  for every  $n$  large enough. Define the test

$$\phi_n := 1_{R_n}, \quad \text{with } R_n := \left\{ x^{(n)} : \sqrt{n} \sup_x |(F_n - F_0)(x)| > K(\log n)^{1/2} \right\},$$

where  $F_n$  is the empirical distribution function, that is, the distribution function associated with the empirical measure  $\mathbb{P}_n$  of the sample  $X^{(n)}$ . Since  $x \mapsto F_0(x)$  is *continuous* by assumption, in virtue of Dvoretzky-Kiefer-Wolfowitz (DKW) (3) inequality, with the tight universal constant in Massart (12), the type I error probability  $P_0^n \phi_n$  can be bounded above as follows

$$P_0^n \phi_n = P_0^n(R_n) \leq 2 \exp(-2K^2 \log n).$$

Then,

$$E_0^n[\Pi_n(A_n^c | X^{(n)})\phi_n] \leq P_0^n \phi_n \leq 2 \exp(-2K^2 \log n), \quad (5)$$

where  $E_0^n$  denotes expectation with respect to  $P_0^n$ , and

$$\begin{aligned} E_0^n[\Pi_n(A_n^c | X^{(n)})] &= E_0^n[\Pi_n(A_n^c | X^{(n)})\phi_n] + E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)] \\ &\leq 2 \exp(-2K^2 \log n) + E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)]. \end{aligned}$$

It remains to control the term  $E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)]$ . Defined the set

$$D_n := \left\{ x^{(n)} : \int_{\mathcal{G}} \prod_{i=1}^n \frac{P_G}{P_0}(x_i) \Pi_n(dG) \leq \Pi_n(B_{\text{KL}}(P_0; \varepsilon_n^2)) \exp(-(C+1)n\varepsilon_n^2) \right\},$$

consider the following decomposition

$$E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)] = E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)(1_{D_n} + 1_{D_n^c})].$$

It is known from Lemma 8.1 of Ghosal *et al.* (7), p. 524, that  $P_0^n(D_n) \leq (C^2 n \varepsilon_n^2)^{-1}$ . It follows that

$$E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)1_{D_n}] \leq P_0^n(D_n) \leq (C^2 n \varepsilon_n^2)^{-1}. \quad (6)$$

By the assumption in (3) and Fubini's theorem,

$$E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n)1_{D_n^c}] \leq \exp((2C+1)n\varepsilon_n^2) \int_{A_n^c} P_G^n(1 - \phi_n) \Pi_n(dG). \quad (7)$$

The following arguments are aimed at finding an exponential upper bound on  $\sup_{G \in A_n^c} P_G^n(1 - \phi_n)$ . By the triangular inequality, over the set  $R_n^c$ ,

$$\begin{aligned} M_n(\log n)^{1/2} &< \sqrt{n} \sup_x |(F_G - F_0)(x)| \\ &\leq \sqrt{n} \sup_x |(F_G - F_n)(x)| + \sqrt{n} \sup_x |(F_n - F_0)(x)| \\ &\leq \sqrt{n} \sup_x |(F_G - F_n)(x)| + K(\log n)^{1/2} \end{aligned}$$

for every  $G \in A_n^c$ , which implies that

$$\sqrt{n} \sup_x |(F_G - F_n)(x)| > (M_n - K)(\log n)^{1/2}.$$

Since  $x \mapsto F_G(x) := \int_{-\infty}^x p_G(u) du$  is continuous, by applying again DKW inequality, we obtain

$$\begin{aligned} \sup_{G \in A_n^c} P_G^n(1 - \phi_n) &\leq \sup_{G \in A_n^c} P_G^n \left( \sqrt{n} \sup_x |(F_G - F_n)(x)| > (M_n - K)(\log n)^{1/2} \right) \\ &\leq 2 \exp(-2(M_n - K)^2 \log n). \end{aligned}$$

Combining the above assertion with (7), we see that

$$E_0^n[\Pi_n(A_n^c | X^{(n)})(1 - \phi_n) 1_{D_n^c}] \lesssim 2 \exp(-[2(M_n - K)^2 - (2C + 1)L_n^2] \log n), \quad (8)$$

where the right-hand side of the above inequality tends to zero provided that  $(M_n - K) > \sqrt{(C + 1/2)L_n}$  for every sufficiently large  $n$ . The in-probability convergence in (4) follows from (5), (6) and (8). This concludes the proof.  $\square$

Some remarks and comments on Lemma 1 are in order.

- The first one aims at spelling out the assumptions used in the proof, some of which could otherwise erroneously seem to be confined to the context of finite mixture models, as well as at clarifying their role. Given the prior concentration rate  $\varepsilon_n$  as defined in (3), which depends on the prior distribution  $\Pi_n$  and the “point”  $P_0$ , the only further assumption used is the *continuity* of the distribution functions  $F_0$  and  $F_G$ , which is satisfied for Lebesgue dominated probability measures  $P_0$  and  $P_G$ . This condition is used to control the type I and type II error probabilities of the (sequence of) tests  $(\phi_n)$  by the DKW inequality. It is, instead, in no way used the assumption that the density  $p_G$  is modeled as a mixture, so that, even if the result has its origin in the context of finite mixtures, it applies to general dominated models and a nearly parametric (up to a logarithmic factor) prior concentration rate is the only driver and determinant of posterior contraction.
- Lemma 1 has its roots in Theorem 2 of Ishwaran *et al.* (10), p. 1324 (see pp. 1330–1331 for the proof), which deals with *finite* mixtures having an *unknown* number of components  $d_0$ , yet *bounded* by an integer  $N$ , namely,  $1 \leq d_0 \leq N < +\infty$ , and the prior is supported over the space of all mixing distributions with at most  $N$  components, the mixture weights being assigned an  $N$ -dimensional Dirichlet distribution with a non-informative choice for the shape parameters that are all set equal to  $\alpha/N$  for a positive constant  $\alpha$ . Nonetheless, as previously remarked, Lemma 1 has a broader scope of validity and applies also to *infinite* kernel mixtures with possibly other priors for the mixing distribution than the Dirichlet process, which “locally” attain an almost parametric prior concentration rate. This is the case for Dirichlet location or location-scale mixtures of normal densities and, more in general, for location-scale mixtures of exponential power densities with an even integer for the shape parameter, when the sampling density has the same form as the assumed model, with mixing distribution being either compactly supported or having sub-exponential tails, see Ghosal and van der Vaart (8), Scricciolo (15), Theorem 4.1, Theorem 4.2 and Corollary 4.1. In all these cases, the prior concentration rate is (at worst)  $\varepsilon_n = n^{-1/2} \log n$ , where  $L_n = (\log n)^{1/2}$ . An extension of previous results to convolution mixtures



of super-smooth kernels, with Pitman-Yor or normalized inverse-Gaussian processes as priors for the mixing distribution, for which Lemma 1 also holds, is considered in Scricciolo (16), see Theorem 1, pp. 486–487. Another class of priors on kernel mixtures to which Lemma 1 applies is that of *sieve* priors. For a given kernel, a sieve prior is defined by combining single priors on classes of kernel mixtures, each one indexed by the number of mixture components, with a prior on such random number. A probability measure with kernel mixture density is then generated in two steps: first the model index, *i.e.*, the number of mixture components, is selected; then a probability measure is generated from the chosen model according to a prior on it. When the true density  $p_0$  is itself a kernel mixture, the prior concentration rate can be assessed by bounding below the probability of Kullback-Leibler type neighborhoods of  $P_0$  by the probability of  $\ell^1$ -balls of appropriate dimension. In fact, approximation properties of mixtures under consideration can be exploited to find a good fitting distribution of the sampling density in a proper subclass. More precisely, any finite kernel mixture can be approximated arbitrarily well (in the distance induced by the  $L^1$ -norm) by mixtures having the same number of components, the mixture components and weights taking values in  $\ell^1$ -neighborhoods of the corresponding true elements. The number of mixture components is then constant, this leading to the prior concentration rate  $\varepsilon_n \propto (n/\log n)^{-1/2}$ , where  $L_n \equiv L_0$ . Examples of sieve priors in which, for every choice of the model index, the mixture weights are jointly distributed according to a Dirichlet distribution, are provided by Bernstein polynomials, see Theorem 2.2 of Ghosal (6), pp. 1268–1269, by histograms and polygons, see Theorem 1 of Scricciolo (14), pp. 629–630 (see pp. 636–637 for the proof). If, as a special case, a single prior distribution on kernel mixtures with a sample size-dependent number  $N \equiv L_n$  of mixture components is considered, then the prior concentration rate is  $\varepsilon_n = (n/\log n)^{-1/2}L_n$  for an arbitrary slowly varying sequence  $L_n \rightarrow +\infty$ .

We now state sufficient conditions on the kernel density and the prior distributions for the mixture atoms and weights so that the overall prior on kernel mixtures with (at most)  $N$  components verifies condition (3) for  $\varepsilon_n \propto (n/\log n)^{-1/2}$ , when the sampling density is itself a kernel mixture with  $1 \leq d_0 \leq N$  components. The aim of this analysis is twofold: first, to provide less stringent requirements on the kernel density than those postulated in condition (b) employed in Theorem 2 of Ishwaran *et al.* (10), p. 1324, which relies on Lemma 4 of Ishwaran (9), pp. 2170–2171; second, to generalize the aforementioned result to a class of prior distributions on the mixture weights comprising the Dirichlet distribution. The density  $p_G$  is modeled as

$$p_G(\cdot) = \sum_{j=1}^N w_j k(\cdot | y_j),$$

with a discrete mixing distribution  $G = \sum_{j=1}^N w_j \delta_{y_j}$ . The vector  $\mathbf{w}_N := (w_1, \dots, w_N)$  of mixing weights has a prior distribution  $\tilde{\pi}_N$  on the  $(N-1)$ -dimensional simplex  $\Delta_N := \{\mathbf{w}_N \in \mathbb{R}^N : 0 \leq w_j \leq 1, j = 1, \dots, N, \sum_{j=1}^N w_j = 1\}$  and the atoms  $y_1, \dots, y_N$

are independently and identically distributed according to a prior distribution  $\pi$ . We shall also use the notation  $\mathbf{y}_N$  for  $(y_1, \dots, y_N)$ . The model can be thus described:

- the random vectors  $\mathbf{y}_N$  and  $\mathbf{w}_N$  are independent;
- given  $(\mathbf{y}_N, \mathbf{w}_N)$ , the random variables  $X_1, \dots, X_n$  are conditionally independent and identically distributed according to  $p_G$ .

The overall prior is then  $\Pi = \tilde{\pi}_N \times \pi^{\otimes N}$ . Let the sampling density  $p_0$  be itself a finite kernel mixture, with  $1 \leq d_0 \leq N$  components,

$$p_0(\cdot) \equiv p_{G_0}(\cdot) = \sum_{j=1}^{d_0} w_j^0 k(\cdot | y_j^0),$$

where the mixing distribution is  $G_0 = \sum_{j=1}^{d_0} w_j^0 \delta_{y_j^0}$  for weights  $\mathbf{w}_{d_0}^0 := (w_1^0, \dots, w_{d_0}^0) \in \Delta_{d_0}$  and support points  $\mathbf{y}_{d_0}^0 := (y_1^0, \dots, y_{d_0}^0) \in \mathbb{R}^{d_0}$ . A caveat applies: if  $d_0$  is strictly smaller than  $N$ , that is,  $1 \leq d_0 < N$ , then the vectors  $\mathbf{w}_{d_0}^0$  and  $\mathbf{y}_{d_0}^0$  are viewed as degenerate elements of  $\Delta_N$  and  $\mathbb{R}^N$ , respectively, with coordinates  $w_{d_0+1} = \dots = w_N = 0$  and  $y_{d_0+1} = \dots = y_N = 0$ .

We assume that

- i) there exists a constant  $K > 0$  such that

$$\|k(\cdot | y_1) - k(\cdot | y_2)\|_1 \leq K|y_1 - y_2| \quad \text{for all } y_1, y_2 \in \mathcal{Y};$$

- ii) for every  $\varepsilon > 0$  small enough,

$$\tilde{\pi}_N(\{\mathbf{w}_N \in \Delta_N : \|\mathbf{w}_N - \mathbf{w}_N^0\|_{\ell_1} \leq \varepsilon\}) \geq \varepsilon^N;$$

- iii) the prior distribution  $\pi$  of the atoms has a continuous and positive Lebesgue density (also denoted by  $\pi$ ) on an interval containing the support of  $G_0$ .

Some remarks and comments on the previously listed assumptions are in order. Condition *i*) requires the kernel density  $k(\cdot | y)$  to be globally Lipschitz continuous on  $\mathcal{Y}$ . Condition *ii*) is satisfied by a Dirichlet prior distribution  $\tilde{\pi}_N = \text{Dir}(\alpha_1, \dots, \alpha_N)$ , with parameters  $\alpha_1, \dots, \alpha_N$  such that, for constants  $a, A > 0$ ,  $D \geq 1$  and, for  $0 < \varepsilon \leq 1/Dk$ ,

$$A\varepsilon^a \leq \alpha_j \leq D, \quad j = 1, \dots, N.$$

Using Lemma A.1 of Ghosal (6), pp. 1278–1279, we find that  $\tilde{\pi}_N(N(\mathbf{w}_N^0; \varepsilon)) \geq \exp(-c_0 N \log(1/\varepsilon))$  for a constant  $c_0 > 0$  depending only on  $a, A, D$  and  $\sum_{j=1}^N \alpha_j$ .

**Proposition 1.** *Under assumptions (i)–(iii), condition (3) is verified for*

$$\varepsilon_n \propto (n/\log n)^{-1/2}.$$

*Proof.* For every density  $p_G$ , with mixing distribution  $G = \sum_{j=1}^N w_j \delta_{y_j}$  having support points  $\mathbf{y}_N \in \mathbb{R}^N$  and mixture weights  $\mathbf{w}_N \in \Delta_N$ , by assumption (i) we have

$$\begin{aligned} \|p_G - p_0\|_1 &\lesssim \sum_{j=1}^N w_j^0 \|k(\cdot | y_j) - k(\cdot | y_j^0)\|_1 + \sum_{j=1}^N |w_j - w_j^0| \|k(\cdot | y_j)\|_1 \\ &\lesssim \|\mathbf{y}_N - \mathbf{y}_N^0\|_{\ell_1} + \|\mathbf{w}_N - \mathbf{w}_N^0\|_{\ell_1}. \end{aligned}$$

Let  $0 < \varepsilon \leq [(1/2) \wedge (1 - e^{-1}) / \sqrt{2}]$  be fixed. For  $\mathbf{y}_N \in \mathbb{R}^N$  and  $\mathbf{w}_N \in \Delta_N$  such that  $\|\mathbf{y}_N - \mathbf{y}_N^0\|_{\ell_1} \leq \varepsilon$  and  $\|\mathbf{w}_N - \mathbf{w}_N^0\|_{\ell_1} \leq \varepsilon$ , by LeCam (11) inequalities, p. 40, relating the  $L^1$ -norm and the Hellinger metric, the squared Hellinger distance between  $p_0$  and  $p_G$  can be bounded above by a multiple of  $\varepsilon$ :

$$\rho_{-1/2}(P_0 \| P_G) = \int (p_G^{1/2} - p_0^{1/2})^2 \leq \|p_G - p_0\|_1 \lesssim \varepsilon.$$

Then, by Lemma A.10 in Scricciolo (15), p. 305, for a suitable constant  $c_1 > 0$ ,

$$\begin{aligned} \left\{ p_G : G = \sum_{j=1}^N w_j \delta_{y_j}, \|\mathbf{w}_N - \mathbf{w}_N^0\|_{\ell_1} \leq \varepsilon, \|\mathbf{y}_N - \mathbf{y}_N^0\|_{\ell_1} \leq \varepsilon \right\} \\ \subseteq B_{\text{KL}} \left( P_0; c_1 \varepsilon \left( \log \frac{1}{\varepsilon} \right)^2 \right). \end{aligned}$$

Next, define the set  $N(\mathbf{w}_N^0; \varepsilon) := \{\mathbf{w}_N \in \Delta_N : \|\mathbf{w}_N - \mathbf{w}_N^0\|_{\ell_1} \leq \varepsilon\}$ . For  $\varepsilon > 0$  small enough, by assumption (ii),

$$\tilde{\pi}_N(N(\mathbf{w}_N^0; \varepsilon)) \gtrsim \exp(-c_0 N \log(1/\varepsilon))$$

with an appropriate constant  $c_0 > 0$ . Denoted by  $B(\mathbf{y}_N^0; \varepsilon)$  the  $\mathbf{y}_N^0$ -centered  $\ell_1$ -ball of radius  $\varepsilon > 0$ ,

$$B(\mathbf{y}_N^0; \varepsilon) := \{\mathbf{y}_N \in \mathbb{R}^N : \|\mathbf{y}_N - \mathbf{y}_N^0\|_{\ell_1} \leq \varepsilon\},$$

by condition (iii), the prior probability of  $B(\mathbf{y}_N^0; \varepsilon)$  under the  $N$ -fold product measure  $\pi^{\otimes N}$  can be bounded below as follows:

$$\begin{aligned} \pi^{\otimes N}(B(\mathbf{y}_N^0; \varepsilon)) &= \prod_{j=1}^N \pi([y_j^0 - (\varepsilon/N), y_j^0 + (\varepsilon/N)]) \\ &= \prod_{j=1}^N \int_{y_j^0 - (\varepsilon/N)}^{y_j^0 + (\varepsilon/N)} \pi(y) dy \gtrsim \exp(-d_1 N \log(1/\varepsilon)) \end{aligned}$$

for a positive constant  $d_1$ . Therefore, for appropriate constants  $c_1, d_2 > 0$ ,

$$\Pi(B_{\text{KL}}(P_0; c_1 \varepsilon |\log \varepsilon|^2)) \gtrsim \tilde{\pi}_N(N(\mathbf{w}_N^0; \varepsilon)) \pi^{\otimes N}(B(\mathbf{y}_N^0; \varepsilon)) \gtrsim \exp(-d_2 N \log(1/\varepsilon)).$$

Set  $\xi := (c_1 \varepsilon)^{1/2} \log(1/\varepsilon)$ , since  $\log(1/\varepsilon) \leq \log(1/\xi)$ , we have  $\Pi(B_{\text{KL}}(P_0; \xi^2)) \geq \exp(-c_2 \log(1/\xi))$  for a real constant  $c_2 > 0$  (possibly depending on  $p_0$ ). Replacing  $\xi$  with  $\varepsilon_n$ , we get  $\Pi(B_{\text{KL}}(P_0; \varepsilon_n^2)) \geq \exp(-c_2 n \varepsilon_n^2)$  for sufficiently large  $n$ , and the proof is complete.  $\square$

Inspection of the proof of Lemma 1 reveals that, under the small ball prior probability estimate in (3), we have

$$E_0^n[\Pi_n(A_n^c | X^{(n)})] = O((n\varepsilon_n^2)^{-1}),$$

which implies that  $\Pi_n(A_n^c | X^{(n)})$  cannot converge to zero in  $P_0^n$ -probability any faster than  $(n\varepsilon_n^2)^{-1} \propto (L_n^2 \log n)^{-1}$ . The assertion of Lemma 1 can be enhanced to have

$$E_0^n[\Pi_n(A_n^c | X^{(n)})] = O(\exp(-B_1 n \varepsilon_n^2))$$

by employing a small ball prior probability estimate involving stronger divergences. The convergence in (4) then becomes almost-sure and, furthermore, due to the fact that the posterior probability vanishes exponentially fast, namely, along almost all simple sequences, for a finite constant  $B > 0$ , we have

$$\Pi_n(A_n^c | X^{(n)}) \leq \exp(-B n \varepsilon_n^2) \text{ for all but finitely many } n,$$

the stochastic order of the maximum absolute difference between  $F_0$  and the posterior expected distribution function can be assessed, see Corollary 1 below.

**Lemma 2.** *Under the conditions of Lemma 1, if the small ball prior probability estimate in (3) is replaced by*

$$\Pi_n(B_{\rho_\alpha}(P_0; \varepsilon_n^2)) \geq \exp(-C n \varepsilon_n^2), \text{ for } \alpha \in (0, 1], \quad (9)$$

then, for  $M_n \geq \sqrt{(C+1/2)L_n}$ ,

$$\Pi_n\left(\sqrt{n} \sup_x |(F_G - F_0)(x)| > M_n (\log n)^{1/2} | X^{(n)}\right) \rightarrow 0 \quad P_0^\infty\text{-almost surely.}$$

*Proof.* The proof is an adaptation of that of Lemma 1. We therefore only highlight the main changes. Taking a sequence  $K_n = \theta M_n$  for any  $\theta \in (0, 1)$ , we have

$$E_0^n[\Pi_n(A_n^c | X^{(n)}) \phi_n] \leq P_0^n \phi_n \leq 2 \exp(-2\theta^2 M_n^2 \log n)$$

and

$$E_0^n[\Pi_n(A_n^c | X^{(n)}) (1 - \phi_n) 1_{D_n^c}] \leq 2 \exp(-[2(1-\theta)^2 M_n^2 - (2C+1)L_n^2] \log n),$$

with

$$M_n > (1-\theta)^{-1} \sqrt{(C+1/2)L_n} \quad (10)$$

for every sufficiently large  $n$ . A straightforward extension of Lemma 2 in Shen and Wasserman (18), p. 691 (and pp. 709–710 for the proof), yields that, for every  $\xi \in (0, 1)$ ,

$$P_0^n(D_n \leq \xi \Pi_n(B_{\rho_\alpha}(P_0; \varepsilon_n^2))) \exp(-(C+1)n\varepsilon_n^2) \leq (1-\xi)^{-1} \exp(-\alpha C n \varepsilon_n^2). \quad (11)$$

Taking  $M_n = IL_n$  for a finite constant  $I > (1-\theta)^{-1} \sqrt{(C+1/2)}$  so that condition (10) is satisfied, by combining partial bounds we obtain that

$$E_0^n[\Pi_n(A_n^c | X^{(n)})] \lesssim \exp(-B_1 n \varepsilon_n^2)$$

for an appropriate finite constant  $B_1 > 0$ . We conclude that

$$P_0^n(\Pi_n(A_n^c | X^{(n)}) \geq \exp(-B n \varepsilon_n^2)) \lesssim \exp(-(B_1 - B)n \varepsilon_n^2).$$

Choose  $0 < B < B_1$ . Since  $\sum_{n=1}^{\infty} \exp(-(B_1 - B)n \varepsilon_n^2) < +\infty$ , almost sure convergence follows by the first Borel-Cantelli lemma.  $\square$

*Remark 1.* The assertion of Lemma 2 still holds if the small ball prior probability estimate in (9) is replaced by the requirement

$$\Pi_n(B_{\rho_{-1/2} \|\cdot\|_\infty}(P_0; \varepsilon_n^2)) \gtrsim \exp(-C n \varepsilon_n^2), \quad (12)$$

which involves a Hellinger type neighborhood of  $P_0$ . Then, a bound similar to that in (11) is given in Lemma 8.4 of Ghosal *et al.* (7), pp. 526–527.

As previously mentioned, Lemma 2 allows to derive the stochastic order of the maximum absolute difference between  $F_0$  and its Bayes' estimator

$$F_n^B(\cdot) := \int_{\mathcal{G}} F_G(\cdot) \Pi(dG | X^{(n)}),$$

namely, the posterior expected distribution function.

**Corollary 1.** *Under the conditions of Lemma 2,*

$$\sqrt{n} \sup_x |(F_n^B - F_0)(x)| = O_{\mathbf{P}}(M_n(\log n)^{1/2}).$$

*Proof.* By standard arguments,

$$\begin{aligned}
\sqrt{n} \sup_x |(F_n^B - F_0)(x)| &= \sqrt{n} \sup_x \left| \int_{\mathcal{G}} F_G(x) \Pi_n(dG | X^{(n)}) - F_0(x) \right| \\
&\leq \int_{\mathcal{G}} \sqrt{n} \sup_x |(F_G - F_0)(x)| \Pi_n(dG | X^{(n)}) \\
&= \left( \int_{A_n} + \int_{A_n^c} \right) \sqrt{n} \sup_x |(F_G - F_0)(x)| \Pi_n(dG | X^{(n)}) \\
&\leq M_n (\log n)^{1/2} + 2 \sqrt{n} \Pi_n(A_n^c | X^{(n)}) \\
&\lesssim M_n (\log n)^{1/2} \quad \text{for sufficiently large } n,
\end{aligned}$$

because condition (9) yields that, with probability one, for a finite constant  $B > 0$ , the posterior probability  $\sqrt{n} \Pi_n(A_n^c | X^{(n)}) \lesssim \sqrt{n} \exp(-Bn\varepsilon_n^2) \rightarrow 0$  for all but finitely many  $n$ . The assertion follows. This concludes the proof.  $\square$

### Posterior Concentration of the Mixing Distribution in Kantorovich Metric

In this section, we deal with the case where the prior distribution  $\Pi$  is supported over the collection of finite kernel mixtures with at most  $N$  components. Sufficient conditions are stated in Theorem 1 so that the posterior rate of convergence, relative to the Kantorovich or  $L^1$ -Wasserstein metric, for the mixing distribution of overfitted mixtures is, up to a slowly varying sequence, (at worst) equal to  $(n/\log n)^{-1/4}$ , the optimal rate being  $n^{-1/4}$ , cf. Chen (1), § 3, pp. 224–226.

In order to state the result, we introduce some more notation. We denote by  $k'(\cdot | y)$  the first partial derivative of the kernel  $k(\cdot | y)$  with respect to  $y$ ,

$$k'(\cdot | y) := \frac{\partial k(\cdot | y)}{\partial y}.$$

For clarity of exposition, we recall that  $F_0$  is the distribution function of the density  $p_0 \equiv p_{G_0}$  corresponding to the mixing distribution  $G_0$  having an *unknown* number of components  $d_0$ , *bounded* by a fixed integer  $N$ .

**Theorem 1.** *Under the conditions of Lemma 1, if, in addition,*

- a)  $\mathcal{Y}$  is compact,
- b)  $\{\int_{-\infty}^x k(u | y) du : y \in \mathcal{Y}\}$  is strongly identifiable in the sense of Definition 2 in Chen (1), p. 225,
- c)  $k'(\cdot | y)$  satisfies a uniform Lipschitz condition: there exist constants  $K' > 0$  and  $\beta > 0$  such that

$$|k'(\cdot | y_1) - k'(\cdot | y_2)| \leq K' |y_1 - y_2|^\beta \quad \text{for all } y_1, y_2 \in \mathcal{Y},$$

then, for  $M_n \gtrsim \sqrt{(C+1/2)L_n}$ ,

$$\Pi(n^{1/4} W_1(G, G_0) > \sqrt{M_n} (\log n)^{1/4} | X^{(n)}) = o_{\mathbf{P}}(1).$$

*Proof.* Since Lemma 1 holds, we have

$$\Pi\left(\sqrt{n}\sup_x|(F_G - F_0)(x)| > M_n(\log n)^{1/2} \mid X^{(n)}\right) = o_{\mathbf{P}}(1). \quad (13)$$

Consistently with the notation introduced in Lemma 1, we set

$$A_n := \left\{ G : \sqrt{n}\sup_x|(F_G - F_0)(x)| \leq M_n(\log n)^{1/2} \right\}.$$

Under assumptions *a)–c)*, Lemma 2 of Chen (1), p. 225 (see pp. 231–232 for the proof) holds true, this implying that, for every  $G \in A_n$ , the Kolmogorov distance between the distribution functions  $F_G$  and  $F_0$  is bounded below (up to a constant) by the squared  $L^1$ -distance between the mixing distributions  $G$  and  $G_0$ , respectively: there exists a constant  $C_0 > 0$  such that, for every  $G \in A_n$ ,

$$C_0\|G - G_0\|_1^2 \leq \sup_x|(F_G - F_0)(x)| \leq M_n n^{-1/2}(\log n)^{1/2}. \quad (14)$$

Taking into account the following representation of the  $L^1$ -Wasserstein distance

$$W_1(G, G_0) = \|G - G_0\|_1,$$

see, *e.g.*, Shorack and Wellner (19), pp. 64–66, which was obtained by Dall’Aglione (2), the assertion follows by combining (13) with (14). This concludes the proof.  $\square$

Some comments on the applicability and consequences of Theorem 1 are in order.

- Theorem 1, like Lemma 1, has its roots in Theorem 2 of Ishwaran *et al.* (10), p. 1324, which is tailored for finite Dirichlet mixtures. However, thanks to Proposition 1, which implies the conclusion of Lemma 1 meanwhile ensuring applicability to a larger family of prior distributions, under conditions *a)–c)*, the assertion that, for sufficiently large constant  $M > 0$ , the convergence

$$\Pi(n^{1/4}W_1(G, G_0) > M(\log n)^{1/4} \mid X^{(n)}) = o_{\mathbf{P}}(1)$$

takes place, still holds. The present result differs from that of Theorem 5 in Nguyen (13), pp. 383–384, under various respects: the latter, in fact, gives an assessment of posterior contraction in the  $L^2$ -Wasserstein, as opposed to the  $L^1$ -Wasserstein metric, for finite mixtures of multivariate distributions, under more stringent conditions and following a completely different line of reasoning.

- As previously observed on the occasion of the transition from Lemma 1 to Lemma 2, if the small ball prior probability estimate in (3) is replaced with either that in (9) or in (12), then the almost-sure version of Theorem 1

$$\Pi(n^{1/4}W_1(G, G_0) > \sqrt{M_n}(\log n)^{1/4} \mid X^{(n)}) \rightarrow 0 \quad P_0^\infty\text{-almost surely}$$

holds and the rate of convergence for the Bayes' estimator of the mixing distribution can be assessed as follows.

**Corollary 2.** *Under the conditions of Theorem 1, with the small ball prior probability estimate in (9), we have*

$$W_1(G_n^B, G_0) = O_{\mathbf{P}}(\sqrt{M_n}(n/\log n)^{-1/4}),$$

where  $G_n^B(\cdot) := \int_{\mathcal{G}} G(\cdot) \Pi(dG | X^{(n)})$  is the Bayes' estimator of the mixing distribution.

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