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# Efficient semiparametric estimation and model selection for multidimensional mixtures

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## Abstract

In this paper, we consider nonparametric multidimensional finite mixture models and we are interested in the semiparametric estimation of the population weights. Here, the i.i.d. observations are assumed to have at least three components which are independent given the population. We approximate the semiparametric model by projecting the conditional distributions on step functions associated to some partition. Our first main result is that if we refine the partition slowly enough, the associated sequence of maximum likelihood estimators of the weights is asymptotically efficient, and the posterior distribution of the weights, when using a Bayesian procedure, satisfies a semiparametric Bernstein von Mises theorem. We then propose a cross-validation like procedure to select the partition in a finite horizon. Our second main result is that the proposed procedure satisfies an oracle inequality. Numerical experiments on simulated data illustrate our theoretical results.

## 1 Introduction

We consider in this paper multidimensional mixture models that describe the probability distribution of a random vector  $X$  with at least three coordinates. The model is a probability mixture of  $k$  populations such that, given the population, the coordinates of the random vector are independently distributed. We call emission distributions the conditional distributions of the coordinates and  $\theta$  the parameter that contains the probability weights of each population. It has been known for some time that such a model is identifiable. An algebraic result by Kruskal [23] in 1977 (see also [27]) proved it when the coordinates of  $X$

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take finitely many values. Kruskal's result was recently used by [1] to obtain identifiability under almost no assumption on the possible emission distributions: only the fact that, for each coordinate, the  $k$  emission distributions are linearly independent. Spectral methods were proposed by [2], which allowed [10] to derive estimators of the emission densities having the minimax rate of convergence when the smoothness of the emission densities is known. Moreover, [11] proposes an estimation procedure in the case of repeated measurements (where the emission distributions of each coordinate given a population are the same).

Our paper focusses on the semiparametric estimation of the population weights when nothing is known about the emission distributions. This is a semiparametric model, where the finite dimensional parameter of interest is  $\theta$  and the infinite dimensional nuisance parameters are the emission distributions.

We are in particular interested in constructing optimal procedures for the estimation of  $\theta$ . Optimal may be understood as efficient, in Le Cam's theory point of view which is about asymptotic distribution and asymptotic (quadratic) loss. See [24], [8], [32], [33]. The first question is: is the parametric rate attainable in the semiparametric setting? We know here, for instance using spectral estimates, that the parametric rate is indeed attainable. Then, the loss due to the nuisance parameter may be seen in the efficient Fisher information and efficient estimators are asymptotically equivalent to the empirical process on efficient influence functions. The next question is thus: how can we construct asymptotically efficient estimators? In the parametric setting, maximum likelihood estimators (m.l.e.'s) do the job, but the semiparametric situation is more difficult, because one has to deal with the unknown nuisance parameter, see Theorems in chapter 24 of [32] where it is necessary to control various bias/approximation terms.

From a Bayesian perspective, the issue is the validity of the Bernstein-Von Mises property of the marginal posterior distribution of the parameter of interest  $\theta$ . In other words: is the marginal posterior distribution of  $\theta$  asymptotically Gaussian? Is it asymptotically centered around an efficient estimator? Is the asymptotic variance of the posterior distribution the inverse of the efficient Fisher information matrix? Semiparametric Bernstein-Von Mises theorems have been the subject of recent research, see [30], [12], [28], [15], [14], [9], [17] and [28].

The results of our paper are twofold: first we obtain asymptotically efficient semiparametric estimators using a likelihood strategy, then we propose a data driven method to perform the strategy in a finite horizon with an oracle inequality as theoretical guarantee.

Let us describe our ideas. For the multidimensional mixture model we consider, we will take advantage of the fact that, for some finite approximations of the nuisance parameter, the model is still valid for the observation process. This may be seen as a *no bias* situation. Indeed, when approximating the emission densities by step functions, the density of the observation is the multinomial distribution of the indicator function of the sets in the partition. Hence, this is a common and fairly crude modelling of densities by histograms. The no bias property of this modelling implies that, for each of these finite dimensional models, the parameter of interest, i.e. the weights of the mixture, may be efficiently estimated within the finite dimensional model. Then, under weak assumptions, and using the fact that one can approximate any density on  $[0, 1]$  by such histograms based on partitions with radius

(i.e. the size of the largest bin) going to zero, it is possible to prove that asymptotically efficient semiparametric estimators may be built using the sequence of m.l.es in a growing (with sample size) sequence of approximation models. In the same way, using Bayesian posteriors in the growing sequence of approximation models, one gets a Bernstein-Von Mises result. One of the important implications of the Bernstein von Mises property is that credible regions, such as highest posterior density regions or credible ellipses are also confidence regions. In the particular case of the semiparametric mixtures, this is of great interest, since the construction of a confidence region is not necessarily trivial. This is our first main result which is stated in Theorem 1: by considering partitions refined slowly enough when the number of observations increases, we can derive efficient estimation procedures for the parameter of interest  $\theta$  and in the Bayesian approach for a marginal posterior distribution on  $\theta$  which satisfies the renown Bernstein von Mises property.

We still need however in practice to choose a good partition, for a finite sample size. This can be viewed as a model selection problem. There is now a huge literature on model selection, both in the frequentist and in the Bayesian literature. Roughly speaking the methods can be split into two categories: penalized likelihood types of approaches, which include in particular AIC, BIC, MDL and marginal likelihood (Bayesian) criteria or approaches which consist in estimating the risk of the estimator in each model using for instance bootstrap or cross validation methods. In all these cases theory and practice are nowadays well grounded, see for instance [22], [29], [6], [25], [7], [5], [16], [3]. Most of the existing results above cover parametric or nonparametric models. Penalized likelihoods in particular target models which are best in terms of Kullback-Leibler divergences typically and therefore aim at estimating the whole nonparametric parameter. Risk estimation via bootstrap or cross-validation methods are more naturally defined in semiparametric (or more generally setups with nuisance parameters) models, however the theory remains quite limited in cases where the estimation strategy is strongly non linear as encountered here.

In our context, the natural risk for  $\theta$  is the quadratic risk, which can not be written as some risk of the distribution of the observations, which is the basic stone in the theory of model selection based on risk estimation. To propose specific procedures, one has thus to find some way to estimate the risk of the estimator in each approximation model, and then select the model with the smallest estimated risk. We propose to use a cross-validation method similar to the one proposed in [13]. To get theoretical results on such a strategy, the usual basic tool is to write the cross-validation criterion as a function of the empirical distribution which is not possible in our semiparametric setting. We thus divide the sample in non overlapping blocks of size  $a_n$  ( $n$  being the the sample size) to define the cross validation criterion. This enables us to prove our second main result: Theorem 2 which states an oracle inequality on the quadratic risk associated with a sample of size  $a_n$  observations, and which also leads to criterion to select  $a_n$ . Simulations indicate moreover that the approach behaves well in practice.

In Section 2, we first describe the model, set the notations and our basic assumptions. We recall the semiparametric tools in Section 2.2, where we define the score functions and the efficient information matrices. Using the fact that spectral estimators are smooth func-

tions of the empirical distribution of the observations, we obtain that, for large enough approximation model, the efficient Fisher information matrix is full rank, see Proposition 1. Intuition says that with better approximation spaces, more is known about all parameters of the distribution, in particular about  $\theta$ . We prove in Proposition 2 that indeed the efficient Fisher information matrix increases when the partition is refined. We are finally able to prove our main general result in Section 2.3. In Lemma 1, we first prove that semiparametric score functions and semiparametric efficient Fisher information matrix are the limits of the parametric ones obtained in the approximation parametric models. Thus, the fact that the semiparametric efficient Fisher information matrix is full rank is a consequence of previous results and stated in Proposition 3. In Theorem 1, we prove that it is possible to let the approximation parametric models grow with the sample size so that the sequence of maximum likelihood estimators are asymptotically efficient in the semiparametric model and so that a semiparametric Bernstein - von Mises Theorem holds. In Section 3, we first discuss in Section 3.1 the reasons to perform model selection and the fact that choosing a too large approximation space does not work, see Proposition 4 and Corollary 1. Then we propose in Section 3.2 our cross-validation criterion, for which we prove an oracle inequality in Theorem 2 and Proposition 5. Results of simulations are described in Section 4, we investigate several choices of the number and length of blocks for performing cross validation, and investigate practically also V-fold strategies. We discuss possible extensions, open questions and further work in Section 5. Finally Section 6 is dedicated to proofs of intermediate propositions and lemmas.

## 2 Asymptotic efficiency

### 2.1 Model and notations

Let  $(X_n)_{n \geq 1}$  be a sequence of independent and identically distributed random variables taking values in  $[0, 1]^3$ . We assume the possible marginal distribution of an observation  $X_n$ ,  $n \geq 1$  is a population mixture of  $k$  distributions such that, given the population, the coordinates are independent and have some density with respect to the Lebesgue measure on  $[0, 1]$ . The possible densities of  $X_n$ ,  $n \geq 1$ , are, if  $\mathbf{x} = (x_1, x_2, x_3) \in [0, 1]^3$ :

$$g_{\theta, \mathbf{f}}(\mathbf{x}) = \sum_{j=1}^k \theta_j \prod_{c=1}^3 f_{j,c}(x_c), \quad \sum_{j=1}^k \theta_j = 1, \quad \theta_j \geq 0, \quad \forall j \quad (1)$$

Here,  $k$  is the number of populations,  $\theta_j$  is the probability to belong to population  $j$  for  $j \leq k$  and we set  $\theta = (\theta_1, \dots, \theta_{k-1})$ . For each  $j = 1, \dots, k$ ,  $f_{j,c}$ ,  $c = 1, 2, 3$ , is the density of the  $c$ -th coordinate of the observation, given the observation coming from population  $j$  and we set  $\mathbf{f} = ((f_{j,c})_{1 \leq c \leq 3})_{1 \leq j \leq k}$ . We denote by  $\mathbb{P}^*$  the true (unknown) distribution of the sequence  $(X_n)_{n \geq 1}$ , such that  $\mathbb{P}^* = P_{\theta^*, \mathbf{f}^*}^{\otimes \mathbb{N}}$ ,  $dP_{\theta^*, \mathbf{f}^*}(\mathbf{x}) = g_{\theta^*, \mathbf{f}^*}(\mathbf{x}) d\mathbf{x}$ , for some  $\theta^* \in \Theta$  and  $\mathbf{f}^* \in \mathcal{F}^{3k}$ , where  $\Theta$  is the set of possible parameters  $\theta$  and  $\mathcal{F}$  the set of probability densities on  $[0, 1]$ .

We approximate the densities by step functions on some partitions of  $[0, 1]$ . We assume that we have a collection of partitions  $\mathcal{I}_M$ ,  $M \in \mathcal{M}$ ,  $\mathcal{M} \subset \mathbb{N}$ , so that for each  $M \in \mathcal{M}$ ,  $\mathcal{I}_M = (I_m)_{1 \leq m \leq M}$  is a partition of  $[0, 1]$  by borelian sets. It is clear that  $I_m$  changes when  $M$  changes. For each  $M \in \mathcal{M}$ , we now consider the model of possible densities

$$g_{\theta, \omega; M}(\mathbf{x}) = \sum_{j=1}^k \theta_j \prod_{c=1}^3 \left( \sum_{m=1}^M \frac{\omega_{j,c,m}}{|I_m|} \mathbb{1}_{I_m}(x_c) \right). \quad (2)$$

Here,  $\omega = ((\omega_{j,c,m})_{1 \leq m \leq M-1})_{1 \leq c \leq 3})_{1 \leq j \leq k}$ , and for each  $j = 1, \dots, k$ , each  $c = 1, 2, 3$ , each  $m = 1, \dots, M-1$ ,  $\omega_{j,c,m} \geq 0$ ,  $\sum_{m=1}^{M-1} \omega_{j,c,m} \leq 1$ , and we denote  $\omega_{j,c,M} = 1 - \sum_{m=1}^{M-1} \omega_{j,c,m}$ . Thus,  $\omega_{j,c,m}$  may be thought of as

$$\omega_{j,c,m} = \int_0^1 f_{j,c} \mathbb{1}_{I_m}(u) du.$$

We denote  $\Omega_M$  the set of possible parameters  $\omega$  when using model (2) with the partition  $\mathcal{I}_M$ .

Let  $\ell_n(\theta, \omega; M)$  be the log-likelihood using model (2), that is

$$\ell_n(\theta, \omega; M) = \sum_{i=1}^n \log g_{\theta, \omega; M}(X_i).$$

It appears as the model of population mixture of multinomial distributions for the observations  $Y_i := ((\mathbb{1}_{I_m}(X_{i,c}))_{1 \leq m \leq M})_{1 \leq c \leq 3}$ , for which the true (unknown) parameter is given by

$$\theta = \theta^*, \quad \omega = \omega_M^* := \left( \left( \left( \int_0^1 f_{j,c}^* \mathbb{1}_{I_m}(u) du \right)_{1 \leq m \leq M-1} \right)_{1 \leq c \leq 3} \right)_{1 \leq j \leq k}.$$

We denote, for each  $M \in \mathcal{M}$ ,  $(\hat{\theta}_M, \hat{\omega}_M)$  the m.l.e., that is a maximizer of  $\ell_n(\theta, \omega; M)$  over  $\Theta \times \Omega_M$ .

Let  $\Pi_M$  denote a prior distribution, that is a probability distribution on the parameter space  $\Theta \times \Omega_M$ . The posterior distribution  $\Pi_M(\cdot | X_1, \dots, X_n)$  is defined as follows. For any borelian subset  $A$  of  $\Theta \times \Omega_M$ ,

$$\Pi_M(A | X_1, \dots, X_n) = \frac{\int_A \prod_{i=1}^n g_{\theta, \omega; M}(X_i) d\Pi_M(\theta, \omega)}{\int_{\Theta \times \Omega_M} \prod_{i=1}^n g_{\theta, \omega; M}(X_i) d\Pi_M(\theta, \omega)}.$$

The first requirement to get consistency of estimators or posterior distributions is the identifiability of the model. We use the following assumption.

**Assumption (A1).**

- For all  $j = 1, \dots, k$ ,  $\theta_j^* > 0$ .
- For all  $c = 1, 2, 3$ , the measures  $f_{1,c}^* dx, \dots, f_{k,c}^* dx$  are linearly independent.

It is proved in Theorem 8 of [1] that under (A1) identifiability holds up to label switching, that is, if  $\mathcal{T}_k$  is the set of permutations of  $\{1, \dots, k\}$ ,

$$\forall \theta \in \Theta, \forall \mathbf{f} \in \mathcal{F}^{3k}, g_{\theta, \mathbf{f}} = g_{\theta^*, \mathbf{f}^*} \implies \exists \sigma \in \mathcal{T}_k \text{ such that } \sigma\theta = \theta^*, \sigma\mathbf{f} = \mathbf{f}^*,$$

where  $\sigma\theta \in \Theta$ ,  $\sigma\mathbf{f} \in \mathcal{F}^{3k}$  and  $\sigma\theta_j = \theta_{\sigma(j)}$ ,  $\sigma f_{j,c} = f_{\sigma(j),c}$ , for all  $c \in \{1, 2, 3\}$ ,  $j \in \{1, \dots, k\}$ . We need that identifiability holds for model (2) also. It is straightforward that this is the case if the partition is refined enough. For any partition  $M$ , any  $\omega = (\omega_m)_{1 \leq m \leq M-1}$  such that  $\omega_m \geq 0$ ,  $m = 1, \dots, M$ , with  $\omega_m = 1 - \sum_{m=1}^{M-1} \omega_m$ , denote  $f_\omega$  the step function given by

$$f_\omega(x) = \sum_{m=1}^M \frac{\omega_m}{|I_m|} \mathbb{1}_{I_m}(x). \quad (3)$$

Introduce the following assumption on the sequence of partitions  $\mathcal{I}_M$ ,  $M \in \mathcal{M}$ .

**Assumption (A2).**

- For all  $M$ , the sets  $I_m$  in  $\mathcal{I}_M$  are intervals with non empty interior.
- As  $M$  tends to infinity,  $\max_{1 \leq m \leq M} |I_m|$  tends to 0.

Assumption (A2) is used to get that all functions  $f_{\omega_{j,c;M}^*}$  tend to  $f_{j,c}^*$  Lebesgue almost everywhere. To extend the results when the coordinates  $x_c$  may be multivariate, the first point of (A2) has to be replaced by:

- There exists  $a > 0$  such that for all  $M$ , for all  $I_m$  in  $\mathcal{I}_M$ , there exists an open ball  $I$  such that  $I_m \subset I$  and  $|I_m| \geq a|I|$ . Here  $|I|$  is the Lebesgue measure of the set  $I$ .

Then, if (A1) and (A2) hold, for  $M$  large enough, we have that for all  $c = 1, 2, 3$ , the measures  $f_{\omega_{1,c;M}^*} dx, \dots, f_{\omega_{k,c;M}^*} dx$  are linearly independent, where

$$\omega_{j,c;M}^* := \left( \int_0^1 f_{j,c;M}^* \mathbb{1}_{I_m}(u) du \right)_{1 \leq m \leq M-1}, \quad c = 1, 2, 3, \quad j = 1, \dots, k.$$

We give a formal proof of this fact in Section 6.1. Thus, using again the identifiability result in [1], under (A1) and (A2), for  $M$  large enough,

$$\forall \theta \in \Theta, \forall \omega \in \Omega_M, g_{\theta, \omega;M} = g_{\theta^*, \omega_M^*;M} \implies \exists \sigma \in \mathcal{T}_k \text{ such that } \sigma\theta = \theta^*, \sigma\omega = \omega_M^*,$$

where  $\sigma\omega \in \Omega_M$  and  $\sigma\omega_{j,c,m} = \omega_{\sigma(j),c,m;M}$ , for all  $m \in \{1, \dots, M\}$ ,  $c \in \{1, 2, 3\}$ ,  $j \in \{1, \dots, k\}$ .

## 2.2 Efficient influence functions and information

We now study the estimation of  $\theta$  in model (1) and (2) from the semiparametric point of view, following Le-Cam's theory. We start with model (2) which is easier to analyze since it is a parametric model. For any  $M$ ,  $g_{\theta, \omega;M}(\mathbf{x})$  is a polynomial function of the parameter  $(\theta, \omega)$

and the model is differentiable in quadratic mean. Denote by  $S_M^* = (S_{\theta,M}^*, S_{\omega,M}^*)$  the score function for parameter  $(\theta, \omega)$  at point  $(\theta^*, \omega_M^*)$  in model (2). We have for  $j = 1, \dots, k-1$

$$(S_{\theta,M}^*)_j = \frac{\prod_{c=1}^3 f_{j,c;M}^* - \prod_{c=1}^3 f_{k,c;M}^*}{g_{\theta^*, \omega_M^*; M}} \quad (4)$$

and for  $j = 1, \dots, k, c = 1, 2, 3, m = 1, \dots, M-1$

$$(S_{\omega,M}^*)_{j,c,m} = \frac{\theta_j^* \left( \frac{\mathbb{1}_{I_m}(x_c)}{|I_m|} - \frac{\mathbb{1}_{I_M}(x_c)}{|I_M|} \right) \prod_{c' \neq c} f_{j,c';M}^*}{g_{\theta^*, \omega_M^*; M}} \quad (5)$$

Denote by  $J_M$  the Fisher information, that is the variance of  $S_M^*(X)$ :

$$J_M = \mathbb{E}^* [S_M^*(X) S_M^*(X)^T]$$

Here,  $\mathbb{E}^*$  denotes expectation under  $\mathbb{P}^*$ , and  $S_M^*(X)^T$  is the transpose vector of  $S_M^*(X)$ .

When considering the question of efficient estimation of  $\theta$  in the presence of a nuisance parameter, the relevant mathematical objects are the efficient influence function and the efficient Fisher information. Let us recall well known facts, see [32] or [33] for details. The efficient score function is the projection of the score function with respect to parameter  $\theta$  on the orthogonal subspace of the closure of the linear subspace spanned by the tangent set with respect to the nuisance parameter (that is the set of scores in parametric models regarding the nuisance parameter). The efficient Fisher information is the variance matrix of the efficient score function. For parametric models, direct computation gives the result. If we partition the Fisher information  $J_M$  according to the parameters  $\theta$  and  $\omega$ , that is

$$[J_M]_{\theta,\theta} = \mathbb{E}^* [S_{\theta,M}^*(X) S_{\theta,M}^*(X)^T], \quad [J_M]_{\omega,\omega} = \mathbb{E}^* [S_{\omega,M}^*(X) S_{\omega,M}^*(X)^T],$$

$$[J_M]_{\theta,\omega} = \mathbb{E}^* [S_{\theta,M}^*(X) S_{\omega,M}^*(X)^T], \quad [J_M]_{\omega,\theta} = [J_M]_{\theta,\omega}^T,$$

we get that, in model (2), if we denote  $\tilde{\psi}_M$  the efficient score function for the estimation of  $\theta$ ,

$$\tilde{\psi}_M = S_{\theta,M}^* - [J_M]_{\theta,\omega} ([J_M]_{\omega,\omega})^{-1} S_{\omega,M}^*,$$

and the efficient Fisher information  $\tilde{J}_M$  is

$$\tilde{J}_M = [J_M]_{\theta,\theta} - [J_M]_{\theta,\omega} ([J_M]_{\omega,\omega})^{-1} [J_M]_{\omega,\theta}^T.$$

To discuss efficiency of estimators, invertibility of the efficient Fisher information is needed. Spectral methods have been proposed recently to get estimators in model (2), see [2]. It is possible to obtain upper bounds of their local maximum quadratic risk with rate  $n^{-1/2}$ , which as a consequence excludes the possibility that the efficient Fisher information be singular. This is stated in Proposition 1 below and proved in Section 6.1.

**Proposition 1.** *Assume (A1) and (A2). Then, for large enough  $M$ ,  $\tilde{J}_M$  is non singular.*



In the context of mixture models, all asymptotic results are given up to label switching. We define here formally what we mean by ‘up to label switching’ for frequentist efficiency results with Equation (7) and Bayesian efficiency results with Equation (9).

Then, if (A1) and (A2) hold, for large enough  $M$   $\tilde{J}_M$  is non singular, and an estimator  $\hat{\theta}$  is asymptotically a regular efficient estimator of  $\theta^*$  if and only if

$$\sqrt{n} \left( \hat{\theta} - \theta^* \right) = \frac{\tilde{J}_M^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}_M(X_i) + o_{\mathbb{P}^*}(1), \quad \text{up to label switching,} \quad (6)$$

which formally means that there exists a sequence  $(\sigma_n)_n$  of  $\mathcal{T}_k$  such that

$$\sqrt{n} \left( \sigma_n \hat{\theta} - \theta^* \right) = \frac{\tilde{J}_M^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}_M(X_i) + o_{\mathbb{P}^*}(1). \quad (7)$$

To get an asymptotically regular efficient estimator, one may for instance apply a one step improvement (see Section 5.7 in [32]) of a preliminary spectral estimator, described in [2]. Also, using the trick given in [32] p. 63 to get consistency of the maximum likelihood estimator (m.l.e.), one sees also that the m.l.e.  $\hat{\theta}_M$  is asymptotically a regular efficient estimator of  $\theta^*$ .

In the Bayesian context, Bernstein-von Mises Theorem holds for large enough  $M$  if the prior has a positive density in the neighborhood of  $(\theta^*, \omega_M^*)$ , see Theorem 10.1 in [32]. That is, if  $\|\cdot\|_{TV}$  denotes the total variation distance, with  $\Pi_{M,\theta}$  the marginal distribution on the parameter  $\theta$ ,

$$\left\| \Pi_{M,\theta}(\cdot | X_1, \dots, X_n) - \mathcal{N} \left( \hat{\theta}; \frac{\tilde{J}_M^{-1}}{n} \right) \right\|_{TV} = o_{\mathbb{P}^*}(1), \quad \text{up to label switching,} \quad (8)$$

where  $\hat{\theta}$  verifies Equation (6), which formally means that

$$\sup_{A \subset \Theta} \left| \Pi_{M,\theta}(\exists \sigma \in \mathcal{T}_k : \sigma \theta \in A | X_1, \dots, X_n) - \mathcal{N} \left( \sigma_n \hat{\theta}; \frac{\tilde{J}_M^{-1}}{n} \right) (A) \right| = o_{\mathbb{P}^*}(1), \quad (9)$$

where  $(\sigma_n)$  and  $\hat{\theta}$  satisfy Equation (7).

A naive heuristic idea is that, when using the  $Y_i$ 's as summaries of the  $X_i$ 's, one has less information, but more and more if the partition  $\mathcal{I}_M$  is refined. Thus, efficient Fisher information should grow when partitions  $\mathcal{I}_M$  are refined. The following proposition is proved in Section 6.2.

**Proposition 2.** *Let  $\mathcal{I}_{M_1}$  be a coarser partition than  $\mathcal{I}_{M_2}$ , that is such that for any  $I \in \mathcal{I}_{M_1}$ , there exists  $A \subset \mathcal{I}_{M_2}$  such that  $I = \cup_{I' \in A} I'$ . Then*

$$\tilde{J}_{M_2} \geq \tilde{J}_{M_1}$$

in which “ $\geq$ ” denotes the partial order between symmetric matrices.

Thus, it is of interest to let the partitions grow so that one reaches the largest efficient Fisher information.

Let us now come back to model (1). Let, for  $j = 1, \dots, k$ ,  $c = 1, 2, 3$ ,  $\mathcal{H}_{j,c}$  be the subset of functions  $h$  in  $L^2(f_{j,c}^* dx)$  such that  $\int h f_{j,c}^* dx = 0$ . Then the tangent set for  $\mathbf{f}$  at point  $(\theta^*, \mathbf{f}^*)$  is the subspace  $\dot{\mathcal{P}}$  of  $L^2(g_{\theta^*, \mathbf{f}^*}(\mathbf{x}) d\mathbf{x})$  spanned by the functions

$$\mathbf{x} \mapsto \frac{h(x_c) \prod_{c'=1}^3 f_{j,c'}^*(x_{c'})}{g_{\theta^*, \mathbf{f}^*}(\mathbf{x})}, \quad h \in \mathcal{H}_{j,c}, \quad j = 1, \dots, k, \quad c = 1, 2, 3,$$

and the efficient score function  $\tilde{\psi}$  for the estimation of  $\theta$  in the semiparametric model (1) is given, for  $j = 1, \dots, k-1$ , by

$$\tilde{\psi}_j = (S_\theta^*)_j - \mathbb{A} (S_\theta^*)_j, \quad (S_\theta^*)_j = \frac{\prod_{c=1}^3 f_{j,c}^* - \prod_{c=1}^3 f_{k,c}^*}{g_{\theta^*, \mathbf{f}^*}}, \quad (10)$$

with  $\mathbb{A}$  the orthogonal projection onto the closure of  $\dot{\mathcal{P}}$  in  $L^2(g_{\theta^*, \mathbf{f}^*}(\mathbf{x}) d\mathbf{x})$ . Then, the efficient Fisher information  $\tilde{J}$  is the variance matrix of  $\tilde{\psi}$ .

If  $\tilde{J}$  is non singular, an estimator  $\hat{\theta}$  is asymptotically a regular efficient estimator of  $\theta^*$  if and only if

$$\sqrt{n} (\hat{\theta} - \theta^*) = \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i) + o_{\mathbb{P}^*}(1), \quad \text{up to label switching} \quad (11)$$

and a Bayesian method using a nonparametric prior  $\Pi$  satisfies a semiparametric Bernstein-von Mises Theorem if, with  $\Pi_\theta$  the marginal distribution on the parameter  $\theta$ ,

$$\left\| \Pi_\theta(\cdot | X_1, \dots, X_n) - \mathcal{N}\left(\hat{\theta}; \frac{\tilde{J}^{-1}}{n}\right) \right\|_{TV} = o_{\mathbb{P}^*}(1), \quad \text{up to label switching} \quad (12)$$

for a  $\hat{\theta}$  satisfying (11).

### 2.3 General result

When the sequence of models is a good approximation of model (1) by model (2), we expect that efficient score functions in (2) are good approximations of efficient score functions in (1) so that asymptotically efficient estimators in model (2) become efficient estimators in model (1). This is what Theorem 1 below states. The approximation assumption we shall use is the following.

**Assumption (A3).** *There exists  $\delta > 0$  such that for all  $\mathbf{x}$  in  $[0, 1]^3$ ,  $\delta \leq g_{\theta^*, \mathbf{f}^*}(\mathbf{x}) \leq 1/\delta$ , and*

$$\lim_{M \rightarrow +\infty} \|g_{\theta^*, \omega_M^*; M} - g_{\theta^*, \mathbf{f}^*}\|_\infty = 0.$$

Note that when (A2) is satisfied, (A3) holds true as soon as the functions  $f_{j,c}^*$ ,  $j = 1, \dots, k$ ,  $c = 1, 2, 3$ , are positive continuous functions.

We first obtain:

**Lemma 1.** *Under Assumptions (A1), (A2) and (A3), the sequence of score functions  $(\tilde{\psi}_M)_M$  converges in  $L^2(g_{\theta^*, \mathfrak{f}^*} d\mathbf{x})$  to the score function  $\tilde{\psi}$ , and the sequence of efficient Fisher informations  $(\tilde{J}_M)_M$  converges to the efficient Fisher information matrix  $\tilde{J}$ .*

Lemma 1 is proved in Section 6.3.

To get that  $\tilde{J}$  is invertible, it is enough that subsequences of approximation spaces are embedded. Introduce the following assumption.

**Assumption (A4).** *There exists a sequence  $(M_p)_{p \geq 1}$  such that for all  $p$ ,  $\mathcal{I}_{M_p}$  is a coarser partition than  $\mathcal{I}_{M_{p+1}}$*

The proof of the following proposition is straightforward using Lemma 1, Proposition 1 and Proposition 2.

**Proposition 3.** *Under Assumptions (A1), (A2), (A3) and (A4),  $\tilde{J}$  is non singular.*

We are now ready to state Theorem 1.

**Theorem 1.** *Under Assumptions (A1), (A2), (A3) and (A4), there exists a sequence  $M_n$  tending to infinity sufficiently slowly such that the m.l.e.  $\hat{\theta}_{M_n}$  is asymptotically a regular efficient estimator of  $\theta^*$  and satisfies*

$$\sqrt{n} \left( \hat{\theta}_{M_n} - \theta^* \right) = \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i) + o_{\mathbb{P}^*}(1), \quad \text{up to label switching.}$$

*Under the same assumptions and if for all  $M$ , the prior  $\Pi_M$  has a positive density in the neighborhood of  $(\theta^*, \omega_M^*)$ , then there exists a sequence  $L_n$  tending to infinity sufficiently slowly such that moreover*

$$\left\| \Pi_{L_n, \theta}(\cdot | X_1, \dots, X_n) - \mathcal{N} \left( \theta^* + \frac{\tilde{J}^{-1}}{n} \sum_{i=1}^n \tilde{\psi}(X_i); \frac{\tilde{J}^{-1}}{n} \right) \right\|_{TV} = o_{\mathbb{P}^*}(1), \quad \text{up to label switching.}$$

*Proof.* If  $\hat{\theta}_M$  is the m.l.e. when using model (2) with partition  $\mathcal{I}_M$  one has

$$\sqrt{n} \left( \sigma_{n,M} \hat{\theta}_M - \theta^* \right) = \frac{\tilde{J}_M^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}_M(X_i) + R_n(M)$$

where for each  $M$ ,  $(R_n(M))_{n \geq 1}$  is a sequence of random vectors converging to 0 in  $\mathbb{P}^*$ -probability as  $n$  tends to infinity. But then, there exists a sequence  $M_n$  tending to infinity sufficiently slowly so that, as  $n$  tends to infinity,  $R_n(M_n)$  tends to 0 in  $\mathbb{P}^*$ -probability. Now,

$$\begin{aligned} \frac{\tilde{J}_{M_n}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}_{M_n}(X_i) &= \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i) + \frac{\tilde{J}_{M_n}^{-1} - \tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i) + \frac{\tilde{J}_{M_n}^{-1}}{\sqrt{n}} \sum_{i=1}^n (\tilde{\psi}_{M_n} - \tilde{\psi})(X_i) \\ &= \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i) + o_{\mathbb{P}^*}(1) \end{aligned}$$

since, by Lemma 1,  $\mathbb{E}^* \left\| \frac{1}{\sqrt{n}} \sum_{i=1}^n (\tilde{\psi}_{M_n} - \tilde{\psi})(X_i) \right\|^2 = \|\tilde{\psi}_{M_n} - \tilde{\psi}\|_{L^2(g_{\theta^*, f^*}(\mathbf{x})d\mathbf{x})}^2$  tends to 0 as  $n$  tends to infinity and  $(\tilde{J}_{M_n})^{-1}$  converges to  $(\tilde{J})^{-1}$  as  $n$  tends to infinity, so that the first part of the theorem is proved.

On the Bayesian side, for all  $M$ , there exists a sequence  $V_n(M)$  of random vectors converging to 0 in  $\mathbb{P}^*$ -probability as  $n$  tends to infinity such that

$$\sup_{A \subset \Theta} \left| \Pi_{M, \theta}(\exists \sigma \in \mathcal{T}_k : \sigma \theta \in A | X_1, \dots, X_n) - \mathcal{N} \left( \sigma_{n, M} \hat{\theta}_M; \frac{\tilde{J}_M^{-1}}{n} \right) \right| = V_n(M).$$

Arguing as previously, there exists a sequence  $L_n$  tending to infinity sufficiently slowly so that, as  $n$  tends to infinity, both  $V_n(L_n)$  and  $R_n(L_n)$  tend to 0 in  $\mathbb{P}^*$ -probability. Using the fact that the total variation distance is invariant through one-to-one transformations we get

$$\begin{aligned} & \left\| \mathcal{N} \left( \sigma_{n, M} \hat{\theta}_M; \frac{\tilde{J}_M^{-1}}{n} \right) - \mathcal{N} \left( \theta^* + \frac{\tilde{J}^{-1}}{n} \sum_{i=1}^n \tilde{\psi}(X_i); \frac{\tilde{J}^{-1}}{n} \right) \right\|_{TV} \\ &= \left\| \mathcal{N} \left( \sqrt{n} (\sigma_{n, M} \hat{\theta}_M - \theta^*) - \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i); \tilde{J}_M^{-1} \right) - \mathcal{N} (0; \tilde{J}^{-1}) \right\|_{TV} \\ &= \left\| \mathcal{N} \left( \tilde{J}_M^{1/2} [\sqrt{n} (\sigma_{n, M} \hat{\theta}_M - \theta^*) - \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i)]; Id \right) - \mathcal{N} (0; \tilde{J}_M \tilde{J}^{-1}) \right\|_{TV} \\ &\leq \left\| \mathcal{N} \left( \tilde{J}_M^{1/2} [\sqrt{n} (\sigma_{n, M} \hat{\theta}_M - \theta^*) - \frac{\tilde{J}^{-1}}{\sqrt{n}} \sum_{i=1}^n \tilde{\psi}(X_i)]; Id \right) - \mathcal{N} (0; Id) \right\|_{TV} \\ &\quad + \left\| \mathcal{N} (0, Id) - \mathcal{N} (0; \tilde{J}_M \tilde{J}^{-1}) \right\|_{TV}. \end{aligned}$$

But for vectors in  $m \in \mathbb{R}^{k-1}$  and symmetric positive  $(k-1) \times (k-1)$  matrices  $\Sigma$  we have

$$\|\mathcal{N}(m, Id) - \mathcal{N}(0; Id)\|_{TV} \leq \|m\|$$

and

$$\begin{aligned} \|\mathcal{N}(0, Id) - \mathcal{N}(0; \Sigma)\|_{TV} &\leq \mathbb{P} \left( \|\Sigma^{1/2} U\|^2 - \|U\|^2 \geq \log[\det(\Sigma)] \right) \\ &\quad - \mathbb{P} \left( \|U\|^2 - \|\Sigma^{-1/2} U\|^2 \geq \log[\det(\Sigma)] \right) \end{aligned}$$

where  $U \sim \mathcal{N}(0, Id)$ . Thus the last part of the theorem follows from the triangular inequality and the fact that using Lemma 1, as  $n$  tends to infinity,  $\tilde{J}_{L_n} \tilde{J}^{-1}$  tends to  $Id$  and  $V_n(L_n)$  and  $R_n(L_n)$  tend to 0 in  $\mathbb{P}^*$ -probability.  $\square$

### 3 Model selection

In Theorem 1, we prove the existence of some increasing partition leading to efficiency. In this section, we propose a method to choose a partition when the number of observations  $n$  is fixed.

### 3.1 Reasons to do model selection

We first explain why the choice of the model is important. We have seen in Proposition 2 that for a sequence of increasing partitions, the efficient matrix is non decreasing. This suggests to choose the coarsest partition and thus  $M_n$  increasing as fast as possible. Yet, one needs to pay attention to the bias in a finite horizon (i.e. when the number of observations  $n$  is fixed). Note that in this model, we don't know any unbiased estimator of  $\theta$ . Besides, typically the bias of an estimator of  $\theta$  may increase when  $M$  increases. This prevents us to choose a sequence  $M_n$  tending to  $+\infty$  too quickly (see Corollary 1).

We now illustrate this issue using the m.l.e. If the m.l.e. is unbiased asymptotically, it is biased for a finite sample. In Proposition 4, we give the limit of the m.l.e. when the number  $n$  of observations is fixed but  $M$  tends to infinity.

**Proposition 4.** *For almost all observations  $X_1, \dots, X_n$ ,  $\hat{\theta}_M(X_1, \dots, X_n)$  tends to*

$$\underline{\theta}_n = \underbrace{(\lfloor n/k \rfloor / n, \dots, \lfloor n/k \rfloor / n)}_{r := n - k \lfloor n/k \rfloor}, \underbrace{(\lceil n/k \rceil / n, \dots, \lceil n/k \rceil / n)}_{k-r}$$

*up to label switching, when  $M$  tends to infinity.*

Proposition 4 is proved in Section 6.4.

Using Proposition 4, we can deduce a constraint (leading to an upper bound in some cases), depending on the considered sequence of partitions  $(\mathcal{I}_M)_{M \in \mathcal{M}}$ , on sequences  $M_n$  leading to efficiency. We believe that this constraint is very conservative and leads to very conservative bounds. Corollary 1 below is proved in Section 6.5.

**Corollary 1.** *Suppose Assumption (A3), if  $\hat{\theta}_{M_n}$  tends to  $\theta^*$  in probability, and  $\theta^*$  is different from  $(1/k, \dots, 1/k)$ ,*

*then there exists  $N > 0$  and a constant  $C > 0$  such that for all  $n \geq N$ ,*

$$n^2 \left( \max_{m \leq M_n} |I_m| \right)^2 M_n \geq C.$$

*Moreover, in the particular case where there exists  $0 < C_1 \leq C_2$  such that for all  $n \in \mathbb{N}$  and  $1 \leq m \leq M_n$ ,*

$$\frac{C_1}{M_n} \leq |I_m| \leq \frac{C_2}{M_n} \tag{13}$$

*then there exists a constant  $C > 0$  such that,*

$$M_n \leq Cn^2.$$

Note that Assumption (13) holds as soon as the partition is regular, so that in the two following cases:

- for the uniform partition, when  $\mathcal{M} = \mathbb{N}$  and for all  $M \in \mathcal{M}$   $I_m = [(m-1)/M, m/M)$  for all  $m < M$ ,  $I_M = [(M-1)/M, 1]$ ,
- or for the dyadic regular partitions, when  $\mathcal{M} = \{2^p, p \in \mathbb{N}^*\}$  and for all  $M \in \mathcal{M}$   $I_m = [(m-1)/M, m/M)$  for all  $m < M$ ,  $I_M = [(M-1)/M, 1]$ , which form an embedded sequence of partition.

### 3.2 Criterion for model selection

In this section, we propose a criterion to choose the partition when  $n$  is fixed. This criterion can be used to choose the size  $M$  of a family of partitions but also to choose between two families of partition. With a dataset, we can compute the m.l.e. (with the EM algorithm) when using model (2) with partition  $\mathcal{I}$ , or we can get an estimator of  $\theta$  using its posterior distribution (the posterior mean or the posterior median for instance). We thus shall index all our estimators by  $\mathcal{I}$ . Note that the results of this section are valid for any family of estimators ( $\tilde{\theta}_{\mathcal{I}}$ ) and not only for the m.l.e.

Proposition 4 and Corollary 1 show the necessity to choose an appropriate partition among a collection of partitions  $\mathcal{I}_M$ ,  $M \in \mathcal{M}$ . To choose the partition we need a criterion. Since the aim is to get efficient estimators, we choose the quadratic risk as the criterion to minimize. We thus want to minimize over all possible partitions

$$R_n(\mathcal{I}) = \mathbb{E}^* \left[ \|\tilde{\theta}_{\mathcal{I}}(X_{1:n}) - \theta^*\|_{\mathcal{T}_k}^2 \right], \quad (14)$$

where  $X_{1:n} = (X_i)_{i \leq n}$  and for all  $\theta, \tilde{\theta} \in \Theta$ ,

$$\|\theta - \tilde{\theta}\|_{\mathcal{T}_k} = \min_{\sigma \in \mathcal{T}_k} \|\sigma\theta - \tilde{\theta}\|_2 = \|\circ\theta - \circ\tilde{\theta}\|_2, \quad (15)$$

with  $\circ\theta = \sigma\theta$  for a permutation  $\sigma \in \mathcal{T}_k$  which orders the components of  $\sigma\theta$ , i.e. such that  $\sigma\theta_1 \leq \dots \leq \sigma\theta_k$ . As usual, this criterion cannot be computed in practice (since we do not know  $\theta^*$ ). To do this on data we need for each partition  $\mathcal{I}$  some estimator  $C(\mathcal{I})$  of  $R_n(\mathcal{I})$ . We want to emphasize here that the choice of the criterion for this problem is not easy. Indeed, the quadratic risk  $R_n(\mathcal{I})$  cannot be written as the expectation of an excess loss expressed thanks to a contrast function, i.e. in the form  $\mathbb{E}^* \left[ \mathbb{E}^* \left[ \gamma(\tilde{\theta}(X_{1:n}), X) - \gamma(\theta^*, X) | X_{1:n} \right] \right]$ , where  $\gamma : \Theta \times \mathcal{X} \rightarrow [0, +\infty)$ . Yet, the last framework is the framework of most theoretical results in model selection, see [5] or [25] for instance. Moreover the quadratic risk has not a usual behaviour. Indeed if we decompose it as an approximation error plus an estimation error as explained in [5]:

$$R_n(\mathcal{I}) = \underbrace{\inf_{\theta \in \Theta_{\mathcal{I}}} \|\theta - \theta^*\|_{\mathcal{T}_k}^2}_{\text{approximation error}} + \underbrace{R_n(\mathcal{I}) - \inf_{\theta \in \Theta_{\mathcal{I}}} \|\theta - \theta^*\|_{\mathcal{T}_k}^2}_{\text{estimation error}}, \quad \text{where } \Theta_{\mathcal{I}} = \Theta,$$

we see that the approximation error is always zero in our model (and not decreasing as often). For these reasons, we cannot apply the usual methods and we use instead a variant of usual cross validation technique.

Consider a partition of  $\{1, \dots, n\}$  in the form  $(B_b, B_{-b}, b \leq b_n)$ , in other words the partition is made of  $2 \times b_n$  subsets of  $\{1, \dots, n\}$ . By definition  $B_{b_1} \cap B_{-b_2} = \emptyset$  for all  $b_1, b_2 \leq b_n$ . Because the maximum likelihood estimator based on any finite sample size is not unbiased, the following naive estimator of the risk is not appropriate:

$$C_{CV1}(\mathcal{I}) = \frac{1}{2b_n} \sum_{b=1}^{b_n} \|\tilde{\theta}_{\mathcal{I}}(X_{B_b}) - \tilde{\theta}_{\mathcal{I}}(X_{B_{-b}})\|_{\mathcal{T}_k}^2.$$

Indeed, using Proposition 4,  $C_{CV1}(\mathcal{I})$  is tending to 0 when  $\max_m |I_m|$  tends to 0. So that minimizing this criterion leads to choosing a partition  $\hat{\mathcal{I}}_n \in \arg \min_{\mathcal{I}} C_{CV1}(\mathcal{I})$  which has a large number of sets and so  $\hat{\theta}_{\hat{\mathcal{I}}_n}(X_{1:n})$  may be close to  $(1/k, \dots, 1/k)$  and then may not even be consistent. This can be seen when decomposing the risk  $R_n(\mathcal{I})$  as:

$$R_n(\mathcal{I}) = \underbrace{\text{Var}^* \left[ \overset{o}{\tilde{\theta}}_{\mathcal{I}}(X_{1:n}) \right]}_{\text{variance}} + \underbrace{\left\| \mathbb{E}^* \left[ \overset{o}{\tilde{\theta}}_{\mathcal{I}}(X_{1:n}) \right] - \theta^* \right\|_{\mathcal{T}_k}^2}_{\text{bias}} \quad (16)$$

and computing the expectation of  $C_{CV1}(\mathcal{I})$  in the case where the sizes of  $B_b, B_{-b}, b \leq b_n$ , are all equal,

$$\mathbb{E}^* [C_{CV1}(\mathcal{I})] = \text{Var}^* \left[ \overset{o}{\tilde{\theta}}_{\mathcal{I}}(X_{B_b}) \right]$$

suggests that  $C_{CV1}(\mathcal{I})$  does not estimate the bias of Equation (16). As an illustration, see Figure 2 where the trends of  $R_n(\mathcal{I})$ ,  $\text{Var}^* \left[ \overset{o}{\hat{\theta}}_{\mathcal{I}}(X_{1:n}) \right]$  and  $\left\| \mathbb{E}^* \left[ \overset{o}{\hat{\theta}}_{\mathcal{I}}(X_{1:n}) \right] - \theta^* \right\|_{\mathcal{T}_k}^2$  respectively are plotted.

To address the bad behaviour of  $C_{CV1}(\mathcal{I})$ , we use an idea of [13]. Choose a (fixed) base partition  $\mathcal{I}_0$  (for which the criterion may also be computed) which is believed to be (almost) unbiased. And set

$$C_{CV}(\mathcal{I}) = \frac{1}{b_n} \sum_{b=1}^{b_n} \left\| \overset{o}{\tilde{\theta}}_{\mathcal{I}}(X_{B_b}) - \overset{o}{\tilde{\theta}}_{\mathcal{I}_0}(X_{B_{-b}}) \right\|_{\mathcal{T}_k}^2.$$

Equivalently, we could choose any unbiased estimator  $\tilde{\theta}$  instead of using an estimator  $\theta_{\mathcal{I}_0}$  of the considered family of estimator. Figure 3 gives an idea of the behaviour of  $C_{CV}$  and  $C_{CV1}$  using the m.l.e.. It shows in particular that in our simulation study  $C_{CV}$  follows the same behaviour as  $R_n(\mathcal{I})$ , contrarywise to  $C_{CV1}$ . More details are provided in Section 4.

We now provide some theoretical results on the behaviour of the minimizer of  $C_{CV}(\cdot)$  over a finite family of candidate partitions  $\mathcal{M}_n$  compared to the minimizer of  $R_{a_n}(\cdot)$  over the same family.

Let  $m_n = \#\mathcal{M}_n$  be number of candidate partitions.

To do so we consider the following set of assumptions:

**Assumption (A5).**

(A5.1)  $B_b, B_{-b}, b \leq b_n$  are disjoint sets of equal size

$$\#B_b = \#B_{-b} = a_n, \quad \text{for all } b \leq b_n$$

(A5.2)  $\tilde{\theta}_{\mathcal{I}_0, b, 2}$  is not biased i.e.  $\mathbb{E}^*[\tilde{\theta}_{\mathcal{I}_0, b, 2}] = \theta^*$ ,

we obtain the following oracle inequality.

**Theorem 2.** *Suppose Assumption (A5). For any sequences  $0 < \epsilon_n, \delta_n < 1$ , with probability greater than*

$$1 - 2m_n \exp \left( -2b_n \left( \epsilon_n \inf_{\mathcal{I} \in \mathcal{M}_n} R_{a_n}(\mathcal{I}) + \delta_n \right)^2 \right),$$

we have

$$R_{a_n}(\widehat{\mathcal{I}}_n) \leq \frac{1 + \epsilon_n}{1 - \epsilon_n} \inf_{\mathcal{I} \in \mathcal{M}_n} R_{a_n}(\mathcal{I}) + \frac{2\delta_n}{1 - \epsilon_n}, \quad (17)$$

where  $\widehat{\mathcal{I}}_n \in \arg \min_{\mathcal{I} \in \mathcal{M}_n} C_{CV}(\mathcal{I})$ .

As a consequence of Theorem 2, the following Proposition holds. Recall that  $n = 2b_n a_n$ .

**Proposition 5.** *Assume (A5). If  $b_n \gtrsim n^{2/3} \log^2(n)$ ,  $a_n \lesssim n^{1/3}/(\log^2(n))$ , and  $m_n \leq C_\alpha n^\alpha$ , for some  $C_\alpha > 0$  and  $\alpha \geq 0$ , then*

$$\mathbb{E}^* \left[ a_n R_{a_n}(\widehat{\mathcal{I}}_n) \right] \leq \inf_{\mathcal{I} \in \mathcal{M}_n} a_n R_{a_n}(\mathcal{I}) + o(1),$$

where  $\widehat{\mathcal{I}}_n \in \arg \min_{\mathcal{I} \in \mathcal{M}_n} C_{CV}(\mathcal{I})$ .

Note that for each  $\mathcal{I}$ ,  $R_{a_n}(\mathcal{I})$  is of order of magnitude  $1/a_n$  so that the remaining term is indeed small regarding the main term. Note also that this is an exact oracle inequality (with constant 1).

In Theorem 2 and Proposition 5,  $\widehat{\mathcal{I}}_n$  is built with  $n$  observations while the risk is associated with  $a_n < n$  observations. This leads to a conservative choice of  $\widehat{\mathcal{I}}_n$ , i.e. we may choose a sequence  $\widehat{\mathcal{I}}_n$  (optimal with  $a_n$  observations) increasing more slowly than the optimal one (with  $n$  observation). We think however that this conservative choice should not change the good behaviour of  $\widehat{\theta}_{\widehat{\mathcal{I}}_n}$ , since Theorem 1 implies that any sequence of partitions which grows slowly enough to infinity leads to an efficient estimator. Hence, once the sequence  $M_n$  growing to infinity is chosen, then any other sequence growing to infinity more slowly also leads to an efficient estimator.

In Proposition 5 and Theorem 2, the reference point estimate  $\tilde{\theta}_{\mathcal{I}_0}(X_{B_{-b}})$  is assumed to be unbiased. This is a strong assumption, which is not exactly satisfied in our simulation study. To consider a reasonable approximation of it,  $\tilde{\theta}_{\mathcal{I}_0}(X_{B_{-b}})$  is chosen as the m.l.e. associated to a partition with a small number of bins. The heuristic behind this choice is that the maximum likelihood is asymptotically unbiased and a small number of bins implies a smaller number of parameters to estimate, so that the asymptotic regime is attained faster. Our simulations confirm this heuristic, see Section 4.

## 4 Simulations

In this section, we illustrate the results obtained in Sections 3.1 and 3.2 with simulations. We compare six criteria for the model selection based on  $C_{CV}$  with different choices of size of training and testing sets. We choose the regular embedded dyadic partitions, i.e. when  $\mathcal{M} = \{2^p, p \in \mathbb{N}^*\}$  and for all  $M \in \mathcal{M}$ ,  $I_m = [(m-1)/M, m/M)$  for all  $m < M$ ,  $I_M = [(M-1)/M, 1]$ . Following Corollary 1, when  $n$  is fixed, we only consider  $M = 2^P \leq M_n = n^3$  (i.e.  $P \leq P_n := \lfloor 3/2 \log(n) \rfloor$ ). In this part, we only consider m.l.e. estimators with ordered components and approximated thanks to the EM algorithm.

For  $n$  fixed, the choice of the model, through  $P$ , is done thanks to the criterion  $C_{CV}$  with two types of choice for  $(B_b), (B_{-b})$ . First, we use the framework under which we were able



to prove something, i.e. Assumption (A5.1) where all the training and testing sets are disjoint. We use different sizes  $a_n$  and  $b_n$ :

- $b_n = \lceil n^{2/3} \log(n)/(20) \rceil$  and  $a_n = \lfloor n/(2b_n) \rfloor$  (Assumption of Proposition 5, up to  $\log(n)$ ), leading to the criterion  $C_{CV}^{D,1}$  and the choice of  $P$  noted  $\hat{P}_n^{D,1} \in \arg \min_{P \leq P_n} C_{CV}^{D,1}(\mathcal{I}_{2^P})$ ,
- $b_n = \lceil n^{1/3} \rceil$ ,  $a_n = \lfloor n/(2b_n) \rfloor$ , leading to the criterion  $C_{CV}^{D,2}$  and the choice of  $P$  noted  $\hat{P}_n^{D,2} \in \arg \min_{P \leq P_n} C_{CV}^{D,2}(\mathcal{I}_{2^P})$ ,
- $a_n = \lfloor n/10 \rfloor$ ,  $b_n = \lfloor n/(2a_n) \rfloor$ , leading to the criterion  $C_{CV}^{D,3}$  and the choice of  $P$  noted  $\hat{P}_n^{D,3} \in \arg \min_{P \leq P_n} C_{CV}^{D,3}(\mathcal{I}_{2^P})$

We also consider the famous V-fold, where the dataset is cut into  $b_n$  disjoint sets  $\tilde{B}_b$  of size  $a_n$ , leading to training sets  $B_b = \tilde{B}_b$  and testing sets  $B_{-b} = \{1, \dots, n\} \setminus \tilde{B}_b$ . We also use different sizes  $a_n$  and  $b_n$ :

- $a_n = \lfloor n^{1/3} \rfloor$ ,  $b_n = \lfloor n/a_n \rfloor$ , leading to the criterion  $C_{CV}^{V,1}$  and the choice of  $P$  noted  $\hat{P}_n^{V,1} \in \arg \min_{P \leq P_n} C_{CV}^{V,1}(\mathcal{I}_{2^P})$ ,
- $a_n = \lfloor n^{2/3}/2 \rfloor$ ,  $b_n = \lfloor n/a_n \rfloor$ , leading to the criterion  $C_{CV}^{V,2}$  and the choice of  $P$  noted  $\hat{P}_n^{V,2} \in \arg \min_{P \leq P_n} C_{CV}^{V,2}(\mathcal{I}_{2^P})$ ,
- $a_n = \lfloor n/10 \rfloor$ ,  $b_n = \lfloor n/a_n \rfloor$ , leading to the criterion  $C_{CV}^{V,3}$  and the choice of  $P$  noted  $\hat{P}_n^{V,3} \in \arg \min_{P \leq P_n} C_{CV}^{V,3}(\mathcal{I}_{2^P})$ .

Note that for criteria

- $C_{CV}^{j,1}$ ,  $j \in \{D, V\}$ ,  $a_n$  is proportional to  $n^{1/3}$  up to a logarithm term,
- $C_{CV}^{j,2}$ ,  $j \in \{D, V\}$ ,  $a_n$  is proportional to  $n^{2/3}$ ,
- $C_{CV}^{j,3}$ ,  $j \in \{D, V\}$ ,  $a_n$  is proportional to  $n$ .

We know explain how we choose  $\mathcal{I}_0$ . We do not know any unbiased estimate of  $\theta$ , which would match the Assumption (A5.2). Particularly the m.l.e.  $\hat{\theta}_M$  is unbiased asymptotically but biased with finite  $n$ . We propose to choose a m.l.e.  $\hat{\theta}_{M_0}$  with a small  $M_0$  with the idea that when  $M$  is small the asymptotic is attained more quickly. Yet,  $M_0$  should not be taken too small neither since otherwise the model would not be identifiable. We propose to choose the smallest  $M_0 = 2^{P_0}$  such that  $M_0 \geq k + 2$  (equivalently  $P_0 \geq \log(k + 2)/\log(2)$ ). This lower bound ensures that generically on  $\mathcal{I}_0$  the model (2) is identifiable.

In the simulation part, we work in the repeated setting, that is  $f_{j,1}^* = f_{j,2}^* = f_{j,3}^*$  and we assume that we know it, i.e. when we search for the m.l.e. in the model (2) associated to  $M \in \mathcal{M}$ , we only search for  $\theta \in \Delta_k$ ,  $\omega \in \Delta_M^k$  (and not  $\omega \in \Delta_M^{3k}$ ) assuming that  $\omega_{j,1,m} = \omega_{j,2,m} = \omega_{j,3,m} = \omega_{j,m}$ . We first use three different true parameters for the simulations, in easy situations. In the three cases,  $k = 2$  and the other parameters are given in Table 1. So that, we work with  $P_0 = 2$  and  $M_0 = 2^2 = 4$ .

The different emission distributions are represented in Figure 1.

Simu.	$k$	$p^*$	$f_{1,1}^*d\lambda = f_{1,2}^*d\lambda = f_{1,3}^*d\lambda$	$f_{2,1}^*d\lambda = f_{2,2}^*d\lambda = f_{2,3}^*d\lambda$
1	2	(0.3, 0.7)	$\mathcal{N}(4/5, 0.07^2)$ truncated to $[0, 1]$	$\mathcal{N}(1/3, 0.1^2)$ truncated to $[0, 1]$
2	2	(0.2, 0.8)	$\mathcal{U}((0, 1))$	$\mathcal{N}(2/3, 0.05^2)$ truncated to $[0, 1]$
3	2	(0.3, 0.7)	$\beta(1, 2)$	$\beta(5, 3)$

Table 1: Values of the true parameters for simulation 1 to 3

Figure 2 gives a taste of the trend of the risk  $R_n(\mathcal{I}_{2^P})$ , along with the variance  $Var^* \left[ \hat{\theta}_{2^P}(X_{1:n}) \right]$

and the squared bias  $\left\| \mathbb{E}^* \left[ \hat{\theta}_{2^P}(X_{1:n}) \right] - \theta^* \right\|_{\mathcal{T}_k}^2$  defined in Equation (16) when  $P$  increases.

We illustrate these trends thanks to different true parameters and numbers of observations  $n$ . The different risks, bias and variances are estimated by Monte Carlo by repeating 1000 times the estimation of  $\theta$  with the m.l.e. (approximated with the EM algorithm). A typical behaviour of the bias is being constant or decreasing, with small increasing values of  $P$ , then increasing a lot when  $P$  increases, and finally stabilizing to the value  $\|\underline{\theta}_n - \theta^*\|$ , which is a consequence of Proposition 4. Typically, the variance is constant or decreasing for small increasing values of  $P$ , sometimes it then increases, before decreasing to zero (which also is a consequence of Proposition 4) when  $P$  gets large. Then, the risk, which is the sum of the squared bias and the variance, is usually constant or decreasing for small increasing values of  $P$  and then increasing to  $\|\underline{\theta}_n - \theta^*\|^2$  when  $P$  gets large.

Now we have an idea of the behaviour of the risk  $R_n(\mathcal{I}_{2^P})$ , we can check the behaviour of the different criteria  $C_{CV}$  and  $C_{CV1}$ . Figure 3 gives an idea of the pattern of some criteria for one sequence of observations  $X_{1:n}$ , distributed from two different true parameters, with respect to  $P$ . We do not show all the criteria since they all look alike. Moreover the purpose of figure 3 is to illustrate the ‘bad’ behaviour of  $C_{CV1}$  compared to  $C_{CV}$  and not comparing the six criteria (which would anyway be impossible with one sequence of observations  $X_{1:n}$ ). Note that we do not compare the values but the behaviour. Indeed, the criteria are used to choose the best  $P$  by taking the minimum of the criterion so that the values are not important by themselves. Besides, we know that the criterion  $C_{CV}$  is biased by a constant depending on  $\mathcal{I}_0$ . As theoretically explained in Section 3 and as a consequence of Proposition 4, we can see that the criteria  $C_{CV1}$  are tending to 0 when  $P$  increases while it is not the case for the criteria  $C_{CV}$ . Looking at Figure 3, the behaviour of  $C_{CV}$  seems to be correct, we precise this impression with table 2.

Finally we compare the six criteria  $C_{CV}^{j,c}$ ,  $j \in \{D, V\}$ ,  $c \in \{1, 2, 3\}$ , by estimating the squared risk of the associated estimator  $\hat{\theta}_{2^{\hat{P}_n}^{j,c}}$ , presented in Table 2. Different sizes  $n$  of samples and different true parameters are used to simulate the data. We can compare the six squared risk to  $\sqrt{\min_{P \leq P_n} R_n(2^P)}$  and  $\sqrt{R_n(2^{P_0})}$ . The different risks are estimated by Monte Carlo by repeating 100 times the estimation. The differences of performance between the different criteria are not obvious. Besides, the performances of all the criteria are satisfactory, compared to  $\sqrt{\min_{P \leq P_n} R_n(2^P)}$ . Yet, we suggest not to use criterion  $C_{CV}^{V,1}$  because it is longer than the others, particularly when  $n$  is large (because of large  $b_n$ ). Furthermore, there is a little advantage to criteria  $C_{CV}^{D,1}$  and  $C_{CV}^{V,2}$ .

These results confirm that by using  $M_0$  small, the criterion behaves correctly. Moreover,

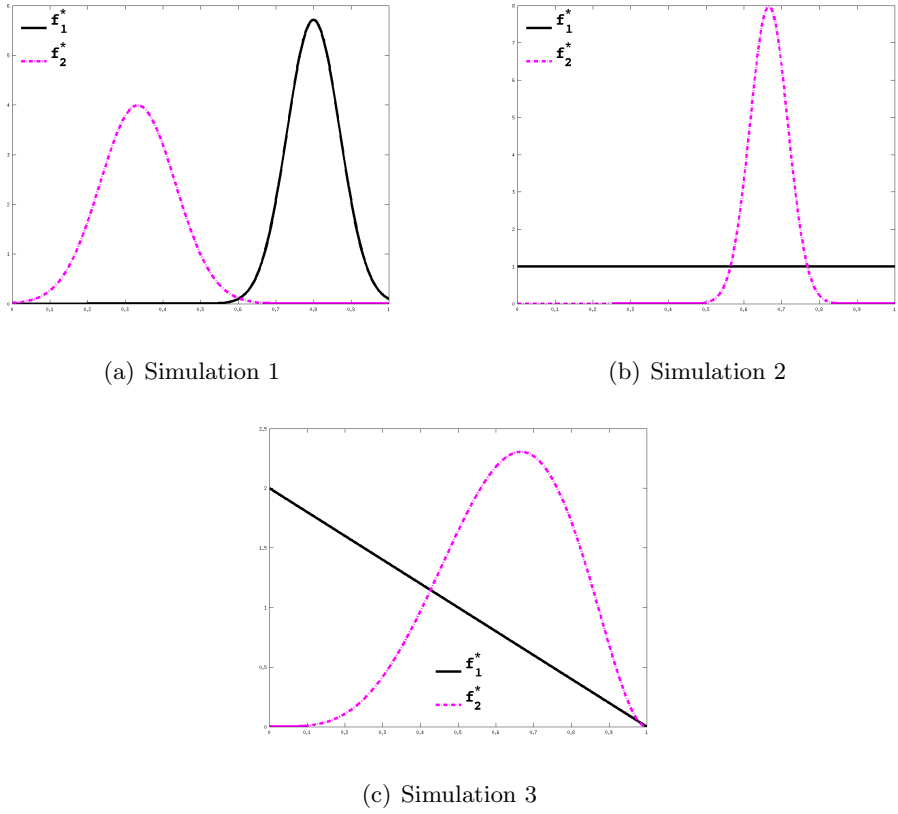
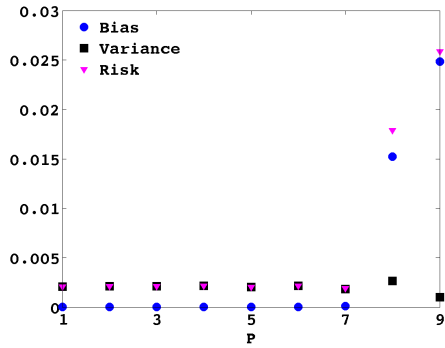


Figure 1: Representation of the true emission distributions for simulations 1, 2 and 3.

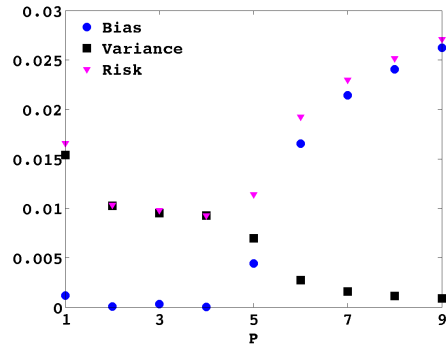
the fact that the choice of  $\hat{I}_n$  corresponds to a risk associated with  $a_n < n$  observations does not seem to be a conservative choice even in a finite horizon (i.e. when  $n$  is fixed). We were expecting this behaviour asymptotically but not in a finite horizon.

## 5 Discussion

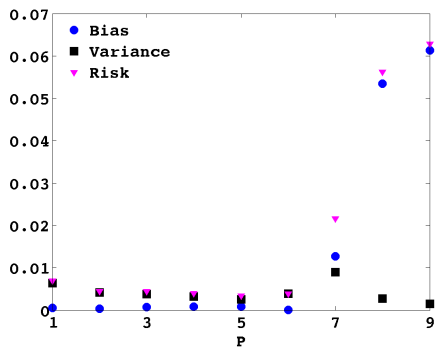
Finite mixture models all have the property that, when the approximation space for the emission distributions is that of step functions (histograms), then the model stays true for observation process. Thus there is no approximation bias regarding the parameter that describes the probability distribution of the latent variables. Extension of the results we obtain in this paper should be possible to other nonparametric finite mixture models. This should also be the case for nonparametric hidden Markov models with translated emission distributions studied in [21] or for general nonparametric finite state space hidden Markov models studied in [18], [34] and [19]. Here, the parameter describing the probability distribution of the latent variable is the transition matrix of the hidden Markov chain. However, semiparametric asymptotic theory for dependent observations is much more involved, see [26] for the ground principles. It seems difficult to identify the score functions and the



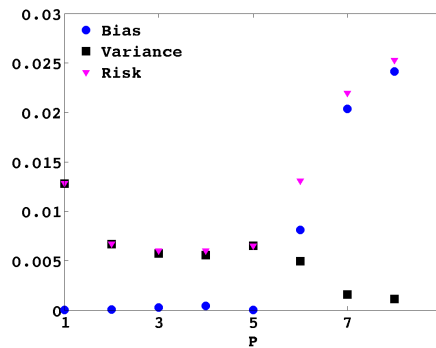
(a) Simulation 1,  $n = 100$



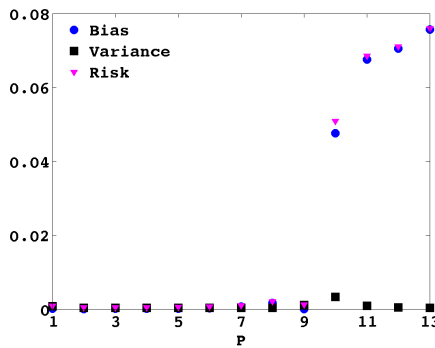
(b) Simulation 3,  $n = 50$



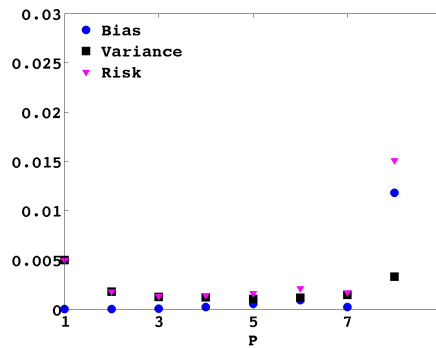
(c) Simulation 2,  $n = 50$



(d) Simulation 3,  $n = 100$



(e) Simulation 2,  $n = 500$



(f) Simulation 3,  $n = 500$

Figure 2: Patterns of the risk (with black squares), the squared bias (with blue dots) and variance (with magenta triangles) with respect to  $P = \log(M)/\log(2)$  for simulations 1, 2 and 3 and different values of  $n$ .

efficient Fisher information matrices for hidden Markov models even in the parametric approximation model, so that to get results such as Theorem 1 could be quite challenging.

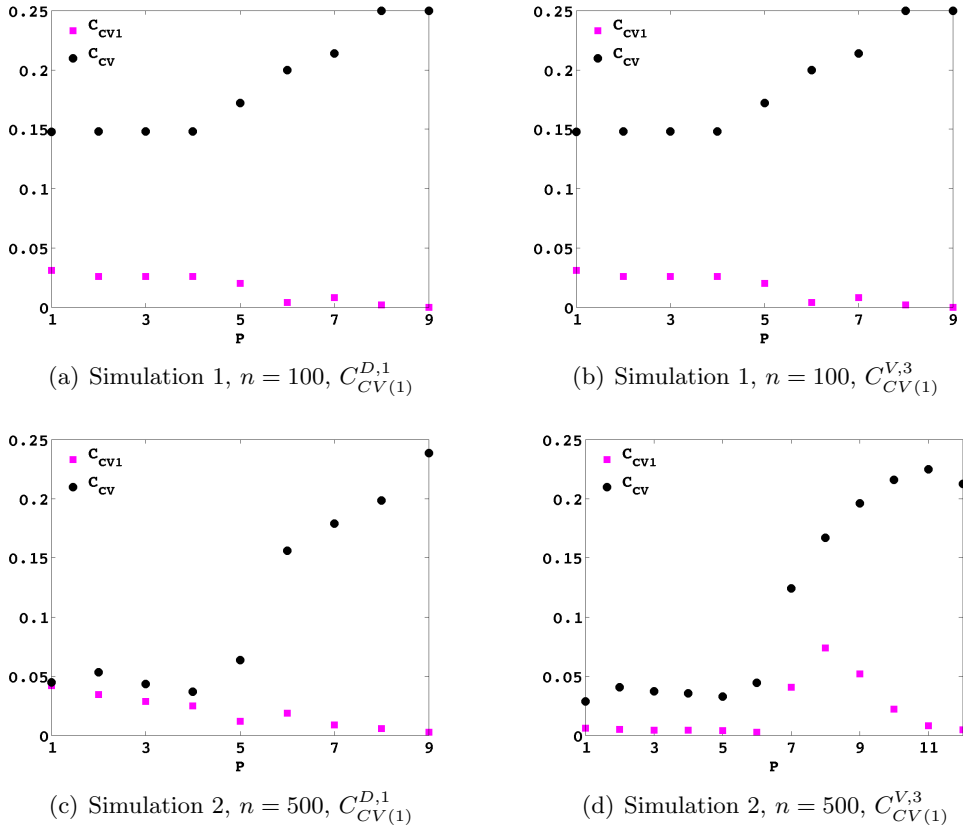


Figure 3: Taste of the behaviour of  $C_{CV1}$  vs  $C_{CV}$ .

## 6 Proofs

### 6.1 Proof of Proposition 1

Let us first prove that for large enough  $M$ , the measures  $f_{\omega_{1,c;M}^*} dx, \dots, f_{\omega_{k,c;M}^*} dx$  are linearly independent. Indeed, if it is not the case, there exists a subsequence  $M_p$  tending to infinity as  $p$  tends to infinity and a sequence  $(\alpha^{(p)})_{p \geq 1}$  in the unit ball of  $\mathbb{R}^k$  such that for all  $p \geq 1$ ,

$$\sum_{j=1}^k \alpha_j^{(p)} f_{\omega_{j,c;M_p}^*}(x) = 0$$

Lebesgue a.e. Let  $\alpha = (\alpha_1, \dots, \alpha_k)$  be a limit point of  $(\alpha^{(p)})_{p \geq 1}$  in the unit ball of  $\mathbb{R}^k$ . Using Assumption (A.2) and Corollary 1.7 in Chapter 3 of [31], we have that as  $p$  tends to infinity,  $f_{\omega_{j,c;M_p}^*}(x)$  converges to  $f_{j,c}^*(x)$  Lebesgue a.e. so that we obtain  $\sum_{j=1}^k \alpha_j f_{j,c}^*(x) = 0$  Lebesgue a.e., contradicting Assumption (A1).

Fix now  $M$  large enough so that the measures  $f_{\omega_{1,c;M}^*} dx, \dots, f_{\omega_{k,c;M}^*} dx$  are linearly independent. Then, one may use the spectral method described in [2] to get estimators  $\hat{\theta}_{sp}$  and

Simulation	1	1	1	1	1	2	2	2	3	3	3
$n$	50	100	500	1000	2000	50	100	500	50	100	500
$\sqrt{\min_{P < \tilde{P}_n} R_n(2^P)}$	0.062	0.043	0.020	0.014	0.010	0.058	0.046	0.020	0.096	0.078	0.036
$\sqrt{R_n(2^{\tilde{P}_0})}$	0.063	0.046	0.021	0.015	0.010	0.067	0.046	0.022	0.10	0.082	0.042
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^D,1}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.069	0.047	0.019	0.014	0.011	0.075	0.056	0.019	0.12	0.087	0.037
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^D,2}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.073	0.046	0.022	0.015	0.010	0.065	0.056	0.025	0.10	0.087	0.046
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^D,3}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.086	0.047	0.021	0.014	0.010	0.087	0.056	0.026	0.11	0.087	0.041
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^V,1}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.091	0.046	0.021	0.013	0.009	0.104	0.055	0.022	0.11	0.087	0.053
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^V,2}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.069	0.046	0.019	0.013	0.010	0.070	0.049	0.022	0.12	0.084	0.036
$\sqrt{\mathbb{E}^* \left[ \ \hat{\theta}_{2^{\tilde{P}_n}^V,3}(X_{1:n}) - \theta^*\ ^2 \right]}$	0.103	0.046	0.019	0.014	0.009	0.10	0.049	0.022	0.14	0.083	0.035

Table 2: Comparison of the squared risk of estimators associated to different criteria

$\hat{\omega}_{M;sp}$  of the parameters  $\theta$  and  $\omega_M$  from a sample of the multinomial distribution associated to density  $g_{\theta,\omega;M}$ . The estimator uses eigenvalues and eigenvectors computed from the empirical estimator of the multinomial distribution. But in a neighborhood of  $\theta^*$  and  $\omega_M^*$ , this is a continuously derivative procedure, and since on this neighborhood, classical deviation probabilities on empirical means hold uniformly, we get easily that for any vector  $V \in \mathbb{R}^k$ , there exists  $K > 0$  such that for all  $c > 0$ , for large enough  $n$  (the size of the sample):

$$\sup_{\|\theta - \theta^*\| \leq \frac{c}{\sqrt{n}}} \left( \langle \hat{\theta}_{sp} - \theta, V \rangle \right)^2 \leq K.$$

Now, the multinomial model is differentiable in quadratic mean, and following the proof of Theorem 4 in [20] one gets that, if  $V^T \tilde{J}_M V = 0$ , then

$$\lim_{c \rightarrow +\infty} \lim_{n \rightarrow +\infty} \sup_{\|\theta - \theta^*\| \leq \frac{c}{\sqrt{n}}} \left( \langle \hat{\theta}_{sp} - \theta, V \rangle \right)^2 = +\infty.$$

Thus for all  $V \in \mathbb{R}^k$ ,  $V^T \tilde{J}_M V \neq 0$ , so that  $\tilde{J}_M$  is not singular.

## 6.2 Proof of Proposition 2

We prove the proposition when  $M_1 = M$ ,  $M_2 = M + 1$ ,  $\mathcal{I}_M = \{I_1, \dots, I_M\}$  and  $\mathcal{I}_{M+1} = \{I_1, \dots, I_{M,0}, I_{M,1}\}$  with  $I_M = I_{M,0} \cup I_{M,1}$ , which is sufficient by induction. We denote  $(\omega_{j,c,m}^{(M)})_{j,c,1 \leq m \leq M}$  the parameter  $\omega$  in the model with partition  $\mathcal{I}_M$  and  $(\omega_{j,c,m}^{(M+1)})_{j,c,1 \leq m \leq M+1}$  the parameter  $\omega$  in the model with partition  $\mathcal{I}_{M+1}$ . Define  $b \in (0, 1)$ ,  $\alpha_{j,c} \in (0, 1)$ ,  $j = 1, \dots, k$ ,  $c = 1, 2, 3$  so that

$$|I_{M,0}| = (1 - b)|I_M|, |I_{M,1}| = b|I_M|, \omega_{j,c,M}^{(M+1)} = (1 - \alpha_{j,c})\omega_{j,c,M}^{(M)}, \omega_{j,c,M+1}^{(M+1)} = \alpha_{j,c}\omega_{j,c,M}^{(M)}.$$

Then, we may write

$$g_{\theta,\omega;M}(\mathbf{x}) = \sum_{j=1}^k \theta_j \prod_{c=1}^3 \prod_{m=1}^M \left( \frac{\omega_{j,c,m}^{(M)}}{|I_m|} \right)^{\mathbb{1}_{I_m}(x_c)}$$

and

$$\begin{aligned} g_{\theta,\omega;M+1}(\mathbf{x}) &= \sum_{j=1}^k \theta_j \prod_{c=1}^3 \prod_{m=1}^{M-1} \left( \frac{\omega_{j,c,m}^{(M+1)}}{|I_m|} \right)^{\mathbb{1}_{I_m}(x_c)} \left[ \left( \frac{\omega_{j,c,M}^{(M+1)}}{|I_{M,0}|} \right)^{\mathbb{1}_{I_{M,0}}(x_c)} \left( \frac{\omega_{j,c,M+1}^{(M+1)}}{|I_{M,1}|} \right)^{\mathbb{1}_{I_{M,1}}(x_c)} \right] \\ &= \sum_{j=1}^k \theta_j \prod_{c=1}^3 \prod_{m=1}^M \left( \frac{\omega_{j,c,m}^{(M)}}{|I_m|} \right)^{\mathbb{1}_{I_m}(x_c)} \left[ \left( \frac{\alpha_{j,c}}{b} \right)^{\mathbb{1}_{I_{M,1}}(x_c)} \left( \frac{1 - \alpha_{j,c}}{1 - b} \right)^{\mathbb{1}_{I_{M,0}}(x_c)} \right]. \end{aligned}$$

Thus, when  $x_c \notin I_M$  for  $c = 1, 2, 3$ ,  $g_{\theta,\omega;M+1}(\mathbf{x}) = g_{\theta,\omega;M}(\mathbf{x})$  and computations have to take care of  $\mathbf{x}$ 's such that for some  $c$ ,  $x_c \in I_M$ . If we parametrize the model with partition  $\mathcal{I}_{M+1}$  using the parameter  $(\theta, (\omega_{j,c,m}^{(M)}), (\alpha_{j,c}))$  we get the same efficient Fisher information for  $\theta$  as when parametrizing with  $(\theta, (\omega_{j,c,m}^{(M+1)}))$ . Define the function  $D$  as the difference between the gradient of  $\log g_{\theta,\omega;M+1}$  and that of  $\log g_{\theta,\omega;M}(\mathbf{x})$  with respect to the parameter  $(\theta, (\omega_{j,c,m}^{(M)}), (\alpha_{j,c}))$ :

$$D(\mathbf{x}) := \nabla \log g_{\theta,\omega;M+1}(\mathbf{x}) - \nabla \log g_{\theta,\omega;M}(\mathbf{x}),$$

in particular the last coordinates of  $\nabla \log g_{\theta,\omega;M}(\mathbf{x})$  corresponding to the derivatives with respect to  $(\alpha_{j,c})$  are zero. Let us denote  $K^{(M+1)}$  the Fisher information obtained for this new parametrization, that is  $K^{(M+1)} = \mathbb{E}^*[(\nabla \log g_{\theta,\omega;M+1}(X))(\nabla \log g_{\theta,\omega;M+1}(X))^T]$ . Easy but tedious computations give

$$\mathbb{E}^*[(\nabla \log g_{\theta,\omega;M}(X))(D(X))^T] = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \vdots & \vdots \\ 0 & \cdots & 0 \end{pmatrix},$$

so that

$$K^{(M+1)} = \begin{pmatrix} J_M & 0 \\ 0 & 0 \end{pmatrix} + \Delta$$

where  $\Delta = \mathbb{E}^*[D(X)D(X)^T]$  is positive semi-definite. As said before,  $\tilde{J}_{M+1}$  is obtained from  $K^{(M+1)}$  using the similar formula as from  $J_{M+1}$ . Then usual algebra gives that  $\tilde{J}_{M+1} \geq \tilde{J}_M$  since  $\Delta$  is positive semi-definite.

### 6.3 Proof of Lemma 1

*Proof.* Notice first that under (A3),  $g_{\theta^*,\mathbf{f}^*}/g_{\theta^*,\omega_{M^*}^*}$  is positively lower and upper bounded, so that the set of functions which are in  $L^2(g_{\theta^*,\mathbf{f}^*}d\mathbf{x})$  is the same as the set of functions which

are in  $L^2(g_{\theta^*, \omega_M^*, M} d\mathbf{x})$ . Also, any step function which is constant over  $I_{m_1} \times I_{m_2} \times I_{m_3}$ ,  $m_1, m_2, m_3 = 1, \dots, M$ , has the same hilbertian product with  $g_{\theta^*, \mathbf{f}^*}$  and with  $g_{\theta^*, \omega_M^*, M}$ . Thus, if for any  $M$ ,  $\mathbb{A}_M$  is the orthogonal projection in  $L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})$  onto  $\dot{\mathcal{P}}_M$ , the set of step functions spanned by the functions  $\left(S_{\omega, M}^*\right)_{j,c,m}$ ,  $j = 1, \dots, k$ ,  $c = 1, 2, 3$ ,  $m = 1, \dots, M-1$ , then for all  $j = 1, \dots, k-1$ ,

$$(\tilde{\psi}_M)_j = (S_{\theta, M}^*)_j - \mathbb{A}_M (S_{\theta, M}^*)_j,$$

so that

$$(\tilde{\psi})_j - (\tilde{\psi}_M)_j = (S_{\theta}^*)_j - (S_{\theta, M}^*)_j - \mathbb{A}_M \left[ (S_{\theta}^*)_j - (S_{\theta, M}^*)_j \right] + (\mathbb{A}_M - \mathbb{A}) (S_{\theta}^*)_j. \quad (18)$$

Notice that using (A3),

$$\dot{\mathcal{P}}_M \subset \dot{\mathcal{P}} \quad (19)$$

so that  $\mathbb{A}_M \mathbb{A} = \mathbb{A}_M$ . We then obtain

$$\left\| (\tilde{\psi})_j - (\tilde{\psi}_M)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})} \leq \left\| (S_{\theta}^*)_j - (S_{\theta, M}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})} + \left\| (\mathbb{A}_M \mathbb{A} - \mathbb{A}) (S_{\theta}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})}.$$

Using Assumption (A2) and Corollary 1.7 in Chapter 3 of [31], we have that as  $M$  tends to infinity,  $\left(S_{\theta, M}^*\right)_j$  converges to  $(S_{\theta}^*)_j$  Lebesgue a.e. Both functions are uniformly upper bounded by the finite constant  $1/\theta_j^*$  using Assumption (A.1), so that  $\left(S_{\theta, M}^*\right)_j$  converges to  $(S_{\theta}^*)_j$  in  $L^2(g_{\theta^*, \mathbf{f}^*}(\mathbf{x}) d\mathbf{x})$  as  $M$  tends to  $+\infty$  and  $\left\| (S_{\theta}^*)_j - (S_{\theta, M}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})}$  converges to 0 as  $M$  tends to  $+\infty$ . Using the same argument, for any function  $S \in \dot{\mathcal{P}}$  there exists a sequence of functions  $S_M \in \dot{\mathcal{P}}_M$  that converges to  $S$  in  $L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})$ . Let  $(S_M)_M$  be the sequence of functions converging to  $\mathbb{A} (S_{\theta}^*)_j$  in  $L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})$ . Since for all  $M$ ,  $S_M \in \dot{\mathcal{P}}_M$ , we have that

$$\left\| \mathbb{A}_M \left[ \mathbb{A} (S_{\theta}^*)_j \right] - \mathbb{A} (S_{\theta}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})} \leq \left\| S_M - \mathbb{A} (S_{\theta}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})}$$

so that also  $\left\| (\mathbb{A}_M \mathbb{A} - \mathbb{A}) (S_{\theta}^*)_j \right\|_{L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})}$  converges to 0 as  $M$  tends to  $+\infty$ . We thus obtain that  $(\tilde{\psi})_j$  converges to  $(\tilde{\psi}_M)_j$  in  $L^2(g_{\theta^*, \mathbf{f}^*} d\mathbf{x})$ . As a consequence,  $\tilde{J}_M$  converges to  $\tilde{J}$  as  $M$  tends to  $+\infty$ .  $\square$

## 6.4 Proof of Proposition 4

Proposition 4 is easily implied by Lemma 2 which formalizes the following. When the sequence of observations  $X_1, \dots, X_n$  and  $n$  are fixed, then almost surely there exists a sufficiently fine partition  $\mathcal{I}_M$  such that there exists at most one component of an observation in each set  $I_m$ ,  $m \leq M$ . Then we can reorder the sets  $I_m$  so that  $X_{i,c} \in I_{i+n(c-1)}$ , for all  $c \in \{1, 2, 3\}$  and  $i \leq n$ . In this case, the likelihood  $\ell_n(\cdot, \cdot; M)$  is maximised at each parameter  $(\theta, \omega)$  belonging to the set  $\mathcal{S}_M \subset \Delta_k \times (\Delta_M)^{3k}$  that we explain now (and formalise in



Lemma 2). Each element of  $\mathcal{S}_M$  corresponds to one clustering of the observations in  $k$  sets (represented by the  $(A_j^*)_{j \leq k}$  in Lemma 2) of size as equal as possible. For each clustering, for all  $j \leq k$ ,

- $\theta_j = \#A_j^*/n$  is the proportion of observations associated to  $A_j^*$  (then the  $\theta_j$  are almost equal to  $1/k$ ),
- for all  $c \in \{1, 2, 3\}$  and for all  $l \leq M$ ,

$$\omega_{j,c,l} = \begin{cases} 1/\#A_j^* & \text{if } l - n(c-1) \in A_j^* \text{ (i.e. } X_{l-n(c-1)} \in I_l \text{ is associated to the hidden state } j), \\ 0 & \text{if } l - n(c-1) \in \{1, \dots, n\} \setminus A_j^* \text{ (i.e. } X_{l-n(c-1)} \in I_l \text{ is not associated to } j), \\ 0 & \text{otherwise (i.e. there is no observation in } I_l). \end{cases}$$

**Lemma 2.** Let  $X_1, \dots, X_n$  be fixed observations, as soon as for all  $i \leq n$  and  $c \in \{1, 2, 3\}$ ,  $X_{i,c} \in I_{i+n(c-1)}$  then the likelihood  $\ell_n(\cdot, \cdot; M)$  is maximised at  $(\hat{\theta}_M, \hat{\omega}_M)$  if and only if  $(\hat{\theta}_M, \hat{\omega}_M) \in \mathcal{S}_M$  where

$$\begin{aligned} \mathcal{S}_M = \{(\theta, \omega) : & \theta_j = \#A_j^*/n, \omega_{j,c,l} = \mathbf{1}_{l-n(c-1) \in A_j^*} / \#A_j^*, \\ & (J_1, J_2) \text{ partition of } \{1, \dots, k\}, \#J_2 = n - k \lfloor n/k \rfloor =: r \\ & (A_j^*)_{j \leq k} \text{ partition of } \{1, \dots, n\}, \\ & \#A_{j_1}^* = \lfloor n/k \rfloor =: q, \text{ for } j_1 \in J_1, \#A_{j_2}^* = \lfloor n/k \rfloor + 1 =: q + 1, \text{ for } j_2 \in J_2\}, \end{aligned}$$

and  $n = kq + r$ ,  $0 \leq r \leq k - 1$ .

*Proof.* Since the set of parameters is compact and the likelihood is a continuous function of the parameters then the maximum is attained.

If  $(\theta, \omega)$  maximises the likelihood  $\ell_n(\cdot, \cdot; M)$ ,

(P1) then, for all  $1 \leq i \leq n$ , there exists  $1 \leq j \leq k$  such that  $\omega_{j,c,i+n(c-1)} > 0$  for all  $c \in \{1, 2, 3\}$ .

Indeed, if there exists  $1 \leq i \leq n$  such that for all  $1 \leq j \leq k$ ,  $\omega_{j,c,i+n(c-1)} = 0$  for some  $c \in \{1, 2, 3\}$ , then

$$\ell_n(\theta, \omega; M) = \sum_{i=1}^n \log \left( \sum_{j=1}^k \theta_j \prod_{c=1}^3 \omega_{j,c,i+n(c-1)} \right) + \underbrace{\sum_{i=1}^n \log (1/(|I_i||I_{i+n}||I_{i+2n}|))}_{\text{constant}} = -\infty.$$

(P2) and if there exists  $j, c, i$  such that  $\omega_{j,c,i+n(c-1)} = 0$  and  $\theta_j > 0$  then  $\omega_{j,d,i+n(d-1)} = 0$  for all  $d$ .

Indeed otherwise you can give the weight  $\omega_{j,d,i+n(d-1)}$ , to one of the other  $\omega_{j,d,s+n(d-1)}$  for which  $\omega_{j,e,s+n(e-1)} > 0$ , for all  $e \neq d$  (which exist otherwise take  $\theta_j = 0$  which would increase the likelihood) and this increases the likelihood.

(P3) and if  $\theta_j > 0$ , then  $\omega_{j,c,l} = 0$  if  $l - n(c-1) \notin \{1, \dots, n\}$ .

Indeed, in this case, there is no observation in  $I_l$  so that  $\omega_{j,c,l}$  does not appear in the likelihood and we conclude similarly as the previous point.



and then summing the result over  $i \in A_j$  and finally subtracting (21) multiplied by  $\bar{\theta}_j$  to the result (ie making  $\sum_{i \in A_j} \bar{\omega}_{j,c,i+n(c-1)}(22) - \bar{\theta}_j(21)$ ), we get

$$0 = -\mu_{j,c} - n\bar{\theta}_j. \quad (26)$$

Then using again Equations (22), (25) and (26), we get

$$\bar{\omega}_{j,c,i+n(c-1)}^2 = n \sum_{s \in J(i)} \bar{\theta}_s \bar{\omega}_{s,1,i}^3, \quad \forall j \in J(i), \forall c \in \{1, 2, 3\},$$

so that  $\bar{\omega}_{j,c,i+n(c-1)}$  does not depend on  $j \in J(i)$  and

$$\bar{\omega}_{j,c,i+n(c-1)} = \mathbf{1}_{i \in A_j} / \left( n \sum_{s \in J(i)} \bar{\theta}_s \right), \quad \forall j \in J(i). \quad (27)$$

For each  $\mathcal{S}_{J,A_1,\dots,A_k} =: \mathcal{S}$ , we have obtained the zeros of the derivative of the log-likelihood, that we now denote  $({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega})$ , to emphasize the dependence with the considered set  $\mathcal{S}$ . We now want to know which of these zeros  $({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega})$  are local maxima thanks to the second partial derivatives.

We consider sets  $\mathcal{S}_{J,A_1,\dots,A_k}$  for which there exists  $i \leq n$  such that there exist  $j$  and  $l$  are in  $J(i)$  and  $j \neq i$ . We consider a second partial derivative of

$$\tilde{\ell}_n(\theta, \tilde{\omega}; M) = \sum_{i=1}^n \log \left( \sum_{j=1}^k \theta_j (\tilde{\omega}_{j,1,i})^3 \right)$$

that is the log-likelihood (up to an additive constant) associated to the model where for all  $1 \leq m \leq k$ ,  $1 \leq s \leq n$ ,  $\omega_{m,1,s} = \omega_{m,2,s+n} = \omega_{m,3,s+2n}$ . Assume without loss of generality that  $\theta_l \geq \theta_j$ , then (using that  $\theta_k = 1 - \sum_{m < k} \theta_m$  and  $\omega_{j,1,n} = 1 - \sum_{s < n} \omega_{j,1,s}$ ),

$$\frac{\partial^2 \tilde{\ell}_n}{\partial \tilde{\omega}_{j,1,i}^2}({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega}; M) = C \left( 6 {}^{\mathcal{S}}\bar{\theta}_j \sum_{m \in J(i) \setminus \{j\}} {}^{\mathcal{S}}\bar{\theta}_m - 3 {}^{\mathcal{S}}\bar{\theta}_j^2 \right) \geq C (6 {}^{\mathcal{S}}\bar{\theta}_j {}^{\mathcal{S}}\bar{\theta}_l - 3 {}^{\mathcal{S}}\bar{\theta}_j^2) > 0,$$

where  $C > 0$ . This implies that for all sets  $\mathcal{S}_{J,A_1,\dots,A_k} := \mathcal{S}$  where there exists  $i \leq n$  such that  $\#J(i) > 1$ , every zeros  $({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega})$  is not a local maximum. So that the only possible local maxima of  $\ell_n(\theta, \omega; M)$  are the zeros  $({}^{\mathcal{S}_{J,A_1,\dots,A_k}}\bar{\theta}, {}^{\mathcal{S}_{J,A_1,\dots,A_k}}\bar{\omega})$  where  $\#J(i) = 1$  for all  $i \leq n$ , i.e. when  $(A_j)_{j \in J}$  forms a partition of  $\{1, \dots, n\}$ .

So we now only consider sets  $A_j$ ,  $j \in J$  which form a partition of  $\{1, \dots, n\}$  and  $\bar{\omega}_{j,c,i+n(c-1)} = \mathbf{1}_{i \in A_j} / (n\bar{\theta}_j)$  for  $i \in A_j$ , using Equation (27). As  $\sum_{i \in A_j} \bar{\omega}_{j,1,i} = 1$ , we then obtain that  $\bar{\theta}_j = \#A_j/n = 1/(n\bar{\omega}_{j,1,i})$ , for all  $i \in A_j$ . So that we now only have to choose the best partition  $(A_j)_{j \in J}$  of  $\{1, \dots, n\}$  and  $J$ . Let  $N_j = \#A_j$ , we know that  $\sum_j N_j = n$  and the log-likelihood at the local maximum  $({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega})$  associated to  $\mathcal{S}_{J,A_1,\dots,A_k} =: \mathcal{S}$  is

$$\ell_n({}^{\mathcal{S}}\bar{\theta}, {}^{\mathcal{S}}\bar{\omega}; M) = \sum_{s \in J} N_s \log(N_s^{-2}) + constant.$$

So that we want to minimize

$$\sum_{s \in J} N_s \log(N_s) \text{ under the constraint } \sum_{s \in J} N_s = n \quad (28)$$

over  $J \subset \{1, \dots, k\}$  and  $N_j \in \mathbb{N}$ ,  $j \in J$ . This minimization is equivalent to the minimization of

$$\sum_{s \leq k} N_s \log(N_s) \text{ under the constraint } \sum_{s \leq k} N_s = n \quad (29)$$

over  $N_j \in \mathbb{N}$ ,  $j \leq k$  (since then the problem (29) is less constrained than for the minimization of (28) when  $J$  is fixed).

And, when  $k$  divides  $n$ , the minimum of (29) is attained at  $N_s = n/k$ . Otherwise, when  $k$  does not divide  $n$ , consider only two indices  $s_1, s_2$  in  $\{1, \dots, k\}$  and assume that  $N_s$ ,  $s \notin \{s_1, s_2\}$  are fixed such that  $N_{s_1} + N_{s_2} = S_N$  is also fixed. Then we want to minimise  $-N_{s_1} \log(N_{s_1}) - (S_N - N_{s_1}) \log(S_N - N_{s_1})$ . Studying the function  $x \in (0, S_N) \mapsto -x \log(S_N - x) - (S_N - x) \log(x)$ , we obtain that the minimum is attained when  $N_{s_1}$  and  $N_{s_2} = S_N - N_{s_1}$  are the closest of  $S_N/2$ . Then in both cases, the m.l.e. is attained at every  $(\theta, \omega) \in \mathcal{S}_M$ . □

## 6.5 Proof of Corollary 1

Suppose that for all  $N > 0$  and all  $C > 0$ , there exists  $n \geq N$  such that

$$n^2 \left( \max_{m \leq M_n} |I_m| \right)^2 M_n \leq C.$$

So that there exists a subsequence  $(\phi(n))_{n \in \mathbb{N}}$  of  $(n)_{n \in \mathbb{N}}$  such that

$$(\phi(n))^2 \left( \max_{m \leq M_{\phi(n)}} |I_m| \right)^2 M_{\phi(n)} \xrightarrow{n \rightarrow \infty} 0. \quad (30)$$

Set  $\epsilon > 0$ , by Proposition 4, there exists  $N_1 > 0$  such that for all  $n \geq N_1$ ,

$$\begin{aligned} & P \left( \left| \widehat{\theta}_{M_n}(X_{1:\phi(n)}) - (1/k, \dots, 1/k) \right| \leq \epsilon \right) \\ & \geq P \left( \{ \exists 1 \leq i_1, i_2 \leq \phi(n), 1 \leq c, d \leq 3, m \leq M_{\phi(n)} : X_{i_1, c} \in I_m, X_{i_2, d} \in I_m \}^c \right) \\ & \geq 1 - \sum_{i_1=1}^{\phi(n)} \sum_{i_2=1}^{\phi(n)} \sum_{m=1}^{M_{\phi(n)}} P(X_{i_1, c} \in I_m, X_{i_2, d} \in I_m) \\ & \geq 1 - (\phi(n))^2 M_{\phi(n)} \max(\sup g, (\sup g)^2) \left( \max_{m \leq M_{\phi(n)}} |I_m| \right)^2. \end{aligned} \quad (31)$$

Using Equations (30) and (31) and Assumption (A3), then  $\widehat{\theta}_{M_n}(X_{1:\phi(n)})$  tends in probability to  $(1/k, \dots, 1/k)$  which contradicts the convergence in law of  $\widehat{\theta}_{M_n}$  to  $\theta^*$ . This concludes the proof.

## 6.6 Proof of Theorem 2

We first recall Lemma 2.1 in [4]:

**Lemma 3** (Sylvain Arlot). *Let  $A, B, C, R : \mathcal{M} \rightarrow \mathbb{R}$ . If for all  $m, m' \in \mathcal{M}$ ,*

$$(C(m) - R(m)) - (C(m') - R(m')) \leq A(m) + B(m'),$$

*then for all  $\hat{m} \in \mathcal{M}$  such that  $C(\hat{m}) \leq \inf_{m \in \mathcal{M}} C(m) + \rho$ ,  $\rho > 0$ ,*

$$R(\hat{m}) - B(\hat{m}) \leq \inf_{m \in \mathcal{M}} \{R(m) + A(m)\} + \rho.$$

We are going to use this lemma with  $R(\mathcal{I}) = R_{a_n}(\mathcal{I})$ ,  $C(\mathcal{I}) = C_{CV}(\mathcal{I})$  and

$$A(\mathcal{I}) = B(\mathcal{I}) = \epsilon_n R(\mathcal{I}) + \delta_n.$$

Using Hoeffding's inequality,

$$P(\{-B(\mathcal{I}) \leq C_{CV}(\mathcal{I}) - R_{a_n}(\mathcal{I}) \leq A(\mathcal{I})\}^c) \leq 2 \exp(-2b_n A(\mathcal{I})^2),$$

since  $\|\hat{\theta}_{\mathcal{I}}(X_{B_b}) - \hat{\theta}_{\mathcal{I}_0}(X_{B_{-b}})\|^2 \leq 1$ , for all  $b$ . We introduce the sets

$$\mathcal{S}_{\mathcal{I}} = \{-B(\mathcal{I}) \leq C_{CV}(\mathcal{I}) - R_{a_n}(\mathcal{I}) \leq A(\mathcal{I})\} \quad (32)$$

for all  $\mathcal{I} \in \mathcal{M}_n$ . Using Lemma 3, on the set  $\cap_{\mathcal{I} \in \mathcal{M}_n} \mathcal{S}_{\mathcal{I}}$ , Equation (17) holds and using Equation (32), we obtain

$$P(\cap_{\mathcal{I} \in \mathcal{M}_n} \mathcal{S}_{\mathcal{I}}) \geq 1 - 2m_n \exp\left(-2b_n \left(\epsilon_n \inf_{\mathcal{I} \in \mathcal{M}_n} R_{a_n}(\mathcal{I}) + \delta_n\right)^2\right).$$

## 6.7 Proof of Proposition 5

Using Theorem 2,

$$\begin{aligned} & \mathbb{E}^* \left[ a_n R_{a_n}(\hat{\mathcal{I}}_n) \right] \\ & \leq a_n \left( \frac{1 + \epsilon_n}{1 - \epsilon_n} \inf_{\mathcal{I} \in \mathcal{M}_n} R_{a_n}(\mathcal{I}) + \frac{2\delta_n}{1 - \epsilon_n} \right) + 2a_n m_n \exp\left(-2b_n \left(\epsilon_n \inf_{\mathcal{I} \in \mathcal{M}_n} R_{a_n}(\mathcal{I}) + \delta_n\right)^2\right) \end{aligned}$$

we can conclude by taking  $\epsilon_n = \delta_n = 1/(\log(n)a_n)$ .

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