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## Fundamental limits for learning hidden Markov model parameters

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## Abstract

We study the frontier between learnable and unlearnable hidden Markov models (HMMs). HMMs are flexible tools for clustering dependent data coming from unknown populations. The model parameters are known to be identifiable as soon as the clusters are distinct and the hidden chain is ergodic with a full rank transition matrix. In the limit as any one of these conditions fails, it becomes impossible to identify parameters. For a chain with two hidden states we prove nonasymptotic minimax upper and lower bounds, matching up to constants, which exhibit thresholds at which the parameters become learnable.

#### 1 Introduction

We consider the learnability of hidden Markov model parameters. Hidden Markov models offer an attractive approach to clustering problems. Such problems are ubiquitous in machine learning. A natural probabilistic approach to modelling the clusters views data as independent draws from a mixture of distributions and seeks to identify the labels. Without strong assumptions about the form of the distributions, this approach fails: an unconstrained mixture model is non-identifiable. This difficulty can be overcome by assuming that the clusters are well separated.

An alternative approach is to remove the assumption that the data points are independent. Perhaps the simplest, but nevertheless a powerful, alternative structure is to model the cluster labels as a time-homogeneous Markov chain; then the data itself is described as following a hidden Markov model (HMM). In sharp contrast to the independent setting, with hidden Markov structure one can recover the distribution of data for each cluster absent virtually any constraint on these distributions: indeed, once all submodels in which the data is in fact independent are ruled out, no further constraint is necessary when there are two hidden states. [With more than two hidden states, current state-of-the-art results have the mild further requirement that the Markov transition matrix be full-rank.] Note that, given consistent estimators of the model parameters, one can construct an empirical Bayes classifier which mimics the optimal clustering performance of the Bayes classifier.

The present work initiates an exploration of the limits of learnability of the hidden Markov parameters as the independent subcase is approached. We focus on the setting of two hidden states and multinomial data, and exhibit principles which should generalise to much wider settings. Our main result, Theorem 1, gives upper and lower bounds showing the minimax estimation rate for the model parameters, exhibiting that these parameters can be learned if and only if the sample size n is large enough compared to a suitable measure of the closeness of the data to the independent subcase.

## 2 Related work

Clustering is one of the most classical tasks in modern machine learning. Given data  $(Y_1, \ldots, Y_n)$ , ones seeks a partition where  $Y_i$  and  $Y_j$  are in the same block if they share similarities: typically a proximity condition to a certain centroid. Algorithms for clustering can be divided into two categories according to whether they rely on geometric arguments or probabilistic modelling. Geometric approaches usually do not assume any generating model for  $(Y_1, \ldots, Y_n)$ , but rather that the clusters can be identified from the data via a suitable separation condition. Undoubtedly the most famous algorithm of this type is the celebrated *k-means* algorithm [29] whose ability to recover well-separated clusters has been investigated in [22].

The other main class of clustering algorithms posit a probabilistic generating model for  $(Y_1, \ldots, Y_n)$  and seeks to recover hidden cluster labels associated with the generating model. One of the most popular models assumes the  $Y_i$ 's are drawn independently from a mixture of normal distributions, where the cluster labels identify from which component a data point is drawn. The model parameters are traditionally learned using the famous EM algorithm [12], and points are assigned to the cluster with the closest centroid. Let us again emphasise that a general independent mixture model is non-identifiable, so that the assumption of gaussianity plays an essential role in allowing the recovery of the clusters. A solution to allow less rigid modelling of the data distribution for each cluster is to drop the independence condition and to use a dependent probabilistic approach, such as the HMM approach considered here.

HMMs have long been used as a flexible tool for clustering questions: see for instance [9, 25, 23, 35, 38, 37]. In this context the distributions of data for the clusters are known as the emission distributions. The proof that parameters can be identified with minimal assumptions is comparatively recent, given for HMMs taking values in a finite set in [4, 21, 5] and extended to allow for emission distributions modelled nonparametrically (but still with the underlying Markov chain having finite state space) in [15, 3]. Results in [11] control the propagation of errors from parameter estimation to the posterior probabilities when calculating the latter via plug-in, implying that good control on the risk of the estimators will ensure the performance of the empirical Bayes classifier is close to that of the true Bayes classifier (whose optimality for clustering is a standard result in decision theory [13]).

A topic closely related to binary classification/clustering is multiple testing, in which one aims to identify within some large data set a collection of data points which come from a 'discovery' hypothesis, rather than from the conservative null hypothesis. In this setting control of the false discovery rate has been obtained recently for a knockoffs-based method in [34] and for an empirical Bayes method in [1]; in each case estimation of the HMM parameters is an essential first step. Modelling the proportion of non-null signals as vanishingly small, as our results permit, would allow for further links to the setting of *sparse* multiple testing, considered for example (with independent data) in [2, 8].

Theoretical justification of a range of learning methods for HMMs with emission distributions modelled parametrically or nonparametrically have been developed in recent years: moment and tensor methods in [5, 11], and model selection using penalized least squares estimation in [10, 27], using penalized likelihood methods in [28], or using other techniques in [26]. These works all give both asymptotic and nonasymptotic upper bounds controlling the distance between estimators and the unknown parameters. All require the data to truly be dependent, but none quantify explicitly how their sample complexity results depend on the 'distance' to independence. Indeed, quantifying this dependence requires a sharp understanding of how the distances between distributions evolve with respect to the distances between parameters, as done for particular parametric finite mixture models in [18, 20, 14].

To the best of our knowledge no prior theoretical result exists addressing the learning of parameters of a HMM when approaching the independent case. A phase transition between learnable and

unlearnable HMMs as exhibited in our current work was previously exhibited experimentally in [33] when the multinomial emission distributions approach each other.

Finally, let us mention that departure from the independence assumption has been noted to allow much better possible learning also in HMM settings free from the assumption that the Markov chain has a finite state space [17, 6] (at the expense of stricter assumptions on the emission distributions), and also in other problems including dynamic networks [30, 7], image denoising [31], and deconvolution [16].

### **3** Setting

Consider a two-state HMM with multinomial emissions, in which we observe the first *n* entries of a sequence  $\mathbf{Y} = (Y_1, Y_2, ...) \in \{1, ..., K\}^{\mathbb{N}}$  which satisfies

$$\mathbb{P}(Y_n = k \mid \mathbf{X}) = f_{X_i}(k),$$
  

$$\mathbf{X} = (X_n)_{n \in \mathbb{N}} \sim \operatorname{Markov}(\pi, Q),$$
(1)

with the  $Y_j$ ,  $j \in \mathbb{N}$  conditionally independent given X. The vector X of 'hidden states' takes values in  $\{0, 1\}^{\mathbb{N}}$  and, for a parameter  $\theta = (p, q, f_0, f_1)$ , the transition matrix of the chain is given by

$$Q \coloneqq \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix},\tag{2}$$

with the convention that for  $j \ge 1$ ,  $\mathbb{P}_{\theta}(X_{j+1} = 0 | X_j = 0) = 1 - p < 1$  and  $\mathbb{P}_{\theta}(X_{j+1} = 0 | X_j = 1) = q > 0$ . The densities  $f_0, f_1$  are the 'emission densities' with respect to counting measure on  $\{1, \ldots, K\}$ . Grant also that  $X_1$  is drawn from the stationary distribution of the chain, i.e.  $\mathbb{P}_{\theta}(X_1 = 1) = p/(p+q)$ .

In the limit where the sequence Y becomes independent and identically distributed (i.i.d.), learning the parameters becomes impossible due to standard identifiability issues for mixture models. This i.i.d. limit can be approached in three ways:

- 1.  $p \approx 0$  or  $q \approx 0$ , and thus the chain X passes long periods of time in one of the two states;
- 2. the transition matrix Q is nearly singular, so that X itself is almost i.i.d; this is the case if  $|1 p q| \approx 0$ ;
- 3. the emission distributions are close to each other:  $||f_0 f_1|| \approx 0$ , where  $|| \cdot ||$  denotes the usual Euclidean norm,  $||f||^2 = \sum |f(k)|^2$ .

We adopt a minimax point of view and encapsulate all the above scenarios within the class of parameters defined, for some  $\delta, \epsilon \in (0, 1)$  and some  $\zeta > 0$ , by

$$\Theta = \Theta(\delta, \epsilon, \zeta) = \{\theta : p, q \ge \delta, |1 - p - q| \ge \epsilon, ||f_0 - f_1|| \ge \zeta\}.$$

Introduce also the subset

$$\Theta_L = \Theta_L(\delta, \epsilon, \zeta) = \Theta \cap \{1 - |1 - p - q| \ge L\}.$$

**Remark 1.** Note that 1 - |1 - p - q| is the absolute spectral gap of the chain X, and hence the mixing time of the chain can be upper bounded uniformly in  $\Theta_L$ . Here L may be arbitrarily small but we think of it as fixed, in contrast to  $\delta$ ,  $\epsilon$  and  $\zeta$  which are allowed to depend on n. With the introduction of this lower bound we still allow one of p, q to be vanishingly small (or arbitrarily close – even equal – to 1), but not both.

**Remark 2.** If  $\zeta$  is too large compared to 1/K,  $\Theta(\delta, \epsilon, \zeta)$  may be empty, or too small to be an interesting parameter space. To avoid this we assume a mild compatibility condition: that

$$\zeta \le \frac{\sqrt{2\lfloor K/2 \rfloor}}{4K}.\tag{3}$$

## 4 Main results

To avoid a label-switching issue discussed in the next section we assume that  $f_0 - f_1$  lies in some specified half-plane. Our main result is the following.

**Theorem 1.** There exist an estimator  $\hat{\theta} = (\hat{p}, \hat{q}, \hat{f}_0, \hat{f}_1)$  and a constant C = C(K, L) > 0 such that for all  $1 \le x^2 \le n\delta^2\epsilon^4\zeta^6$ 

$$\sup_{\theta \in \Theta_L} \mathbb{P}_{\theta} \Big( \max(|\hat{p} - p|, |\hat{q} - q|) > \frac{Cx}{\sqrt{n\delta^2 \epsilon^4 \zeta^6}} \max(\delta, \epsilon \zeta) \Big) \le e^{-x^2}$$
$$\sup_{\theta \in \Theta_L} \mathbb{P}_{\theta} \Big( \max(\|\hat{f}_0 - f_0\|, \|\hat{f}_1 - f_1\|) > \frac{Cx}{\sqrt{n\delta^2 \epsilon^4 \zeta^4}} \Big) \le e^{-x^2}.$$

Grant condition (3), assume  $\delta \leq 1/6$ ,  $\epsilon \leq 1/3$ ,  $L \leq 1/3$  and  $n\delta^2 \epsilon^4 \zeta^6 \geq 1$ . Then for some c = c(K) > 0,

$$\inf_{\check{\theta}} \sup_{\theta \in \Theta_L} \mathbb{P}_{\theta} \Big( \max(|\check{p} - p|, |\check{q} - q|) > \frac{c}{\sqrt{n\delta^2 \epsilon^4 \zeta^6}} \max(\delta, \epsilon\zeta) \Big) \ge 1/4,$$
$$\inf_{\check{\theta}} \sup_{\theta \in \Theta_L} \mathbb{P}_{\theta} \Big( \max(\|\check{f}_0 - f_0\|, \|\check{f}_1 - f_1\|) > \frac{c}{\sqrt{n\delta^2 \epsilon^4 \zeta^4}} \Big) \ge 1/4,$$

where the infima are over all estimators  $\check{\theta} = (\check{p}, \check{q}, \check{f}_0, \check{f}_1)$ .

The estimator  $\hat{\theta}$  is built via plug-in from those constructed later in Theorem 2. Note that the maxima are genuinely required in the lower bounds: in the extreme case where p is close to zero and q is close to 1, one has many samples with  $X_i = 0$  and few with  $X_i = 1$ , so that p and  $f_0$  are easier to estimate accurately than q and  $f_1$ .

We deduce immediately the sample complexity for learning the parameters.

**Corollary 1.** Fix a target error magnitude E > 0 and a probability level  $\alpha > 0$ . For the same estimators as in Theorem 1, there exists a constant C = C(K, L) such that for any  $\theta \in \Theta_L$  we have

$$n \ge \frac{\log(1/\alpha)}{\delta^2 \epsilon^4 \zeta^6} \max\left(\frac{C\delta^2}{E^2}, \frac{C\epsilon^2 \zeta^2}{E^2}, 1\right) \implies \mathbb{P}_{\theta}(\max(|\hat{p} - p|, |\hat{q} - q|) > E) \le \alpha,$$
$$n \ge \frac{\log(1/\alpha)}{\delta^2 \epsilon^4 \zeta^4} \max\left(\frac{C}{E^2}, \frac{1}{\zeta^2}\right) \implies \mathbb{P}_{\theta}(\max(\|\hat{f}_0 - f_0\|, \|\hat{f}_1 - f_1\|) > E) \le \alpha.$$

Conversely there exists a constant c(K) > 0 such that for all  $0 < E \le c(K)$  and for any estimator  $\check{\theta} = (\check{p}, \check{q}, \check{f}_0, \check{f}_1)$  there exists  $\theta \in \Theta_L$  such that

$$n \leq \frac{\max(\delta^2, \epsilon^2 \zeta^2)}{\delta^2 \epsilon^4 \zeta^6} \quad \Longrightarrow \quad \mathbb{P}_{\theta}(\max(|\check{p} - p|, |\check{q} - q|) > E) \geq 1/4,$$
$$n \leq \frac{1}{\delta^2 \epsilon^4 \zeta^4} \quad \Longrightarrow \quad \mathbb{P}_{\theta}(\max(\|\check{f}_0 - f_0\|, \|\check{f}_1 - f_1\|) > E) \geq 1/4.$$

Note that to apply Theorem 1 for the lower bounds we would initially also need  $n \ge (\delta^2 \epsilon^4 \zeta^6)^{-1}$  but by monotonicity — i.e. the fact that any measurable function of  $(Y_1, \ldots, Y_n)$  is also a measurable function of  $(Y_1, \ldots, Y_N)$  for  $N \ge n$  — the restriction can be removed.

### **5 Proof outline**

We sketch out the main ideas behind the proof of Theorem 1. The full proof is deferred to the supplementary material, along with all other proofs for this article.

The minimax lower bounds are obtained by an argument  $\hat{a}$  la Le Cam. In particular, it is a famous result of Le Cam [24, 36] that the minimax rate (under quadratic loss) of estimating a functional  $g: \Theta \to \mathbb{R}$ is always greater than the maximum value that  $|g(\theta) - g(\tilde{\theta})|^2$  can take for  $\theta, \tilde{\theta} \in \Theta$  under the constraint that  $K(p_{\theta}^{(n)}; p_{\tilde{\theta}}^{(n)}) \leq c$ , where  $K(p_{\theta}^{(n)}; p_{\tilde{\theta}}^{(n)})$  denotes the *Kullback-Leibler* (KL) divergence between the laws of  $(Y_1, \ldots, Y_n)$  under parameters  $\theta$  and  $\tilde{\theta}$ , and 0 < c < 1 is a small positive constant (see Lemma 3 for the precise formulation we use). Understanding bounds on  $|g(\theta) - g(\tilde{\theta})|$  in terms of bounds on  $K(p_{\theta}^{(n)}; p_{\tilde{\theta}}^{(n)})$  is also sufficient for obtaining an upper bound on the minimax estimation rate. Since the observations are not i.i.d, it is not the case that  $K(p_{\theta}^{(n)}; p_{\tilde{a}}^{(n)}) = nK(p_{\theta}^{(1)}; p_{\tilde{a}}^{(1)})$ , and, while it is true that  $K(p_{\theta}^{(n)}; p_{\bar{\theta}}^{(n)}) \leq nK(p_{\theta}^{(1)}; p_{\bar{\theta}}^{(1)})$ , this bound is not useful: if it were, it could equally be applied to give bounds in a general mixture model, in which parameter estimation is known to be impossible. Building on the work of [5, 15] we know that  $\theta$  is identifiable from  $p_{\theta}^{(3)}$  and we record in Lemma 2 the more useful bound  $K(p_{\theta}^{(n)}; p_{\bar{\theta}}^{(n)}) \leq \lceil n/3 \rceil K(p_{\theta}^{(3)}; p_{\bar{\theta}}^{(3)})$ , the right side of which we further bound by a constant multiple of  $n \| p_{\theta}^{(3)} - p_{\bar{\theta}}^{(3)} \|^2$  since the KL divergence is equivalent to the squared Euclidean distance under mild assumptions. The main difficulty of the proof is to relate  $\| p_{\theta}^{(3)} - p_{\bar{\theta}}^{(3)} \|$  to a suitable notion of distance between  $\theta$  and  $\tilde{\theta}$ . We propose a reparametrisation of the model problem to simplify the analysis. Indeed, motivated by a desire to simplify the expression for  $p^{(3)}$  (see equations (9) and (10) in Section 6), we introduce new parameters  $\phi, \psi$ . A key result is Proposition 1, which establishes that  $\| p_{\theta(\phi,\psi)}^{(3)} - p_{\theta(\bar{\phi},\bar{\psi})}^{(3)} \|$  is equivalent to  $\rho(\phi,\psi;\tilde{\phi},\tilde{\psi})$ , where  $\rho$  is defined in the proposition and can be seen as the "natural" statistical distance of the problem. The parameterization ( $\phi, \psi$ ) turns out to be of special interest: the component of  $\phi$  determine how "close" the sequence Y is to being i.i.d in an interpretable way (see Section 6), and the parameter  $\psi$  is related to the stationary distribution of the sequence Y. For this reason, we also establish minimax lower bounds for the estimation problems  $\max_{|\phi, \bar{\phi}, \bar{\phi}|^2$  (respectively  $\max_{|\phi, - \bar{\psi}_j|^2}$ ) subject to  $n\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \leq c$  and  $\theta(\phi,\psi), \theta(\tilde{\phi},\tilde{\psi}) \in \Theta$  for a small enough constant c > 0. Finally the lower bounds for the original parameters in the Theorem 1 are essentially deduced from the bounds for ( $\phi, \psi$ ) and inversion of the parameterization.

The minimax upper bounds are obtained by producing an estimator that attains the bounds. To do so, we leverage that  $p_{\theta}^{(3)}$  can be estimated in Euclidean distance at the parametric rate  $n^{-1/2}$  by the empirical estimator  $\hat{p}_n^{(3)}$  defined in Section 7, Lemma 1. Then, we produce an estimator  $(\hat{\phi}, \hat{\psi})$  for  $(\phi, \psi)$  by solving for  $(\hat{\phi}, \hat{\psi}) \in \arg\min_{\phi, \psi} \|p_{\theta(\phi, \psi)}^{(3)} - \hat{p}_n^{(3)}\|$ . By standard calculations and using the equivalence between  $\|p_{\theta(\phi, \psi)}^{(3)} - p_{\theta(\tilde{\phi}, \tilde{\psi})}^{(3)}\|$  and  $\rho(\phi, \psi; \tilde{\phi}, \tilde{\psi})$  derived in the Proposition 1, we show in Theorem 2 that any such  $(\hat{\phi}, \hat{\psi})$  attains the minimax lower bounds for estimating  $(\phi, \psi)$ . Finally, the upper bounds for the original parameters in the Theorem 1 are obtained by taking  $\hat{\theta} = \theta(\hat{\phi}, \hat{\psi})$ .

### 6 Change of parameterisation

We reparametrise the model in such a way that the i.i.d. limiting cases are highlighted, by changing variables to  $\phi = (\phi_1, \phi_2, \phi_3)$  and  $\psi = (\psi_1, \psi_2)$  defined as

$$\phi(\theta) = \begin{pmatrix} \frac{q-p}{p+q} & 1-p-q & \|f_0 - f_1\| \end{pmatrix}, \quad \psi(\theta) = \begin{pmatrix} \frac{qf_0 + pf_1}{p+q} & \frac{f_0 - f_1}{\|f_0 - f_1\|} \end{pmatrix}$$

Here we have separated the scalar parameters  $\phi$  from the vector parameters  $\psi$ . Defining

$$r(\phi) = \frac{1}{4}(1 - \phi_1^2)\phi_2\phi_3^2,\tag{4}$$

it follows from the discussion in Section 3 that the data Y is close to i.i.d. exactly when  $r(\phi) \approx 0$ . [This is of course true also of other combinations of the components of  $\phi$ , but as equation (10) will show,  $r(\phi)$  is the appropriate combination measuring the "distance" to the i.i.d. case.]

Define

$$\Phi = \Phi(\delta, \epsilon, \zeta) = \{ (\phi(\theta), \psi(\theta)) : \theta \in \Theta(\delta, \epsilon, \zeta) \}, \Phi_L = \Phi_L(\delta, \epsilon, \zeta) = \{ (\phi(\theta), \psi(\theta)) : \theta \in \Theta_L(\delta, \epsilon, \zeta) \},$$

and note that for  $(\phi, \psi) \in \Phi$ , we have

$$-\frac{1-\delta}{1+\delta} \le \phi_1 \le \frac{1-\delta}{1+\delta}, \quad \epsilon \le |\phi_2| \le 1-2\delta, \quad \phi_3 \ge \zeta, \quad |r(\phi)| \ge \delta \epsilon \zeta^2/4, \tag{5}$$

while for  $(\phi, \psi) \in \Phi_L$  we additionally have

$$|\phi_2| \le 1 - L. \tag{6}$$

**Remark 3.** When K = 2, in view of identifiability issues discussed in the next subsection,  $\psi_2$  is not needed in the parametrisation, since we may universally make the choice

$$\psi_2 = \left(\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right).$$

**Remark 4.** The parametrisation  $\theta \mapsto (\phi, \psi)$  is invertible: we calculate

$$p = \frac{1}{2}(1 - \phi_2)(1 - \phi_1),$$
  

$$q = \frac{1}{2}(1 - \phi_2)(1 + \phi_1),$$
  

$$f_0 = \psi_1 - \frac{1}{2}\phi_1\phi_3\psi_2 + \frac{1}{2}\phi_3\psi_2,$$
  

$$f_1 = \psi_1 - \frac{1}{2}\phi_1\phi_3\psi_2 - \frac{1}{2}\phi_3\psi_2.$$

**Remark 5.** Suppose  $\psi_1$  is a probability density function with respect to counting measure on  $\{1, \ldots, K\}$ ,  $\psi_2$  is a function satisfying  $\|\psi_2\| = 1$ ,  $\sum_k \psi_2(k) = 0$ , and  $\phi$  satisfies  $|\phi_1| \le 1$ ,  $|\phi_2| \le 1$  and  $\phi_3 \ge 0$ . Then  $(\phi, \psi)$  lies in  $\Phi(\delta, \epsilon, \zeta)$  if and only if

$$\frac{1}{2}(1-\phi_2)(1-|\phi_1|) \ge \delta, \quad \frac{1}{2}(1-\phi_2)(1+|\phi_1|) \le 1, \quad |\phi_2| \ge \epsilon, \quad \phi_3 \ge \zeta, \tag{7}$$

$$\psi_1(k) - \frac{1}{2}\phi_1\phi_3\psi_2(k) - \frac{1}{2}\phi_3|\psi_2(k)| \ge 0, \quad \forall k \le K.$$
 (8)

#### 6.1 Identifiability of the model

The model (1) is identifiable for the parameter set  $\Theta$  only up to 'label-switching', since Y has the same distribution under the parameters  $(p, q, f_0, f_1)$  and  $(q, p, f_1, f_0)$ ; in the parametrisation  $(\phi, \psi)$ , the distribution of Y is the same under  $(\phi_1, \phi_2, \phi_3, \psi_1, \psi_2)$  and under  $(-\phi_1, \phi_2, \phi_3, \psi_1, -\psi_2)$ . However, it was proved in [5] that aside from this label-switching, the model parameters can be identified from the law of just three consecutive observations. To that end, for any integer m denoting by  $P_{\theta}^{(m)}$  the law of m consecutive observations with parameter  $\theta \in \Theta$ , and by  $p_{\theta}^{(m)}$  the corresponding density with respect to counting measure on  $\{1, \ldots, K\}^m$ , we calculate

$$p_{\theta}^{(3)} = \left(\frac{q}{p+q}\right)g \otimes f_0 \otimes g + \left(\frac{p}{p+q}\right)h \otimes f_1 \otimes h, \tag{9}$$

where  $g = (1-p)f_0 + pf_1$  and  $h = qf_0 + (1-q)f_1$ , and where  $\otimes$  denotes the tensor product so that  $(f \otimes g \otimes h)(a, b, c) = f(a)g(b)h(c), \quad (a, b, c) \in \{1, \dots, K\}^3.$ 

In the  $(\phi, \psi)$  parametrisation, writing, in a slight abuse of notation, just  $p_{\phi,\psi}^{(3)}$  for  $p_{\theta(\phi,\psi)}^{(3)}$ , we have

$$p_{\phi,\psi}^{(3)} = \psi_1 \otimes \psi_1 \otimes \psi_1 + r(\phi) \big( \psi_2 \otimes \psi_2 \otimes \psi_1 + \psi_1 \otimes \psi_2 \otimes \psi_2 \big) \\ + \phi_2 r(\phi) \psi_2 \otimes \psi_1 \otimes \psi_2 - \phi_1 \phi_2 \phi_3 r(\phi) \psi_2 \otimes \psi_2 \otimes \psi_2, \quad (10)$$

where we recall the notation  $r(\phi) = \frac{1}{4}(1 - \phi_1^2)\phi_2\phi_3^2$ ,

Optimal estimation rates can be obtained if we adequately understand the Kullback–Leibler divergence between distributions with different parameters. The Kullback–Leibler divergence between  $P_{\theta(\phi,\psi)}^{(n)}$ and  $P_{\theta(\phi,\tilde{\psi})}^{(n)}$  can be related to the Euclidean distance between the densities  $p_{\phi,\psi}^{(3)}$  and  $p_{\tilde{\phi},\tilde{\psi}}^{(3)}$  (see Lemma 2), and we define a statistical distance  $\rho$  directly on the parameter space  $\Phi$  which is equivalent to this Euclidean distance. The function  $\rho$  is not a true metric because it may not satisfy the triangle inequality and because, due to the identifiability issues reflected by the appearance of factors of  $\operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle)$  in its definition, we may have  $\rho(\phi, \psi; \tilde{\phi}, \tilde{\psi}) = 0$  with  $(\phi, \psi) \neq (\tilde{\phi}, \tilde{\psi})$ . Here  $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on  $\mathbb{R}^K$ ,  $\langle f, g \rangle = \sum_{i=1}^K f(k)g(k)$ .

**Proposition 1.** For r as in equation (4) define m by

$$m(\phi) := (r(\phi), \phi_2 r(\phi), \phi_1 \phi_2 \phi_3 r(\phi)), \tag{11}$$

and define

ρ

$$\begin{aligned} (\phi,\psi;\tilde{\phi},\tilde{\psi}) &= \max\{ |m_1(\phi) - m_1(\tilde{\phi})|, |m_2(\phi) - m_2(\tilde{\phi})|, |m_3(\phi) - \operatorname{sgn}(\langle\psi_2,\tilde{\psi}_2\rangle) \cdot m_3(\tilde{\phi})|, \\ \|\psi_1 - \tilde{\psi}_1\|, \max\{|m_1(\phi)|, |m_1(\tilde{\phi})|\} \cdot \|\psi_2 - \operatorname{sgn}(\langle\psi_2,\tilde{\psi}_2\rangle) \cdot \tilde{\psi}_2\| \}. \end{aligned}$$

There exist constants  $c_1, c_2 > 0$  (which depend on K) such that for all  $(\phi, \psi), (\hat{\phi}, \hat{\psi}) \in \bigcup_{\delta, \epsilon, \zeta} \Phi(\delta, \epsilon, \zeta)$  we have

$$c_1\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \le \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\| \le c_2\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}).$$

## 7 Upper bounds

We obtain the following upper bounds for estimating  $\phi$  and  $\psi$ . Since we are studying limits as the quantities of interest become small, the relative risk may be of as much interest as the absolute risk, and we provide bounds for both quantities. The bounds demonstrate that learning model parameters is possible in the regime where *n* is large enough in relation to  $\delta$ ,  $\epsilon$  and  $\rho$ . Observe firstly that estimation of  $p^{(3)}$  is possible at a parametric rate.

**Lemma 1.** Define the empirical estimator  $\hat{p}_n^{(3)}: \{1, \ldots, K\}^n \to [0, 1]$  by

$$\hat{p}_n^{(3)}(a,b,c) = \frac{1}{n} \sum_{i=1}^{n-2} \mathbb{1}\{Y_i = a, Y_{i+1} = b, Y_{i+2} = c\}.$$

Then for some constant C = C(K, L) and any  $x \ge 1$ 

$$\sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{(\phi,\psi)}(\|\hat{p}^{(3)} - p^{(3)}\| \ge Cx/\sqrt{n}) \le e^{-x^2}.$$

**Theorem 2.** Assume  $\Phi_L$  is non-empty and let  $\hat{\phi}, \hat{\psi}$  be any measurable functions satisfying

$$\|p_{\hat{\phi},\hat{\psi}}^{(3)} - \hat{p}_n^{(3)}\| \le 2 \inf_{(\tilde{\phi},\tilde{\psi})\in\Phi_L} \|p_{\tilde{\phi},\tilde{\psi}}^{(3)} - \hat{p}_n^{(3)}\|.$$

There exists a constant C = C(K, L) > 0 such that the following hold.

1. Assume  $1 \le x^2 \le n\delta^2\epsilon^4\zeta^6$ . Then

$$\sup_{\substack{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)}} \mathbb{P}_{\phi,\psi}\Big(\Big|\frac{1-\hat{\phi}_1^2}{1-\phi_1^2}-1\Big|^2 \ge \frac{2Cx^2}{n\delta^2\epsilon^4\zeta^6}\Big)$$
  
$$\le \sup_{\substack{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)}} \mathbb{P}_{\phi,\psi}\Big(\min(|\hat{\phi}_1-\phi_1|,|\hat{\phi}_1+\phi_1|)^2 \ge \frac{Cx^2}{n\epsilon^4\zeta^6}\Big) \le e^{-x^2}.$$

2. Assume  $1 \le x^2 \le n\delta^2\epsilon^2\zeta^4$ . Then

$$\sup_{\substack{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)}} \mathbb{P}_{\phi,\psi}\Big(\Big|\frac{\hat{\phi}_2}{\phi_2} - 1\Big|^2 \ge C\frac{x^2}{n\delta^2\epsilon^4\zeta^4}\Big) \\ \le \sup_{\substack{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)}} \mathbb{P}_{\phi,\psi}\Big(|\hat{\phi}_2 - \phi_2|^2 \ge C\frac{x^2}{n\delta^2\epsilon^2\zeta^4}\Big) \le e^{-x^2}.$$

3. Assume  $1 \le x^2 \le n\delta^2\epsilon^4\zeta^6$ . Then

$$\sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(\Big|\frac{\hat{\phi}_3}{\phi_3} - 1\Big|^2 \ge C \frac{x^2}{n\delta^2\epsilon^4\zeta^6}\Big) \\ \le \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(|\hat{\phi}_3 - \phi_3|^2 \ge C \frac{x^2}{n\delta^2\epsilon^4\zeta^4}\Big) \le e^{-x^2}.$$

4. Assume  $1 \le x^2 \le n$ . Then

$$\sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(\|\hat{\psi}_1-\psi_1\|^2 \ge \frac{Cx^2}{n}\Big) \le e^{-x^2}.$$

5. Assume  $1 \le x^2 \le n\delta^2\epsilon^2\zeta^4$  and K > 2. Then

$$\sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\left(\min\left(\|\hat{\psi}_2 - \psi_2\|^2, \|\hat{\psi}_2 + \psi_2\|^2\right) \ge \frac{Cx^2}{n\delta^2\epsilon^2\zeta^4}\right) \le e^{-x^2}.$$

Recall that estimating  $\psi_2$  is unnecessary when K = 2 (see Remark 3). Note that the absolute loss in each case is bounded, and one can deduce that the bounds for  $\phi_2$  and for  $\psi$  hold without an upper bound on x, with  $e^{-x^2}$  on the right replaced by zero (for C large enough).

### 8 Lower bounds

We prove lower bounds, matching the previous upper bounds in a suitable regime and demonstrating the impossibility of learning model parameters when n is not large enough in relation to  $\delta$ ,  $\epsilon$  and  $\rho$ . The particular value 1/4 on the right sides in the following is not essential: what is important is that the probabilities are bounded away from zero. The lower bounds over  $\Phi_L$  remain true over the larger set  $\Phi$ .

**Theorem 3.** Grant the compatibility condition (3) and assume  $\epsilon \le 1/3$ ,  $\delta \le 1/6$  and  $L \le 1/3$ . There exists a constant c = c(K) such that the following hold. The infima are over all estimators, i.e. all measurable functions of the data  $(Y_1, \ldots, Y_n)$ .

1. Assume  $n\delta^2\epsilon^4\zeta^6 \ge 1$ . Then

$$\inf_{\hat{\phi}_1} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\left(\min(|\hat{\phi}_1-\phi_1|^2,|\hat{\phi}_1+\phi_1|^2)\geq \frac{c}{n\epsilon^4\zeta^6}\right) \\
\geq \inf_{\hat{\phi}_1} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\left(\left|\frac{1-\tilde{\phi}_1^2}{1-\phi_1^2}-1\right|^2\geq \frac{2c}{n\delta^2\epsilon^4\zeta^6}\right)\geq 1/4.$$

2. Assume  $n\delta^2\epsilon^4\zeta^4 \ge 1$ . Then

$$\begin{split} \inf_{\hat{\phi}_2} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(|\hat{\phi}_2 - \phi_2|^2 \ge \frac{c}{n\delta^2\epsilon^2\zeta^4}\Big) \\ \ge \inf_{\hat{\phi}_2} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(\Big|\frac{\hat{\phi}_2}{\phi_2} - 1\Big|^2 \ge \frac{c}{n\delta^2\epsilon^4\zeta^4}\Big) \ge 1/4. \end{split}$$

3. Assume  $n\delta^2\epsilon^4\zeta^6 \geq 1$ . Then

$$\begin{split} \inf_{\hat{\phi}_2} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(|\hat{\phi}_3 - \phi_3|^2 \ge \frac{c}{n\delta^2\epsilon^4\zeta^4}\Big) \\ \ge \inf_{\hat{\phi}_2} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(\Big|\frac{\hat{\phi}_3}{\phi_3} - 1\Big|^2 \ge \frac{c}{n\delta^2\epsilon^4\zeta^6}\Big) \ge 1/4. \end{split}$$

4. For any n,  $\delta$ ,  $\epsilon$  and  $\zeta$ ,

$$\inf_{\hat{\psi}_1} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi}\Big(\|\hat{\psi}_1-\psi_1\|^2 \ge \frac{c}{n}\Big) \ge 1/4.$$

5. Assume  $n\delta^2\epsilon^2\zeta^4 \ge 1$  and K > 2. Then

$$\inf_{\hat{\psi}_1} \sup_{(\phi,\psi)\in\Phi_L(\delta,\epsilon,\zeta)} \mathbb{P}_{\phi,\psi} \Big( \min(\|\hat{\psi}_2 - \psi_2\|, \|\hat{\psi}_2 + \psi_2\|)^2 \ge \frac{c}{n\delta^2\epsilon^2\zeta^4} \Big) \ge 1/4.$$

#### 9 Conclusions, limitations and future directions

In this work we have quantified the impact on learnability of approaching the i.i.d. boundary within the set of parameters of a hidden Markov model. The limiting cases occur when one hidden state is absorbing, when the underlying Markov chain becomes a sequence of independent variables, or when the emission distributions are equal. We have proved both upper and lower bounds for the estimation rates of the parameters in a hidden Markov models with two hidden states and finitely many possible outcomes. Our results show that a phase transition occurs near the boundary and quantify how large the sample has to be in order to get estimators with prescribed error with high probability.

Some tricky regions of the parameter space are not fully captured in the upper and lower bounds. Specifically, the condition on n in the lower bound for estimating  $\phi_2$  differs by a factor of  $\epsilon^2$  from the corresponding condition in the upper bound. In the upper bound for  $\phi_1$ , in the region  $n\delta^2\epsilon^4\zeta^6 < x^2 \leq n\epsilon^4\zeta^6$  we do not obtain the correct rate of decay in the probability as x increases.

In this range we can obtain something by applying the bound with  $y^2 = \min(x^2, n\delta^2\epsilon^4\zeta^6)$  but we cannot expect that this gives the correct dependence on y. [When  $x^2 \ge n\epsilon^4\zeta^6$  we may replace  $e^{-x^2}$  with zero, as noted after the theorem for  $\phi_2$  and  $\psi$ .] A similar gap exists for estimating  $\phi_3$ . Our results already work for a wide range of parameters, and extending to the few remaining cases is an interesting issue for future research.

Our results are limited to the context of latent variables with two hidden states and multinomial emission distributions. We believe similar results hold with more than two hidden states and with arbitrary nonparametric emission distributions. Investigation of phase transitions for more general HMMs and misspecified modelling will be the object of further work. Developments of our findings for clustering, multiple testing and sparse settings will also be the object of further work, and all will depend fundamentally on the results obtained here.

On the practical side, usual estimation algorithms can be expected to exhibit bad computational behaviour when the unknown true parameters lie near the learning frontier. We have not tackled this issue here and we believe it merits substantive investigation, both in building robust algorithms and in detecting the poor performance in the problematic region. This last question is interesting both from a practical and a theoretical point of view.

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## A Proofs

The following lemma exhibits the fact that  $p^{(3)}$  contains qualitatively the same information as  $p^{(m)}$  for  $m \ge 3$ . The information here is quantified by the Kullback–Leibler divergence, defined for distributions with densities p, q with respect to some common dominating measure by

$$K(p;q) = \mathbb{E}_p\left(\log\frac{p}{q}\right).$$

**Lemma 2.** For any  $n \in \mathbb{N}$  and any  $\theta, \tilde{\theta} \in \Theta$ ,

$$K(p_{\theta}^{(n)}; p_{\tilde{\theta}}^{(n)}) \leq \lceil n/3 \rceil K(p_{\theta}^{(3)}; p_{\tilde{\theta}}^{(3)}).$$

If further for all k we have  $\min(\tilde{f}_0(k), \tilde{f}_1(k)) \ge c$  for some constant c > 0, then

$$K(p_{\theta}^{(n)}; p_{\tilde{\theta}}^{(n)}) \leq \lceil n/3 \rceil c^{-3} \| p_{\theta}^{(3)} - p_{\tilde{\theta}}^{(3)} \|_{2}^{2}.$$

*Proof.* For any  $k, k' \ge 1$  satisfying  $k' \le 3k$ , we have

$$K(p_{\theta}^{(k')}; p_{\tilde{\theta}}^{(k')}) \le K(p_{\theta}^{(3k)}; p_{\tilde{\theta}}^{(3k)}) \le kK(p_{\theta}^{(3)}; p_{\tilde{\theta}}^{(3)}),$$

which yields the first claim.

For the second claim, recall that K(p;q) is upper bounded by the chi-square distance  $\chi^2(p,q) = \mathbb{E}_q[(p/q-1)^2]$  (e.g. [36, Lemma 2.7]). The result then follows from the fact that if  $\tilde{f}_0$ ,  $\tilde{f}_1$  are bounded below by c then  $p_{\tilde{\theta}}^{(3)}$  is lower bounded by  $c^3$ .

#### A.1 Proof of Proposition 1

Recall the definition (11) of m as

$$m(\phi) := (r(\phi), \phi_2 r(\phi), \phi_1 \phi_2 \phi_3 r(\phi)), \quad r(\phi) = \frac{1}{4} (1 - \phi_1^2) \phi_2 \phi_3^2.$$

We write  $\tilde{m} = m(\tilde{\phi})$ , and we write  $\psi_{ijk}$  for  $\psi_i \otimes \psi_j \otimes \psi_k$  and  $\tilde{\psi}_{ijk}$  for  $\tilde{\psi}_i \otimes \tilde{\psi}_j \otimes \tilde{\psi}_k$ . Then from equation (10) we have

$$p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)} = (\psi_{111} - \tilde{\psi}_{111}) + \{m_1(\psi_{221} + \psi_{122}) - \tilde{m}_1(\tilde{\psi}_{221} + \tilde{\psi}_{122})\} + \{m_2\psi_{212} - \tilde{m}_2\tilde{\psi}_{212}\} - \{m_3\psi_{222} - \tilde{m}_3\tilde{\psi}_{222}\}.$$
(12)

Recalling that  $\langle \cdot, \cdot \rangle$  denotes the Euclidean inner product on  $\mathbb{R}^K$ , we have  $\langle \psi_1, 1 \rangle = 1$ ,  $\langle \psi_2, 1 \rangle = 0$ ,  $\|\psi_2\| = 1$  and  $\|1\| = K^{1/2}$ . Let  $\langle \cdot, \cdot \rangle$  also denote the Euclidean inner product on  $\mathbb{R}^{3 \times 3 \times 3}$ , wherein for functions  $f_i, \tilde{f}_i : \{1, \ldots, K\} \to \mathbb{R}, i \leq 3$  we have

$$\langle f_1 \otimes f_2 \otimes f_3, \tilde{f}_1 \otimes \tilde{f}_2 \otimes \tilde{f}_3 \rangle = \langle f_1, \tilde{f}_1 \rangle \langle f_2, \tilde{f}_2 \rangle \langle f_3, \tilde{f}_3 \rangle$$

Lower bounding  $\|p_{\phi,\psi}^{(3)} - p_{\phi,\tilde{\psi}}^{(3)}\|$  For any function  $f : \{1,\ldots,K\} \to \mathbb{R}$ , we have

$$\langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, f \otimes 1 \otimes 1 \rangle = \langle \psi_{111} - \tilde{\psi}_{111}, f \otimes 1 \otimes 1 \rangle = \langle \psi_1 - \tilde{\psi}_1, f \rangle.$$

Then

$$\begin{aligned} \|\psi_{1} - \psi_{1}\| &= \sup_{\|f\|=1} |\langle \psi_{1} - \psi_{1}, f \rangle| \\ &= \sup_{\|f\|=1} |\langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, f \otimes 1 \otimes 1 \rangle| \\ &\leq \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\| \sup_{\|f\|=1} \|f \otimes 1 \otimes 1\| = K \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|, \end{aligned}$$
(13)

and similarly,

$$\langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, 1 \otimes f \otimes f \rangle = \langle \psi_{111} - \tilde{\psi}_{111}, 1 \otimes f \otimes f \rangle + \langle m_1\psi_{122} - \tilde{m}_1\tilde{\psi}_{122}, 1 \otimes f \otimes f \rangle$$

$$= \langle \psi_1 - \tilde{\psi}_1, f \rangle^2 + m_1 \langle \psi_2, f \rangle^2 - \tilde{m}_1 \langle \tilde{\psi}_2, f \rangle^2.$$

$$(14)$$

Choosing  $f = \psi_2 + \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\psi}_2$  (with the convention that  $\operatorname{sgn}(0) = +1$ ), we observe that

$$\langle \psi_2, f \rangle = 1 + |\langle \psi_2, \tilde{\psi}_2 \rangle| = \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \langle \tilde{\psi}_2, f \rangle.$$

In particular we note that  $\langle \psi_2, f \rangle^2 = \langle \tilde{\psi}_2, f \rangle^2 = (1 + |\langle \psi_2, \tilde{\psi}_2 \rangle|)^2 \ge 1$ . Since also  $||f||^2 = 2 + 2|\langle \psi_2, \tilde{\psi}_2 \rangle| \le 4$ , returning to (14) we observe that

$$|m_{1} - \tilde{m}_{1}| \leq ||f||^{2} ||\psi_{1} - \tilde{\psi}_{1}||^{2} + ||1 \otimes f \otimes f|| ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}||$$
  
$$\leq 4 ||\psi_{1} - \tilde{\psi}_{1}||^{2} + 4K^{1/2} ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}||$$
  
$$\leq 4(K^{7/2} + K^{1/2}) ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}||, \qquad (15)$$

where for the last line we have used equation (13) and the fact that  $||p_{\phi,\psi}^{(3)} - p_{\phi,\psi}^{(3)}||^2 \leq K^3$ . We continue by considering the expression  $f \otimes 1 \otimes f$ , for which we have

$$\begin{aligned} \langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, f \otimes 1 \otimes f \rangle &= \langle \psi_{111} - \tilde{\psi}_{111}, f \otimes 1 \otimes f \rangle + \langle m_2 \psi_{212} - \tilde{m}_2 \tilde{\psi}_{212}, f \otimes 1 \otimes f \rangle \\ &= \langle \psi_1 - \tilde{\psi}_1, f \rangle^2 + m_2 \langle \psi_2, f \rangle^2 - \tilde{m}_2 \langle \tilde{\psi}_2, f \rangle^2 \end{aligned}$$

Recognising symmetry with equation (14), we again choose  $f = \psi_2 + \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\psi}_2$  to obtain

$$|m_2 - \tilde{m}_2| \le 4(K^{7/2} + K^{1/2}) ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}||.$$
(16)

Finally, considering the expression  $f \otimes f \otimes f$ , we observe that

$$\begin{split} \langle p_{\phi,\psi}^{(3)} - p_{\bar{\phi},\bar{\psi}}^{(3)}, f \otimes f \otimes f \rangle &= \langle \psi_{111} - \tilde{\psi}_{111}, f \otimes f \otimes f \rangle + \langle m_1(\psi_{221} + \psi_{122}) - \tilde{m}_1(\tilde{\psi}_{221} + \tilde{\psi}_{122}), f \otimes f \otimes f \rangle \\ &+ \langle m_2\psi_{212} - \tilde{m}_2\tilde{\psi}_{212}, f \otimes f \otimes f \rangle - \langle m_3\psi_{222} - \tilde{m}_3\tilde{\psi}_{222}, f \otimes f \otimes f \rangle. \end{split}$$

In other words,

$$\begin{split} \langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, f \otimes f \otimes f \rangle &= \langle \psi_1 - \tilde{\psi}_1, f \rangle^3 + 2 \left( m_1 \langle \psi_2, f \rangle^2 \langle \psi_1, f \rangle - \tilde{m}_1 \langle \tilde{\psi}_2, f \rangle^2 \langle \tilde{\psi}_1, f \rangle \right) \\ &+ \left( m_2 \langle \psi_2, f \rangle^2 \langle \psi_1, f \rangle - \tilde{m}_2 \langle \tilde{\psi}_2, f \rangle^2 \langle \tilde{\psi}_1, f \rangle \right) - \left( m_3 \langle \psi_2, f \rangle^3 - \tilde{m}_3 \langle \tilde{\psi}_2, f \rangle^3 \right) \end{split}$$

Once more choosing  $f = \psi_2 + \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\psi}_2$ , we obtain (recall that by construction  $||f|| \leq 2$ ,  $1 \leq \langle \psi_2, f \rangle^2 = \langle \tilde{\psi}_2, f \rangle^2 \leq 4$ , and also  $\operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \langle \psi_2, f \rangle = \langle \tilde{\psi}_2, f \rangle$ )

$$|m_{3} - \operatorname{sgn}(\langle \psi_{2}, \tilde{\psi}_{2} \rangle) \cdot \tilde{m}_{3}| \leq 8 \|\psi_{1} - \tilde{\psi}_{1}\|^{3} + 8 \|p_{\phi,\psi}^{(3)} - p_{\phi,\psi}^{(3)}\| + 8 |m_{1}\langle \psi_{1}, f \rangle - \tilde{m}_{1}\langle \tilde{\psi}_{1}, f \rangle| + 4 |m_{2}\langle \psi_{1}, f \rangle - \tilde{m}_{2}\langle \tilde{\psi}_{1}, f \rangle|.$$

For some constant C = C(K) we have

$$\begin{split} \left| m_1 \langle \psi_1, f \rangle - \tilde{m}_1 \langle \psi_1, f \rangle \right| &\leq |\langle \psi_1, f \rangle| |m_1 - \tilde{m}_1| + |\tilde{m}_1| |\langle \psi_1 - \psi_1, f \rangle| \\ &\leq 2 \|\psi_1\| |m_1 - \tilde{m}_1| + 2|\tilde{m}_1| \|\psi_1 - \tilde{\psi}_1\| \\ &\leq C \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|, \end{split}$$

where for the last line we have used equations (13) and (15) and that  $\|\psi_1\| \leq K^{1/2}$  and  $|\tilde{m}_1| \leq \tilde{\phi}_3^2/4 \leq \|\tilde{f}_0 - \tilde{f}_1\|^2/4 \leq K/4$ .

Similarly, using equation (16) and the fact that  $|\tilde{m}_2|$  is suitably bounded, we have for some C = C(K)

$$\left|m_{2}\langle\psi_{1},f\rangle-\tilde{m}_{2}\langle\tilde{\psi}_{1},f\rangle\right|\leq C\|p_{\phi,\psi}^{(3)}-p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|.$$

We deduce for some different constant C = C(K) that

$$|m_3 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{m}_3| \le C ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}||.$$
(17)

Finally, for  $\psi_2$  we show that for some C we have

$$\max(|m_1|, |\tilde{m}_1|) \|\psi_2 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\psi}_2 \| \le C \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|.$$
(18)

If  $\psi_2 = \tilde{\psi}_2$  there is nothing to prove, so we assume without loss of generality that  $\psi_2 \neq \tilde{\psi}_2$ . Also assume that  $|m_1| \geq |\tilde{m}_1|$ , the final bound then following by symmetry. Returning to equation (14) with f to be chosen, we see that

$$m_1(\langle \psi_2, f \rangle^2 - \langle \tilde{\psi}_2, f \rangle^2) = \langle \psi_1 - \tilde{\psi}_1, f \rangle^2 - \langle p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}, 1 \otimes f \otimes f \rangle - \langle \tilde{\psi}_2, f \rangle^2 (m_1 - \tilde{m}_1).$$

Since  $\langle \psi_2, f \rangle^2 - \langle \tilde{\psi}_2, f \rangle^2 = \langle \psi_2 - \tilde{\psi}_2, f \rangle \langle \psi_2 + \tilde{\psi}_2, f \rangle$  we obtain

$$|m_1\langle\psi_2 - \tilde{\psi}_2, f\rangle\langle\psi_2 + \tilde{\psi}_2, f\rangle| \le ||f||^2 ||\psi_1 - \tilde{\psi}_1||^2 + K||f||^2 ||p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}|| + |m_1 - \tilde{m}_1|\langle\tilde{\psi}_2, f\rangle^2.$$
(19)

Observe that  $\psi_2 + \tilde{\psi}_2$  is orthogonal to  $\psi_2 - \tilde{\psi}_2$  (this arises from the fact that  $\psi_2$  and  $\tilde{\psi}_2$  have unit norms) and choose

$$f = \frac{\psi_2 + \psi_2}{\|\psi_2 + \tilde{\psi}_2\|} + \frac{\psi_2 - \psi_2}{\|\psi_2 - \tilde{\psi}_2\|}$$

note that

$$\langle \psi_2 - \tilde{\psi}_2, f \rangle \langle \psi_2 + \tilde{\psi}_2, f \rangle = \| \psi_2 - \tilde{\psi}_2 \| \| \psi_2 + \tilde{\psi}_2 \|$$

Since also  $||f|| \le 2$  and  $|\langle \tilde{\psi}_2, f \rangle| \le 2$ , continuing from equation (19) and using equations (13) and (15) we see that for a constant C = C(K)

$$\begin{aligned} |m_1| \|\psi_2 - \tilde{\psi}_2\| \|\psi_2 + \tilde{\psi}_2\| &\leq 4 \|\psi_1 - \tilde{\psi}_1\|^2 + 4K \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\| + 4|m_1 - \tilde{m}_1| \\ &\leq 2C \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|. \end{aligned}$$

Observing that

$$\begin{split} \|\psi_{2} - \tilde{\psi}_{2}\|^{2} \|\psi_{2} + \tilde{\psi}_{2}\|^{2} &= \|\psi_{2} - \operatorname{sgn}(\langle\psi_{2}, \tilde{\psi}_{2}\rangle) \cdot \tilde{\psi}_{2}\|^{2} \|\psi_{2} + \operatorname{sgn}(\langle\psi_{2}, \tilde{\psi}_{2}\rangle) \cdot \tilde{\psi}_{2}\|^{2} \\ &= \|\psi_{2} - \operatorname{sgn}(\langle\psi_{2}, \tilde{\psi}_{2}\rangle) \cdot \tilde{\psi}_{2}\|^{2} \left(2 + 2|\langle\psi_{2}, \tilde{\psi}_{2}\rangle|\right) \\ &\geq 2\|\psi_{2} - \operatorname{sgn}(\langle\psi_{2}, \tilde{\psi}_{2}\rangle) \cdot \tilde{\psi}_{2}\|^{2}, \end{split}$$

and recalling we assumed that  $|m_1| \ge |\tilde{m}_1|$ , equation (18) follows.

The proof that  $\|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|$  is lower bounded up to a constant by  $\rho(\phi,\psi;\tilde{\phi},\tilde{\psi})$  follows by combining equations (13) and (15)–(18)

Upper bounding  $\|p_{\phi,\psi}^{(3)} - p_{\bar{\phi},\bar{\psi}}^{(3)}\|$  From equation (12),

$$\begin{split} \|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\| &\leq \|\psi_{111} - \tilde{\psi}_{111}\| + |m_1 - \tilde{m}_1| \|\psi_{221} + \psi_{122}\| + |\tilde{m}_1| \|\psi_{221} - \tilde{\psi}_{221}\| \\ &+ |\tilde{m}_1| \|\psi_{122} - \tilde{\psi}_{122}\| + |m_2 - \tilde{m}_2| \|\psi_{212}\| + |\tilde{m}_2| \|\psi_{212} - \tilde{\psi}_{212}\| \\ &+ |m_3 - \tilde{m}_3| \|\psi_{222}\| + |\tilde{m}_3| \|\psi_{222} - \tilde{\psi}_{222}\|. \end{split}$$
(20)

Note that the bound remains valid if we replace the final two terms by

$$|m_3 + \tilde{m}_3| \|\psi_{222}\| + |\tilde{m}_3| \|\psi_{222} + \psi_{222}\|_{22}$$

we focus on the case where  $sgn(\langle \psi_2, \tilde{\psi}_2 \rangle) = +1$  for which the original decomposition yields suitable bounds, but the proof in the other case is similar using the alternative decomposition.

As used already in proving the lower bound on  $\|p_{\phi,\psi}^{(3)} - p_{\tilde{\phi},\tilde{\psi}}^{(3)}\|$ , we note that

$$\max(\|\psi_{221}\|, \|\psi_{122}\|, |\tilde{m}_1|, \|\psi_{212}\|, |\tilde{m}_2|, \|\psi_{222}\|, |\tilde{m}_3|) \le C,$$

for some C = C(K). To conclude the proof it thus suffices to bound the tensor product terms  $\|\psi_{ijk} - \tilde{\psi}_{ijk}\|$  in terms of the differences  $\|\psi_1 - \tilde{\psi}_1\|, \|\psi_2 - \tilde{\psi}_2\|$ . First we decompose

$$\begin{split} \|\psi_1 \otimes \psi_1 \otimes \psi_1 - \tilde{\psi}_1 \otimes \tilde{\psi}_1 \otimes \tilde{\psi}_1 \| &\leq \|\psi_1 \otimes \psi_1 \otimes \psi_1 - \tilde{\psi}_1 \otimes \psi_1 \otimes \psi_1 \otimes \psi_1 \| \\ &+ \|\tilde{\psi}_1 \otimes \psi_1 \otimes \psi_1 - \tilde{\psi}_1 \otimes \tilde{\psi}_1 \otimes \psi_1 \| + \|\tilde{\psi}_1 \otimes \tilde{\psi}_1 \otimes \psi_1 - \tilde{\psi}_1 \otimes \tilde{\psi}_1 \otimes \tilde{\psi}_1 \|, \end{split}$$

so that

$$\|\psi_{111} - \tilde{\psi}_{111}\| \le \|\psi_1 - \tilde{\psi}_1\| (\|\psi_1\|^2 + \|\psi_1\| \|\tilde{\psi}_1\| + \|\tilde{\psi}_1\|^2) \le 3K \|\psi_1 - \tilde{\psi}_1\|.$$
(21)

We also note, recalling that  $\psi_2$  and  $\tilde{\psi}_2$  have unit norms, that

$$\begin{aligned} \|\psi_{221} - \tilde{\psi}_{221}\|^2 &= \|\psi_{221}\|^2 + \|\tilde{\psi}_{221}\|^2 - 2\langle\psi_{221}, \tilde{\psi}_{221}\rangle \\ &= \|\psi_1\|^2 + \|\tilde{\psi}_1\|^2 - 2\langle\psi_2, \tilde{\psi}_2\rangle^2\langle\psi_1, \tilde{\psi}_1\rangle \\ &= \|\psi_1 - \tilde{\psi}_1\|^2 + 2\langle\psi_1, \tilde{\psi}_1\rangle \left(1 - \langle\psi_2, \tilde{\psi}_2\rangle^2\right) \\ &\leq \|\psi_1 - \tilde{\psi}_1\|^2 + 2\|\psi_1\| \|\tilde{\psi}_1\| \|1 - \langle\psi_2, \tilde{\psi}_2\rangle^2|. \end{aligned}$$

Observe that

$$\|\psi_2 - \tilde{\psi}_2\|^2 = 2(1 - \langle \psi_2, \tilde{\psi}_2 \rangle), \tag{22}$$

and hence

$$\left|1 - \langle \psi_2, \tilde{\psi}_2 \rangle^2\right| = \left|1 + \langle \psi_2, \tilde{\psi}_2 \rangle\right| \left|1 - \langle \psi_2, \tilde{\psi}_2 \rangle\right| \le 2|1 - \langle \psi_2, \tilde{\psi}_2 \rangle| = \|\psi_2 - \tilde{\psi}_2\|^2$$

We deduce that

$$\|\psi_{221} - \tilde{\psi}_{221}\|^2 \le \|\psi_1 - \tilde{\psi}_1\|^2 + 2\|\psi_1\| \|\tilde{\psi}_1\| \|\psi_2 - \tilde{\psi}_2\|^2 \le \|\psi_1 - \tilde{\psi}_1\|^2 + 2K \|\psi_2 - \tilde{\psi}_2\|^2.$$
(23)

By symmetry, the same bound holds for  $\|\psi_{122} - \tilde{\psi}_{122}\|$  and for  $\|\psi_{212} - \tilde{\psi}_{212}\|$ . Furthermore  $\|\psi_{222}\| = 1$ , and using (22),

$$\|\psi_{222} - \psi_{222}\|^{2} = \|\psi_{222}\|^{2} + \|\psi_{222}\|^{2} - 2\langle\psi_{222},\psi_{222}\rangle$$
  
$$= 2 - 2\langle\psi_{2},\tilde{\psi}_{2}\rangle^{3}$$
  
$$= 2(1 - \langle\psi_{2},\tilde{\psi}_{2}\rangle)(1 + \langle\psi_{2},\tilde{\psi}_{2}\rangle + \langle\psi_{2},\tilde{\psi}_{2}\rangle^{2})$$
  
$$\leq 3\|\psi_{2} - \tilde{\psi}_{2}\|^{2}.$$
 (24)

The claim follows from inserting equations (21), (23) and (24) into equation (20).

#### A.2 Proof of Theorem 2

We start with the proof of Lemma 1, that  $p^{(3)}$  can be estimated at a parametric rate.

*Proof of Lemma 1.* We use a Markov chain concentration result from [32]. Theorem 3.4 therein (but note there is an updated version of the paper on arXiv) tells us that for any stationary Markov chain  $\mathbf{Z} = (Z^{(1)}, Z^{(2)}, ...)$  of pseudo-spectral gap  $\gamma_{ps}$  (defined as in [32]) and any function h satisfying  $\mathbb{E}[h(Z^{(1)})^2] \leq \sigma^2$  and  $\|h\|_{\infty} \leq b$ ,

$$\mathbb{P}(|\sum_{i=1}^{n} h(Z^{(i)}) - Eh(Z^{(1)})| \ge x) \le 2\exp\left(-\frac{x^2\gamma_{\text{ps}}}{8(n+1/\gamma_{\text{ps}})\sigma^2 + 20bx}\right).$$
(25)

We apply to the chain Z defined by  $Z^{(n)} = (X_n, X_{n+1}, X_{n+2}, Y_n, Y_{n+1}, Y_{n+2})$ ; we begin by showing the pseudo-spectral gap of this chain is bounded from below. Proposition 3.4 of the same reference shows that the reciprocal of the pseudo-spectral gap of any chain is bounded above by twice the mixing time  $t_{\text{mix}}^Z$  of the chain, defined as the first time that the law of Z, regardless of the starting distribution, is within 1/4 of its invariant distribution in total variation distance. We note that  $t_{\text{mix}}^Z$  is equal to the mixing time  $t_{\text{mix}}^{X^{(3)}}$  of the chain  $((X_n, X_{n+1}, X_{n+2})_{n\geq 0})$ . This latter quantity is equal to  $t_{\text{mix}}^X + 2$  where  $t_{\text{mix}}^X$  denotes the mixing time of the chain X itself. Finally, the matrix Q has eigenvalues 1 and  $\phi_2$ , and an explicit computation yields that  $\max_{ij} |Q_{ij}^n - \pi_j| = \max_i(\pi_i) |\phi_2|^n$  so that the mixing time of X is at most

$$\Big\lceil \frac{\log 4}{\log(1/|\phi_2|)} \Big\rceil \le \Big\lceil \frac{\log 4}{\log(1/(1-L))} \Big\rceil \le \Big\lceil \frac{\log 4}{L} \Big\rceil,$$

which is a constant since L is fixed. The pseudo-spectral gap of the chain Z is thus lower bounded by some constant  $\gamma = \gamma(L)$ .

Applying equation (25) with  $h(Z) = \mathbb{1}\{Z_4 = a, Z_5 = b, Z_6 = c\}$ , which satisfies  $\mathbb{E}h^2 \leq 1$  and  $\|h\|_{\infty} \leq 1$ , we see that

$$\mathbb{P}_{\phi,\psi}\big(n|\hat{p}^{(3)}(a,b,c) - p^{(3)}_{\phi,\psi}(a,b,c)| \ge x\big) \le 2\exp\Big(-\frac{\gamma x^2}{8n + 8/\gamma + 20x}\Big),$$

hence for some constant c' > 0

$$\mathbb{P}_{\phi,\psi}\big(|\hat{p}^{(3)}(a,b,c) - p^{(3)}_{\phi,\psi}(a,b,c)| \ge x/\sqrt{n}\big) \le 2\exp\Big(-c'\min\Big(x^2, x^2n, x\sqrt{n}\Big)\Big).$$

Using that  $\|\hat{p}^{(3)} - p^{(3)}\| \le K^3 \max_{a,b,c} |\hat{p}^{(3)}(a,b,c) - p^{(3)}(a,b,c)|$  and a union bound, we deduce for some C = C(K,L) and for  $x \le \sqrt{n}$  that

$$\mathbb{P}_{\phi,\psi}(\|\hat{p}^{(3)} - p^{(3)}\| \ge K^3 x / \sqrt{n}) \le 2K^3 \exp(-Cx^2).$$

For  $x \ge 1$  we may absorb the factor  $2K^3$  into the exponential by changing the constant C, and by replacing x with C'x we can remove this constant, yielding the result in the case where  $C'x \le \sqrt{n}$ . In the other case, since  $\|\hat{p}^{(3)} - p^{(3)}\|$  is bounded (by  $K^{3/2}$ ), by increasing the constant C' if necessary we have  $C'x/\sqrt{n} \ge K^{3/2}$  so that the probability in question is equal to  $0 \le e^{-x^2}$ .

To prove Theorem 2, observe that by Lemma 1 there exist events  $A_n$  of probability at least  $e^{-x^2}$  on which

$$\|\hat{p}_n^{(3)} - p_{\phi,\psi}^{(3)}\| \le Cx/\sqrt{n}.$$

The true parameter  $(\phi, \psi)$  lies in  $\Phi_L$  so that any estimators constructed in Theorem 2 satisfy

$$\|p_{\hat{\phi},\hat{\psi}}^{(3)} - \hat{p}_n^{(3)}\| \le 2\|p_{\phi,\psi}^{(3)} - \hat{p}_n^{(3)}\|,$$

and hence on the event  $\mathcal{A}_n$  further satisfy

$$\|p_{\hat{\phi},\hat{\psi}}^{(3)} - p_{\phi,\psi}^{(3)}\| \le \|p_{\hat{\phi},\hat{\psi}}^{(3)} - \hat{p}_n^{(3)}\| + \|p_{\phi,\psi}^{(3)} - \hat{p}_n^{(3)}\| \le 3\|p_{\phi,\psi}^{(3)} - \hat{p}_n^{(3)}\| \le 3Cx/\sqrt{n},$$

By Proposition 1 we deduce for a constant C' that  $\rho(\hat{\phi}, \hat{\psi}; \phi, \psi) \leq C' x/\sqrt{n}$  on  $\mathcal{A}_n$ . For estimating  $\psi$ , observe that  $\|\hat{\psi}_1 - \psi_1\| \leq \rho(\hat{\phi}, \hat{\psi}; \phi, \psi)$  and  $|r(\phi)| \min(\|\hat{\psi}_2 - \psi_2\|, \|\hat{\psi}_2 + \psi_2\|) \leq \rho(\hat{\phi}, \hat{\psi}; \phi, \psi)$ . The upper bound for estimating  $\psi_1$  is immediate and, recalling from equation (5) that  $|r(\phi)| \geq \delta \epsilon \zeta^2/4$ , we also deduce the bound for  $\psi_2$ .

For the bounds on  $\phi$ , observe firstly that it suffices to prove the upper bounds on the absolute risk since, taking  $\phi_2$  as an example, for  $(\phi, \psi) \in \Phi_L(\delta, \epsilon, \zeta)$  we have

$$\mathbb{P}_{\phi,\psi}\left(|\hat{\phi}_2/\phi_2 - 1|^2 \ge \frac{C}{n\delta^2\epsilon^4\zeta^4}\right) = \mathbb{P}_{\phi,\psi}\left(|\hat{\phi}_2 - \phi_2|^2 \ge \frac{C\phi_2^2}{n\delta^2\epsilon^4\zeta^4}\right)$$
$$\le \mathbb{P}_{\phi,\psi}\left(|\hat{\phi}_2 - \phi_2| \ge \frac{C\epsilon^2}{n\delta^2\epsilon^4\zeta^4}\right).$$
(26)

(See also after equation (27) for a similar argument with  $\phi_1$ .) Define

$$\omega_1(\phi,\psi;\eta) \coloneqq \sup\Big\{ |\phi_1 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\phi}_1| : \rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \le \eta \Big\},\$$

and

$$\omega_j(\phi,\psi;\eta) \coloneqq \sup\Big\{ |\phi_j - \tilde{\phi}_j| \, : \, \rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \le \eta \Big\}, \qquad j = 2,3.$$

We have the following.

**Proposition 2.** Let  $\eta \in [0, 1]$ . There exist constants c, C for which the following hold.

$$\eta < c(1 - \phi_1^2)\phi_2^2\phi_3^3 \implies \omega_1(\phi, \psi; \eta) \le \frac{C\eta}{\phi_2^2\phi_3^3},$$
  
$$\eta < c(1 - \phi_1^2)|\phi_2|\phi_3^2 \implies \omega_2(\phi, \psi; \eta) \le \frac{C\eta}{(1 - \phi_1^2)|\phi_2|\phi_3^2},$$
  
$$\eta < c(1 - \phi_1^2)\phi_2^2\phi_3^3 \implies \omega_3(\phi, \psi; \eta) \le \frac{C\eta}{(1 - \phi_1^2)\phi_2^2\phi_3^2}.$$

The conditions of Theorem 2 ensure that on the event  $\mathcal{A}_n$  we may apply Proposition 2 with  $\eta = C'x/\sqrt{n}$ . We deduce the upper bounds for estimating the components of  $\phi$  immediately upon replacing  $\phi_1, \phi_2$  and  $\phi_3$  on the right sides in Proposition 2 by their lower bounds [for  $\phi_1$  we note that  $\min(|\hat{\phi}_1 - \phi_1|, |\hat{\phi}_1 + \phi_1|) \le |\phi_1 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\phi}_1|$ ].

*Proof of Proposition 2.* Recall that  $m(\phi) = (r(\phi), \phi_2 r(\phi), \phi_1 \phi_2 \phi_3 r(\phi))$  with  $r(\phi) = \frac{1}{4}(1 - \phi_1^2)\phi_2\phi_3^2$ . If  $r(\phi) = 0$  then for each item no  $\eta \in [0, 1]$  satisfies the conditions and so there is nothing to prove. Otherwise, note that m is invertible when restricted to  $\{\phi : r(\phi) \neq 0\} \supset \Phi(\delta, \epsilon, \zeta)$  and its inverse is given by  $\phi(m)$  defined by

$$\begin{split} \phi_1(m) &= m_3/(4m_1^2m_2 + m_3^2)^{1/2} \\ \phi_2(m) &= m_2/m_1, \\ \phi_3(m) &= (4m_1^2m_2 + m_3^2)^{1/2}/m_2. \end{split}$$

For arbitrary  $(\phi, \psi; \tilde{\phi}, \tilde{\psi})$  satisfying  $\rho(\phi, \psi; \tilde{\phi}, \tilde{\psi}) \leq \eta$ , we define

$$\Delta_1 \coloneqq m_1(\tilde{\phi}) - m_1(\phi), \quad \Delta_2 \coloneqq m_2(\tilde{\phi}) - m_2(\phi), \quad \Delta_3 \coloneqq \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot m_3(\tilde{\phi}) - m_3(\phi).$$

Define also

$$g(\phi) \coloneqq 4m_1(\phi)^2 m_2(\phi) + m_3(\phi)^2$$
  
=  $\{m_2(\phi)\phi_3\}^2$   
=  $\{\frac{1}{4}(1-\phi_1^2)\phi_2^2\phi_3^3\}^2$ ,

and, for  $\Delta = (\Delta_1, \Delta_2, \Delta_3)$ ,

$$h_{\phi}(\Delta) \coloneqq g(\phi) - g(\phi) \\ = 4(m_1(\phi) + \Delta_1)^2(m_2(\phi) + \Delta_2) + (m_3(\phi) + \Delta_3)^2 - \{4m_1(\phi)^2m_2(\phi) + m_3(\phi)^2\}.$$

Observe that

$$h_{\phi}(\Delta) = 8m_1(\phi)m_2(\phi)\Delta_1 + 8m_1(\phi)\Delta_1\Delta_2 + 4m_2(\phi)\Delta_1^2 + 4\Delta_1^2\Delta_2 + 4m_1(\phi)^2\Delta_2 + 2m_3(\phi)\Delta_3 + \Delta_3^2.$$

## **Bounding** $\omega_1$ We decompose,

$$\begin{split} \phi_1 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\phi}_1 &= \frac{m_3(\phi)}{\sqrt{4m_1(\phi)^2 m_2(\phi) + m_3(\phi)^2}} - \frac{\operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot m_3(\tilde{\phi})}{\sqrt{4m_1(\tilde{\phi})^2 m_2(\tilde{\phi}) + m_3(\tilde{\phi})^2}} \\ &= \frac{m_3(\phi)}{\sqrt{g(\phi)}} - \frac{m_3(\phi) + \Delta_3}{\sqrt{g(\phi) + h_{\phi}(\Delta)}} \\ &= m_3(\phi) \Big\{ \frac{1}{\sqrt{g(\phi)}} - \frac{1}{\sqrt{g(\phi) + h_{\phi}(\Delta)}} \Big\} - \frac{\Delta_3}{\sqrt{g(\phi) + h_{\phi}(\Delta)}} \\ &= \frac{m_3(\phi)}{\sqrt{g(\phi)(g(\phi) + h_{\phi}(\Delta))}} \Big\{ \sqrt{g(\phi) + h_{\phi}(\Delta)} - \sqrt{g(\phi)} \Big\} - \frac{\Delta_3}{\sqrt{g(\phi) + h_{\phi}(\Delta)}} \\ &= \frac{m_3(\phi)}{\sqrt{g(\phi)(g(\phi) + h_{\phi}(\Delta))}} \frac{h_{\phi}(\Delta)}{\sqrt{g(\phi) + h_{\phi}(\Delta)} + \sqrt{g(\phi)}} - \frac{\Delta_3}{\sqrt{g(\phi) + h_{\phi}(\Delta)}}. \end{split}$$

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Now we observe that  $m_3(\phi)/\sqrt{g(\phi)}$  is equal to  $\phi_1,$  so indeed

$$\phi_1 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\phi}_1 = \frac{\phi_1 h_\phi(\Delta) - \Delta_3(\sqrt{g(\phi) + h_\phi(\Delta)} + \sqrt{g(\phi)})}{\sqrt{g(\phi) + h_\phi(\Delta)}(\sqrt{g(\phi) + h_\phi(\Delta)} + \sqrt{g(\phi)})}$$

Call the numerator of this last fraction N and call its denominator D. Writing  $h_{\phi}(\Delta)$  as  $h_{\phi}(\Delta) = \xi_{\phi}(\Delta) + \gamma_{\phi}(\Delta)$ , where  $\gamma_{\phi}(\Delta) \coloneqq 2m_3(\phi)\Delta_3 + \Delta_3^2$ , we see that

$$N = \phi_1 \xi_{\phi}(\Delta) + \phi_1 \gamma_{\phi}(\Delta) - \Delta_3 \{ (g(\phi) + h_{\phi}(\Delta))^{1/2} + g(\phi)^{1/2} \}$$

In order to obtain the optimal upper bound, we need to do a fine analysis of this expression. To this end, we calculate

$$\begin{split} A &\coloneqq \phi_1 \gamma_{\phi}(\Delta) - \Delta_3 \{ (g+h)^{1/2} + g^{1/2} \} \\ &= 2\Delta_3 \{ \phi_1 m_3(\phi) - g^{1/2} \} + \phi_1 \Delta_3^2 - \Delta_3 \{ (g+h)^{1/2} - g^{1/2} \} \\ &= -2\Delta_3 (1-\phi_1^2) g^{1/2} + \phi_1 \Delta_3^2 - \frac{\Delta_3 h}{(g+h)^{1/2} + g^{1/2}} \\ &= -2\Delta_3 (1-\phi_1^2) g^{1/2} - \Delta_3 \frac{\gamma_{\phi}(\Delta) - \phi_1 \Delta_3 ((g+h)^{1/2} + g^{1/2})}{(g+h)^{1/2} + g^{1/2}} - \frac{\Delta_3 \xi_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}}, \end{split}$$

where the last line follows because  $\phi_1 m_3(\phi) = \phi_1^2 g(\phi)^{1/2}$ . We now focus on the middle term of this last display, which we will express as a function of A.

$$\begin{split} B &\coloneqq \gamma_{\phi}(\Delta) - \phi_{1}\Delta_{3}((g+h)^{1/2} + g^{1/2}) \\ &= 2\Delta_{3}(m_{3}(\phi) - \phi_{1}g^{1/2}) + \Delta_{3}^{2} - \phi_{1}\Delta_{3}\{(g+h)^{1/2} - g^{1/2}\} \\ &= \Delta_{3}^{2} - \frac{\phi_{1}\Delta_{3}h}{(g+h)^{1/2} + g^{1/2}} \\ &= \Delta_{3}^{2} - \frac{\phi_{1}\Delta_{3}\gamma_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}} - \frac{\phi_{1}\Delta_{3}\xi_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}} \\ &= \Delta_{3}\frac{\Delta_{3}\{(g+h)^{1/2} + g^{1/2}\} - \phi_{1}\gamma_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}} - \frac{\phi_{1}\Delta_{3}\xi_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}} \\ &= -\frac{\Delta_{3}A}{(g+h)^{1/2} + g^{1/2}} - \frac{\phi_{1}\Delta_{3}\xi_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}}. \end{split}$$

Thus,

$$A = -2\Delta_3(1-\phi_1^2)g^{1/2} - \frac{\Delta_3 B}{(g+h)^{1/2} + g^{1/2}} - \frac{\Delta_3\xi_\phi(\Delta)}{(g+h)^{1/2} + g^{1/2}}$$
  
=  $-2\Delta_3(1-\phi_1^2)g^{1/2} + \frac{\Delta_3^2 A}{\{(g+h)^{1/2} + g^{1/2}\}^2} + \frac{\phi_1\Delta_3^2\xi_\phi(\Delta)}{\{(g+h)^{1/2} + g^{1/2}\}^2} - \frac{\Delta_3\xi_\phi(\Delta)}{(g+h)^{1/2} + g^{1/2}},$ 

from which we deduce that

$$N = \phi_1 \xi_{\phi}(\Delta) + \frac{-2\Delta_3 (1 - \phi_1^2) g^{1/2} + \frac{\phi_1 \Delta_3^2 \xi_{\phi}(\Delta)}{\{(g+h)^{1/2} + g^{1/2}\}^2} - \frac{\Delta_3 \xi_{\phi}(\Delta)}{(g+h)^{1/2} + g^{1/2}}}{1 - \Delta_3^2 / \{(g+h)^{1/2} + g^{1/2}\}^2}$$

Since  $m_2(\phi) \ge 0$ , we see that  $\xi_{\phi}(\Delta)$  has maximal amplitude when  $\Delta_1 = \operatorname{sgn}(m_1(\phi))\eta$  and when  $\Delta_2 = \eta$ , in which case we have

$$\begin{aligned} |\xi_{\phi}(\Delta)| &= 8|m_1(\phi)|m_2(\phi)\eta + 8|m_1(\phi)|\eta^2 + 4m_2(\phi)\eta^2 + 4\eta^3 + 4m_1(\phi)^2\eta \\ &\leq 12m_1(\phi)^2\eta + 12|m_1(\phi)|\eta^2 + 4\eta^3, \end{aligned}$$

where the last line follows since  $m_2(\phi) \le |m_1(\phi)|$ . Now we observe that under the condition of the lemma, we have  $\eta \le |m_1(\phi)|$ , and so we can find a constant C > 0 such that

$$|\xi_{\phi}(\Delta)| \le Cm_1(\phi)^2 \eta$$

Also, we have that  $|\gamma_{\phi}(\Delta)| \leq 2|m_3(\phi)|\eta + \eta^2$ , and so

$$h_{\phi}(\Delta)| \le Cm_1(\phi)^2\eta + 2|m_3(\phi)|\eta + \eta^2,$$

Noting that  $\phi_3 \leq \sqrt{K}$ , for  $c_0 = c_0(K)$  sufficiently small in the assumption of the proposition we have  $|h_{\phi}(\Delta)| \leq g(\phi)/2$ . Consequently, noting also that  $|\Delta_3| \leq \eta$  and  $\eta \leq 4c_0g^{1/2}$ , we find that

$$|N| \lesssim |\phi_1| m_1(\phi)^2 \eta + \eta(1 - \phi_1^2) g(\phi)^{1/2} \lesssim \eta(1 - \phi_1^2)^2 \phi_2^2 \phi_3^3,$$

and

$$D|\gtrsim g(\phi)\gtrsim (1-\phi_1^2)^2\phi_2^4\phi_3^6.$$

Hence we have

$$|\phi_1 - \operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) \cdot \tilde{\phi}_1| \lesssim \frac{\eta}{\phi_2^2 \phi_3^3}$$

**Bounding**  $\omega_2$  We rewrite,

$$\phi_2 - \tilde{\phi}_2 = \frac{m_2(\phi)}{m_1(\phi)} - \frac{m_2(\phi) + \Delta_2}{m_1(\phi) + \Delta_1}$$
$$= \frac{m_2(\phi)(m_1(\phi) + \Delta_1) - (m_2(\phi) + \Delta_2)m_1(\phi)}{m_1(\phi)(m_1(\phi) + \Delta_1)}.$$

Hence,

$$\phi_2 - \tilde{\phi}_2 = \frac{\Delta_1 m_2(\phi) - \Delta_2 m_1(\phi)}{m_1(\phi)(m_1(\phi) + \Delta_1)}.$$

Under the assumptions of the theorem, we have that  $\eta \leq m_1(\phi)/2$ , and thus

$$\begin{aligned} |\phi_2 - \tilde{\phi}_2| &\leq \frac{2\eta(m_2(\phi) + |m_1(\phi)|)}{m_1(\phi)^2} \\ &\leq \frac{4\eta}{|m_1(\phi)|} \\ &= \frac{16\eta}{(1 - \phi_1^2)|\phi_2|\phi_3^2}. \end{aligned}$$

**Bounding**  $\omega_3$  We rewrite,

$$\begin{split} \phi_{3} - \tilde{\phi}_{3} &= \frac{\sqrt{g(\phi)}}{m_{2}(\phi)} - \frac{\sqrt{g(\phi) + h_{\phi}(\Delta)}}{m_{2}(\phi) + \Delta_{2}} \\ &= \frac{m_{2}(\phi)(\sqrt{g(\phi)} - \sqrt{g(\phi) + h_{\phi}(\Delta)})}{m_{2}(\phi)(m_{2}(\phi) + \Delta_{2})} + \frac{\Delta_{2}\sqrt{g(\phi)}}{m_{2}(\phi)(m_{2}(\phi) + \Delta_{2})} \\ &= \frac{-h_{\phi}(\Delta)}{(m_{2}(\phi) + \Delta_{2})(\sqrt{g(\phi) + h_{\phi}(\Delta)} + \sqrt{g(\phi)})} + \frac{\Delta_{2}\phi_{3}}{m_{2}(\phi) + \Delta_{2}} \\ &= \frac{-h_{\phi}(\Delta) + \Delta_{2}\phi_{3}(\sqrt{g(\phi) + h_{\phi}(\Delta)} + \sqrt{g(\phi)})}{(m_{2}(\phi) + \Delta_{2})(\sqrt{g(\phi) + h_{\phi}(\Delta)} + \sqrt{g(\phi)})} \end{split}$$

Let us call the numerator of the rhs of the last display N, and the denominator D. We further decompose  $h_{\phi}(\Delta)$  as  $h_{\phi}(\Delta) = \xi_{\phi}(\Delta) + \gamma_{\phi}(\Delta)$ , where  $\gamma_{\phi}(\Delta) \coloneqq 4m_1(\phi)^2 \Delta_2$ . We see that

$$\begin{split} N &= -\xi_{\phi}(\phi) - 4m_1(\phi)^2 \Delta_2 + \phi_3 \Delta_2 ((g+h)^{1/2} + g^{1/2}) \\ &= -\xi_{\phi}(\phi) - 4m_1(\phi)^2 \Delta_2 + \phi_3 \Delta_2 \{(g+h)^{1/2} + g^{1/2}\} \\ &= -\xi_{\phi}(\phi) - 4m_1(\phi)^2 \Delta_2 + 2\phi_3 \Delta_2 g^{1/2} + \phi_3 \Delta_2 \{(g+h)^{1/2} - g^{1/2}\} \\ &= -\xi_{\phi}(\phi) + \Delta_2 (1+\phi_1^2) \phi_3 g^{1/2} + \frac{\phi_3 \Delta_2 h}{(g+h)^{1/2} + g^{1/2}}, \end{split}$$

where the last line follows because  $m_1(\phi)^2 = \frac{1}{4}(1-\phi_1^2)\phi_3 g^{1/2}$ . Since  $m_2(\phi) \ge 0$ , we see that  $\xi_{\phi}(\Delta)$  has maximal amplitude when  $\Delta_1 = \operatorname{sgn}(m_1(\phi))\eta$  and when  $\Delta_2 = \eta$ , in which case we have

$$\begin{aligned} |\xi_{\phi}(\Delta)| &= 8|m_1(\phi)|m_2(\phi)\eta + 8|m_1(\phi)|\eta^2 + 4m_2(\phi)\eta^2 + 4\eta^3 + 2|m_3(\phi)|\eta + \eta^2 \\ &\lesssim \{|m_1(\phi)|m_2(\phi) + 2|m_3(\phi)|\}\eta + \eta^2 \\ &\lesssim (1 - \phi_1^2)\phi_2^2\phi_3^3 \max\{(1 - \phi_1^2)|\phi_2|\phi_3, |\phi_1|\}\eta + \eta^2, \end{aligned}$$

where the second line follows because under the assumptions of the proposition we have that  $m_2(\phi) \leq |m_1(\phi)|$  and  $\eta \leq m_2(\phi)/2$  (note that  $\phi_3 \leq K^{1/2}$ ). Since  $h_{\phi}(\Delta) = \xi_{\phi}(\Delta) + 4m_1(\phi)^2 \Delta_2$ , we also have

$$|h_{\phi}(\Delta)| \lesssim (1 - \phi_1^2)\phi_2^2\phi_3^3 \max\{(1 - \phi_1^2)\phi_3, |\phi_1|\}\eta + \eta^2,$$

Hence,

$$\begin{split} |N| &\lesssim (1 - \phi_1^2) \phi_2^2 \phi_3^3 \max\{(1 - \phi_1^2) |\phi_2| \phi_3, |\phi_1| \} \eta + \eta^2 \\ &+ \eta \phi_3 g^{1/2} + \frac{\eta^2 \phi_3(1 - \phi_1^2) \phi_2^2 \phi_3^3 \max\{(1 - \phi_1^2) \phi_3, |\phi_1| \} + \eta^3 \phi_3}{g^{1/2}} \\ &\lesssim (1 - \phi_1^2) \phi_2^2 \phi_3^3 \max\{(1 - \phi_1^2) |\phi_2| \phi_3, |\phi_1| \} \eta + \eta^2 \\ &+ \eta \phi_3 g^{1/2} + \eta^2 \phi_3 \max\{(1 - \phi_1^2) \phi_3, |\phi_1| \} + \frac{\eta^3}{(1 - \phi_1^2) \phi_2^2 \phi_3^2} \end{split}$$

But by assumption  $\eta \lesssim (1-\phi_1^2)\phi_2^2\phi_3^3,$  and  $4g^{1/2}=(1-\phi_1^2)\phi_2^2\phi_3^2,$  thus

$$|N| \lesssim (1 - \phi_1^2) \phi_2^2 \phi_3^3 \max\{\phi_3, |\phi_1|\} \eta + \eta^2.$$

Note that  $\max(\phi_3, |\phi|_1) \leq \sqrt{K}$ . Moreover, under the assumptions of the proposition and using that  $\phi_3 \leq \sqrt{K}$ , it is the case that  $|\Delta_2| \leq \eta \leq m_2(\phi)$ . Therefore  $|D| \gtrsim m_2(\phi)\sqrt{g(\phi)}$ , and

$$|\phi_3 - \tilde{\phi}_3| \lesssim \frac{\eta}{(1 - \phi_1^2)\phi_2^2 \phi_3^2} + \frac{\eta^2}{(1 - \phi_1^2)^2 \phi_2^4 \phi_3^5}$$

Finally, since have assumed that  $\eta < \frac{(1-\phi_1^2)\phi_2^2\phi_3^2}{8}$ , we see that the second term is at most a constant times the first, so that it can be absorbed by increasing the constant C.

#### A.3 Proof of Theorem 3

We give a standard two-point testing lower bound, summarising ideas that can be found for example in Chapter 2 of [36].

**Lemma 3.** Given data  $X^{(n)} \sim p_u^{(n)}$  for parameter  $u \in U$ , the following lower bounds hold for estimating u.

Suppose  $\mathcal{U} \subseteq \mathbb{R}$  and for some  $r \leq 1/2$  assume that there exist parameters  $u_0, u_1$  satisfying

*i*. 
$$|u_1/u_0 - 1| \ge 4r$$
,

*ii.*  $K(p_{u_1}^{(n)}; p_{u_0}^{(n)}) \le 1/100.$ 

where we recall K denotes the Kullback-Leibler divergence. Then

$$\inf_{\hat{u}} \sup_{u \in \mathcal{U}} \mathbb{P}_u(|\hat{u}/u - 1| \ge r) \ge 1/4$$

where the infimum is over all estimators  $\hat{u}$  based on the data  $X^{(n)}$ .

If instead  $(\mathcal{U}, d)$  is a pseudo-metric space and for some  $r \ge 0$  there exist parameters  $u_0, u_1$  satisfying

*i.*  $d(u_0, u_1) \ge 2r$ *ii.*  $K(p_{u_1}^{(n)}, p_{u_0}^{(n)}) \le 1/100,$ 

then

$$\inf_{\hat{u}} \sup_{u \in \mathcal{U}} \mathbb{P}_u(d(\hat{u}, u) \ge r) \ge 1/4.$$

*Proof.* Given an estimator  $\hat{u}$  we may construct a test T of  $u = u_0$  vs  $u = u_1$ ,

$$T = \mathbb{1}\left\{ \left| \frac{\hat{u}}{u_0} - 1 \right| > \left| \frac{\hat{u}}{u_1} - 1 \right| \right\}$$

Observe that

$$\begin{aligned} \frac{\hat{u}}{u_0} - 1 \Big| &= \Big| \frac{u_1}{u_0} - 1 + \frac{\hat{u} - u_1}{u_1} \frac{u_1}{u_0} \Big| \\ &\geq 4r - \Big| \frac{\hat{u}}{u_1} - 1 \Big| (1 + 4r). \end{aligned}$$

Then

$$\mathbb{P}_{u_1}(T=0) = \mathbb{P}_{u_1}\left(\left|\frac{\hat{u}}{u_0} - 1\right| \le \left|\frac{\hat{u}}{u_1} - 1\right|\right) \\ \le \mathbb{P}_{u_1}\left(4r - \left|\frac{\hat{u}}{u_1} - 1\right|(1+4r) \le \left|\frac{\hat{u}}{u_1} - 1\right|\right) \\ \le \mathbb{P}_{u_1}\left(\left|\frac{\hat{u}}{u_1} - 1\right| \ge r\right),$$

where for the last line we have used that  $4r/(2+4r) \ge r$  for  $r \le 1/2$ . Also note that on the event  $\{T = 1\} \cap \{|\hat{u}/u_0 - 1| < r\}$  we have also  $|\hat{u}/u_1 - 1| < r$  and hence

$$|u_1/u_0 - 1| = |\hat{u}/u_0 - 1 - (\hat{u}/u_1 - 1) - (\hat{u}/u_1 - 1)(u_1/u_0 - 1) < 2r + r|u_1/u_0 - 1|,$$

so that  $|u_1/u_0 - 1| < 2r/(1 - r)$  on this event. Having assumed  $r \le 1/2$  and  $|u_1/u_0 - 1| \ge 4r$  we deduce that  $\{T = 1\} \cap \{|\hat{u}/u_0 - 1| < r\} = \emptyset$  so that  $\{T = 1\} \subseteq \{|\hat{u}/u_0 - 1| \ge r\}$ , and hence we have shown

$$\inf_{\hat{u}} \sup_{u} \mathbb{P}_u\left(\left|\frac{\hat{u}}{u} - 1\right| \ge r\right) \ge \inf_{\hat{u}} \max_{i=0,1} \mathbb{P}_{u_i}\left(\left|\frac{\hat{u}}{u_i} - 1\right| \ge r\right) \ge \inf_{T} \max_{i=0,1} \mathbb{P}_{u_i}(T \neq i),$$

where the latter infimum is over all tests T. In the pseudo-metric case a reduction considering the test  $T = \mathbb{1}\{d(\hat{u}, u_0) > d(\hat{u}, u_1)\}$  and directly using the triangle inequality likewise yields

$$\inf_{\hat{u}} \sup_{u} \mathbb{P}_u(d(\hat{u}, u) \ge r) \ge \inf_{T} \max_{i=0,1} \mathbb{P}_{u_i}(T \neq i).$$

It remains to lower bound the maximum probability of testing error by 1/4. Introducing the event  $A = \left\{\frac{p_{u_0}^{(n)}}{p_{u_1}^{(n)}} \ge 1/2\right\}$ , we see

$$\mathbb{P}_{u_0}(T \neq 0) \ge \mathbb{E}_{u_1}\left[\frac{p_{u_0}^{(n)}}{p_{u_1}^{(n)}}\mathbb{1}_A T\right] \ge \frac{1}{2}\left[\mathbb{P}_{u_1}(T=1) - \mathbb{P}_{u_1}(A^c)\right]$$

Thus, writing  $p_1 = \mathbb{P}_{u_1}(T = 1)$ , we see

$$\max(\mathbb{P}_{u_0}(T \neq 0), \mathbb{P}_{u_1}(T \neq 1)) \ge \max(\frac{1}{2}(p_1 - \mathbb{P}_{u_1}(A^c)), 1 - p_1)$$
$$\ge \inf_{p \in [0,1]} \max(\frac{1}{2}(p - \mathbb{P}_{u_1}(A^c)), 1 - p).$$

The infimum is attained when  $\frac{1}{2}(p - \mathbb{P}_{u_1}(A^c)) = 1 - p$  and takes the value  $\frac{1}{3}\mathbb{P}_{u_1}(A)$  so that

$$\inf_{T} \max_{i=0,1} \mathbb{P}_{u_i}(T \neq i) \ge \frac{1}{3} \mathbb{P}_{u_1}(A).$$

Next observe

$$\begin{split} \mathbb{P}_{u_1}(A) &= \mathbb{P}_{u_1} \big[ \frac{p_{u_1}^{(n)}}{p_{u_0}^{(n)}} \le 2 \big] = 1 - \mathbb{P}_{u_1}^n \big[ \log \big( \frac{p_{u_1}^{(n)}}{p_{u_0}^{(n)}} \big) > \log 2 \big] \ge 1 - \mathbb{P}_{\theta_1}^n \big[ |\log \big( \frac{p_{u_1}^{(n)}}{p_{u_0}^{(n)}} \big) | > \log 2 \big] \\ &\ge 1 - \big( \log 2 \big)^{-1} \mathbb{E}_{u_1} \big| \log \big( \frac{p_{u_1}^{(n)}}{p_{u_0}^{(n)}} \big) \big|, \end{split}$$

where we have used Markov's inequality to attain the final expression. By the second Pinsker inequality (e.g. Proposition 6.1.7b in [19]), using the upper bound on the Kullback–Leibler divergence we can continue the chain of inequalities to see

$$\mathbb{P}_{u_1}(A) \ge 1 - (\log 2)^{-1} \left[ K(p_{u_1}^{(n)}, p_{u_0}^{(n)}) + \sqrt{2K(p_{u_1}^{(n)}, p_{u_0}^{(n)})} \right] \ge 1 - (\log 2)^{-1} (\mu + \sqrt{2\mu}).$$

For any c < 1/3, we may choose  $\mu = \mu(c)$  small enough that the testing error satisfies

$$\inf_{T} \max_{i=0,1} \mathbb{P}_{u_i}(T \neq i) \ge \frac{1}{3} \left( 1 - \frac{\mu + \sqrt{2\mu}}{\log 2} \right) > c,$$

and in particular a numerical calculation shows that  $\mu = 1 + \frac{1}{4} \log 2 - \sqrt{1 + \frac{1}{2} \log 2} > 1/100$  works for c = 1/4.

In view of Lemma 2 and Proposition 1, for any  $(\phi, \psi), (\tilde{\phi}, \tilde{\psi}) \in \Phi$  corresponding to strictly positive emission densities, we have

$$K(p_{\phi,\psi}^{(n)}, p_{\tilde{\phi},\tilde{\psi}}^{(n)}) \le Cn\rho(\phi,\psi;\tilde{\phi},\tilde{\psi})^2,$$

where C > 0 is a constant depending only on K and a lower bound for the emission densities. To prove Item (1) we apply Lemma 3 to  $u = 1 - \phi_1^2$  to see that there exists a constant  $c_1$  for which the relative risk bound is proved if we can exhibit, for a constant  $c_2$  which we may choose arbitrarily, parameters  $(\phi, \psi), (\tilde{\phi}, \tilde{\psi}) \in \Phi_L(\delta, \epsilon, \zeta)$  satisfying

$$\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \le c_1/\sqrt{n}, \quad \text{and} \quad \left|\frac{1-\tilde{\phi}_1^2}{1-\phi_1^2} - 1\right| \ge c_2/\sqrt{n\delta^2\epsilon^4\zeta^6}.$$
(27)

To prove the absolute risk bound we then note that for any  $a \ge 0$ , since  $|\phi_1| \le 1$  and  $1 - \phi_1^2 \ge \delta$ , so that we may assume the same of  $\hat{\phi}_1$ , we have

$$\mathbb{P}_{\phi,\psi}(\min(|\hat{\phi}_1 - \phi_1|, |\hat{\phi}_1 + \phi_1|) \ge a) \ge \mathbb{P}_{\phi,\psi}(|(1 - \hat{\phi}_1^2) - (1 - \phi_1^2)| \ge 2a) \\ \ge \mathbb{P}_{\phi,\psi}(|(1 - \hat{\phi}_1^2)/(1 - \phi_1^2) - 1| \ge 2a/\delta).$$

(See also equation (26) for a similar calculation with  $\phi_2$ .)

Similar conditions to (27) suffice for proving the other parts of Theorem 3 and we proceed now to verifying the existence of suitable parameters  $(\phi, \psi)$  and  $(\tilde{\phi}, \tilde{\psi})$ , with the help of the following lemma.

**Lemma 4.** For a given  $\phi$ , assume conditions (6) and (7) and assume that  $\phi_3 \leq \sqrt{2\lfloor K/2 \rfloor}/(2K)$ . Then there exists  $\psi$  such that  $(\phi, \psi)$  lies in  $\Phi_L$  and the corresponding emission densities  $f_0, f_1$  are bounded below by some constant c = c(K) > 0.

In particular, for  $|\phi_1| \leq 1 - 3\delta$ ,  $\epsilon \leq \phi_2 \leq \min(1/3, 1 - L)$ ,  $\zeta \leq \phi_3 \leq 2\zeta$ , then such a  $\psi$  exists under the compatibility condition (3).

Proof. Take

$$\psi_1(k) = 1/K, \quad \psi_2(k) = (2\lfloor K/2 \rfloor)^{-1/2} (\mathbb{1}\{k \text{ odd}, k < K\} - \mathbb{1}\{k \text{ even}\}), \quad k \le K.$$

Under the assumed condition on  $\phi_3$  and recalling that  $|\phi_1| \leq 1$  by assumption, we observe from the expressions for  $f_0, f_1$  given in Remark 4 that these are lower bounded by 1/(2K). In the particular case, one simply notes that all the conditions hold for such  $\phi$ .

**Proof of Items (1) and (3)** We prove the lower bounds for estimating  $\phi_1$  and  $\phi_3$  together. For some small constant c > 0, set  $R = c\epsilon^{-2}\zeta^{-3}n^{-1/2}$  and, writing  $S = (2 - 6\delta - R)R/(6\delta - 9\delta^2)$ , set

$$\phi = (1 - 3\delta, \epsilon, \zeta \sqrt{1 + S}),$$
$$\tilde{\phi} = (1 - 3\delta - R, \epsilon, \zeta).$$

Recalling the definition  $r(\phi) = (1 - \phi_1^2)\phi_2\phi_3^2/4$ , the choice of  $\phi_3$  ensures that  $r(\phi) = r(\tilde{\phi})$ , and we note that under the assumptions of the theorem we have  $R \leq \delta \leq 1/6$  so that  $S \leq R/\delta \leq 1$  and  $\zeta \leq \phi_3 \leq 2\zeta$ . By Lemma 4 there exists  $\psi$  such that  $(\phi, \psi), (\tilde{\phi}, \psi) \in \Phi_L$  and for this  $\psi$  we see that

$$\rho(\phi,\psi;\tilde{\phi},\psi) = |\phi_1\phi_2\phi_3r(\phi) - \tilde{\phi}_1\tilde{\phi}_2\tilde{\phi}_3r(\tilde{\phi})| = \phi_2r(\phi)|\phi_1\phi_3 - \tilde{\phi}_1\tilde{\phi}_3|.$$

Using that  $\sqrt{1+t} \le 1+t$  for  $t \ge 0$  we have

$$|\phi_1\phi_3 - \tilde{\phi}_1\tilde{\phi}_3| = (1 - 3\delta)\zeta(\sqrt{1 + S} - 1) + R\zeta \le (S + R)\zeta \le 2R\zeta/\delta,$$

hence since  $r(\phi) = (6\delta - 9\delta^2)\epsilon\zeta^2(1+S)/4 \le 3\delta\epsilon\zeta^2$ , we obtain

$$\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) \le 6\epsilon^2 \zeta^3 R \le 6cn^{-1/2}$$

Recalling that  $R \leq \delta \leq 1/6$  and that  $r(\phi) = r(\tilde{\phi})$  one calculates

$$\frac{1-\tilde{\phi}_1^2}{1-\phi_1^2} - 1 = S \ge R/(12\delta).$$

For c small enough we see that the conditions in equation (27) are satisfied, yielding the claimed bound for estimating  $\phi_1$ .

To prove the lower bound for estimating  $\phi_3$  it suffices to lower bound  $|\phi_3/\tilde{\phi}_3 - 1|$ . Here we use the bound  $\sqrt{1+x} - 1 \ge x/(2\sqrt{1+x}) \ge x/(2\sqrt{2})$  for  $0 \le x \le 1$  to see for a constant c' > 0 that

$$|\phi_3/\phi_3 - 1| \ge c'R/\delta$$

The bound for  $\phi_3$  follows from applying Lemma 3.

**Proof of Item (2)** For a constant 
$$c > 0$$
, define  $R = c\delta^{-1}\epsilon^{-1}\zeta^{-2}n^{-1/2}$ , define  $\phi, \phi$  by  
 $\phi = (1 - 3\delta, \epsilon, \zeta(1 + R/\epsilon)^{1/2})$   
 $\tilde{\phi} = (1 - 3\delta, \epsilon + R, \zeta),$ 

and observe that by construction  $r(\phi) = r(\tilde{\phi})$ . Noting that  $\phi_2 \leq 2\epsilon \leq 1 - L$  and  $\phi_3 \leq 2\zeta$  because the assumptions of Theorem 3 ensure that  $R \leq \epsilon \leq 1/3$ , we deduce using Lemma 4 that there exists some  $\psi = \tilde{\psi}$  such that  $(\phi, \psi), (\tilde{\phi}, \tilde{\psi}) \in \Phi_L(\delta, \epsilon, \zeta)$ .

Next observe, using that  $(1+x)^{1/2} \le 1+x$ ,

$$\phi_1|\phi_2\phi_3 - \tilde{\phi}_2\tilde{\phi}_3| \le |\phi_2||\phi_3 - \tilde{\phi}_3| + |\tilde{\phi}_3||\phi_2 - \tilde{\phi}_2| = \epsilon\zeta(\sqrt{1 + R/\epsilon} - 1) + \zeta R \le 2\zeta R \le R,$$

the last inequality following from the fact that under the compatibility condition (3) we have  $\zeta \leq 1/2$ . We deduce

$$\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) = r(\phi)\max(|\phi_2 - \tilde{\phi}_2|, |\phi_1\phi_2\phi_3 - \tilde{\phi}_1\tilde{\phi}_2\tilde{\phi}_3|) = Rr(\phi).$$

Again using that  $\phi_3 \leq 2\zeta$  and noting also that  $(1 - \phi_1^2) = 6\delta - 9\delta^2 \leq 6\delta$ , we see that for some C' > 0 we have

$$p(\phi,\psi;\tilde{\phi},\tilde{\psi}) \leq C'\delta\epsilon\zeta^2 R \leq cC'n^{-1/2}$$

As with Items (1) and (3), for c small enough in the definition of R we may apply Lemma 3 to deduce the claimed lower bound since  $|\tilde{\phi}_2/\phi_2 - 1| = R/\epsilon$ .

**Proof of Item (4)** Set  $\phi = \tilde{\phi} = (0, \epsilon, \zeta)$ , set, as in Lemma 4,

$$\psi_1(k) = 1/K, \quad \psi_2(k) = (2\lfloor K/2 \rfloor)^{-1/2} (\mathbb{1}\{k \text{ odd}, k < K\} - \mathbb{1}\{k \text{ even}\}), \quad k \le K,$$

and define  $\tilde{\psi}_1 = \psi_1 + cn^{-1/2}\psi_2$ . Note that under the compatibility condition (3) we have  $(\phi, \psi), (\tilde{\phi}, \tilde{\psi}) \in \Phi_L$  for *n* larger than some C = C(K, c), or for all  $n \ge 1$  if *c* is small enough. Then

$$\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) = cn^{-1/2}$$

and we apply Lemma 3 to deduce the result.

**Proof of Item (5)** Set  $\phi = \tilde{\phi} = (1 - 3\delta, \epsilon, \zeta)$ , choose  $\psi_1 = \tilde{\psi}_1$  to be the uniform density on  $\{1, \ldots, K\}$ . As with the previous parts, an application of Lemma 3 will yield the theorem if we can exhibit  $\psi_2, \tilde{\psi}_2$  such that the induced emission densities are bounded below by some c' = c'(K) > 0,  $\|\psi_2 - \tilde{\psi}_2\| = R := c(n\delta^2\epsilon^2\zeta^4)^{-1/2}$  for some c > 0,  $\operatorname{sgn}(\langle \psi_2, \tilde{\psi}_2 \rangle) = +1$ , and  $\rho(\phi, \psi; \tilde{\phi}, \tilde{\psi}) \leq c_1 n^{-1/2}$  for a small constant  $c_1$ . Such a choice is possible, for a small enough constant c, under the compatibility condition (3) and for  $n\delta^2\epsilon^2\zeta^4 \geq 1$ ; for example, define  $\psi_2$  as in Lemma 4 by

$$\psi_2(k) = (2\lfloor K/2 \rfloor)^{-1/2} (\mathbb{1}\{k \text{ odd}, k < K\} - \mathbb{1}\{k \text{ even}\}), \quad k \le K,$$

and, for h defined by  $h(1) = 2^{-1/2}$ ,  $h(3) = -2^{-1/2}$  and h(k) = 0 for all other k, define

$$\tilde{\psi}_2 = (\psi_2 + \alpha h)/(1 + \alpha), \quad \alpha = R/(2 - R).$$

This satisfies  $\|\tilde{\psi}_2 - \psi_2\| = R$ ,  $\|\tilde{\psi}_2\| = 1$ ,  $\langle\tilde{\psi}_2, 1\rangle = 0$  and  $\langle\tilde{\psi}_2, \psi_2\rangle \ge 0$ . For  $k \notin \{1,3\}$  the condition (8) of Remark 5 holds with 1/(2K) in place of 0 on the right, and for  $k \in \{1,3\}$  a direct calculation shows that the condition with 1/(4K) in on the right if R is upper bounded by some c' = c'(K), which is the case for c = c(K) sufficiently small. Then

$$\rho(\phi,\psi;\tilde{\phi},\tilde{\psi}) = |r(\phi)| \|\psi_2 - \tilde{\psi}_2\| \le \delta \epsilon \zeta^2 R \le c n^{-1/2}.$$

#### A.4 Proofs for Section 4

*Proof of Theorem 1.* We begin with the upper bounds. From the inversion formulae in Remark 4 we have

$$\max(\|\hat{f}_0 - f_0\|, \|\hat{f}_1 - f_1\|) \le \|\hat{\psi}_1 - \psi_1\| + \frac{1}{2} \|\hat{\phi}_1 \hat{\phi}_3 \hat{\psi}_2 - \phi_1 \phi_3 \psi_2\| + \frac{1}{2} \|\hat{\phi}_3 \hat{\psi}_2 - \phi_3 \psi_2\|$$

Recalling that  $|\hat{\phi}_1| \leq 1$ , that  $0 \leq \phi_3 \leq K^{1/2}$  and that  $\|\psi_2\| = \|\hat{\psi}_2\| = 1$ , we decompose the second term on the right, with an implicit decomposition of the third term included:

$$\begin{aligned} \|\hat{\phi}_1\hat{\phi}_3\hat{\psi}_2 - \phi_1\phi_3\psi_2\| &\leq |\hat{\phi}_1|\|\hat{\phi}_3\hat{\psi}_2 - \phi_3\psi_2\| + |\phi_3||\hat{\phi}_1 - \phi_1| \\ &\leq |\hat{\phi}_3 - \phi_3| + K^{1/2}\|\hat{\psi}_2 - \psi_2\| + \phi_3|\hat{\phi}_1 - \phi_1|. \end{aligned}$$

It follows that for some constant C we have

$$\max(\|\hat{f}_0 - f_0\|, \|\hat{f}_1 - f_1\|) \le C \max(\|\hat{\psi}_1 - \psi_1\|, \|\hat{\psi}_2 - \psi_2\|, |\hat{\phi}_3 - \phi_3|, \phi_3|\hat{\phi}_1 - \phi_1|).$$

Applying Proposition 2 as in the proof of Theorem 2, one can show that for some C > 0

$$\mathbb{P}_{\phi,\psi}\Big(\phi_3^2|\hat{\phi}_1 - \phi_1|^2 \ge \frac{Cx^2}{n\epsilon^4\zeta^4}\Big) \le e^{-x^2}.$$

The upper bounds for estimating  $f_0$  and  $f_1$  then follow from Theorem 2.

Similarly, Remark 4 and the fact that  $|\phi_2| \leq 1$  give

$$\max(|\hat{p}-p|, |\hat{q}-q|) \le \frac{1}{2}(1+|\hat{\phi}_1|)|\hat{\phi}_2 - \phi_2| + \frac{1}{2}|\hat{\phi}_1 - \phi_1||1 - \phi_2| \le 2\max(|\hat{\phi}_1 - \phi_1|, |\hat{\phi}_2 - \phi_2|).$$
  
The upper bounds then again follow from Theorem 2

The upper bounds then again follow from Theorem 2.

For the lower bounds, writing  $\theta(\phi, \psi) = (p, q, f_0, f_1)$  and  $\theta(\tilde{\phi}, \tilde{\psi}) = (\tilde{p}, \tilde{q}, \tilde{f}_0, \tilde{f}_1)$ , observe by Lemma 3 that it suffices to lower bound  $\max(|p - \tilde{p}|, |q - \tilde{q}|)$  and  $\max(|f_0 - \tilde{f}_0||, ||f_1 - \tilde{f}_1||)$  corresponding to choices of  $(\phi, \psi), (\tilde{\phi}, \tilde{\psi})$  made in the proof of Theorem 3.

From the inversion formulae in Remark 4 we calculate, for any  $\phi$ ,  $\tilde{\phi}$ ,

$$2 \max(|p - \tilde{p}|, |q - \tilde{q}|) \\ \geq \max((1 + |\phi_1|)|\phi_2 - \tilde{\phi}_2| - |1 - \tilde{\phi}_2||\phi_1 - \tilde{\phi}_1|, |\phi_1 - \tilde{\phi}_1||1 - \tilde{\phi}_2| - (1 - |\phi_1|)|\phi_2 - \tilde{\phi}_2|).$$
(28)

If  $\delta > \epsilon \zeta$  set  $\phi = (1 - 3\delta, \epsilon, \zeta(1 + S)^{1/2})$  and  $\tilde{\phi} = (1 - 3\delta - R, \epsilon, \zeta)$ , where  $R = c(n\epsilon^4 \zeta^6)^{-1/2}$  for some c > 0 and where  $S \in [R/(12\delta), R/\delta]$  is, as in the proof of Theorem 3 Item (1), such that

 $r(\phi) = r(\tilde{\phi})$ . If  $\delta \leq \epsilon \zeta$  instead set  $\phi = (1 - 3\delta, \epsilon, \zeta(1 + R/\epsilon)^{1/2}), \tilde{\phi} = (1 - 3\delta, \epsilon + R, \zeta)$  with  $R = c(n\epsilon^2\delta^2\zeta^4)^{-1/2}$ . In either case the proof of Theorem 3 demonstrates that for suitable  $\psi = \tilde{\psi}$  we have  $K(p_{\phi,\psi}^{(n)}, p_{\tilde{\phi},\tilde{\psi}}^{(n)}) \leq 1/100$  for c small enough hence by Lemma 3

$$\inf_{\tilde{\theta}} \sup_{\theta \in \Theta} \mathbb{P}_{\theta} \Big( \max(|\check{p} - p|, |\check{q} - q|) > c' \max(|p - \tilde{p}|, |q - \tilde{q}|) \Big) \ge 1/4.$$

Inserting from equation (28) we conclude the bound in either case.

For  $(f_0, f_1)$ , again set  $\phi = (1-3\delta, \epsilon, \zeta(1+S)^{1/2})$ ,  $\tilde{\phi} = (1-3\delta-R, \epsilon, \zeta)$  where  $R = c\epsilon^{-2}\zeta^{-3}n^{-1/2}$ , and choose  $\psi = \tilde{\psi}$  by Lemma 4. As with p and q we deduce that for some c' > 0 we have

$$\inf_{\check{\theta}} \sup_{\theta \in \Theta} \mathbb{P}_{\theta} \Big( \max(\|\check{f}_0 - f_0\|, \|\check{f}_1 - f_1\|) > c' \max(\|f_0 - \tilde{f}_0\|, \|f_1 - \tilde{f}_1\|) \Big) \ge 1/4.$$

Using the inversion formulae in Remark 4 and the fact that  $\psi = \tilde{\psi}$  and  $\|\psi_2\| = 1$ , one calculates

$$2\max(\|f_0 - \tilde{f}_0\|, \|f_1 - \tilde{f}_1\|) = |\phi_1\phi_3 - \tilde{\phi}_1\tilde{\phi}_3| + |\phi_3 - \tilde{\phi}_3| \ge |\phi_3 - \tilde{\phi}_3|$$

For the current choice of  $\phi$ ,  $\tilde{\phi}$ , calculating as in proving Theorem 3 Item (3), we have  $|\phi_3 - \tilde{\phi}_3| \ge C\zeta R/\delta$  for some C > 0 and we deduce the lower bound.

*Proof of Corollary 1.* It suffices to substitute  $\alpha = e^{-x^2}$  into Theorem 1 and solve for error equal to E, while ensuring that  $x^2 = \log(1/\alpha)$  is suitably bounded.

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