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FUNCTIONAL FINITE MIXTURE REGRESSION MODELS

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Abstract:

The aim of this paper is to develop a set of functional finite mixture regression models with functional predictors in the framework of the reproducing kernel Hilbert space. First, we show the consistency of a penalized likelihood model order estimator for the true model order, denoted as q^* . We further show that the penalty of order $q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}} \log(n)$ yields the strong consistent estimator of q^* , where n and q are the sample size and the model order, respectively, and r is the eigenvalue decay rate of an operator determined jointly by the reproducing and covariance kernels. Second, we establish the minimax rate of convergence for the estimation risk. It is shown that the optimal rate is determined by the alignment of the reproducing kernel and the covariance kernel and the true model order q^* .

An efficient algorithm is also developed to estimate all unknown components of the functional finite mixture model. Simulation studies and a real data analysis are carried out to illustrate the merits of our method.

1. Introduction

With the rapid growth of modern technology, many large-scale biomedical studies (e.g., UK Biobank) have been/are being conducted to collect massive datasets with large volumes of multi-modality imaging, genetic, neurocognitive, and clinical information from increasingly large cohorts. Simultaneously extracting and integrating rich and diverse heterogeneous information in neuroimaging and/or other variables from these big data sets could transform our understanding of how diseases impact the structure and function of the brain and cognitive functions across the lifespan. Therefore, it is imperative to develop new learning methods (Liu and Zhu, 2021; Feng et al., 2020; Wang et al., 2021; Ombao et al., 2016), which are applicable to many neuroimaging studies for neuropsychiatric disorders, major neurodegenerative diseases, and normal brain development.

Mixture models is a powerful probabilistic model for using mixture distributions to represent the presence of subpopulations within an overall population. See a comprehensive review of the theory and applications of mix-

ture models in McLachlan and Peel (2000). The most well-known mixture model is the Gaussian mixture model (Richard and Green, 1997), in which the density of a random vector Y is represented by $p(y) = \sum_{i=1}^q \phi_i N(\mu_i, \Sigma_i)$, where the i -th vector component is characterized by a normal distribution with a weight ϕ_i , a mean μ_i , and a covariance Σ_i . This framework can be extended naturally to the regression setting. The Gaussian mixture regression model (Ghahramani and Jordan, 1994; Calinon et al., 2007; Stulp and Sigaud, 2015) assumes that the conditional distribution of multiple response responses given one or more predictors follows a Gaussian mixture distribution and the conditional mean is a function of the predictors. In this paper, we investigate major mathematical challenges in the conditional analysis of clinical response variables given ultra high-dimensional imaging predictors under the framework of functional finite mixture regression models.

Functional data analysis has been an active area of research, and well-known monographs in this area include Ramsay and Sloverman (2005), Bowman (2010), and Ferraty and Vieu (2006). Functional regression, particularly the functional linear regression model, has been extensively studied. The literature on functional linear regression is vast. For example, scalar-on-function regression (a continuous response variable regressed on functional covariates), which corresponds to our proposed mixture model

(1.1) with a single component, has been studied by (Cai and Hall, 2006; Crambes et al., 2009; Wang et al., 2016; Yuan and Cai, 2010; Hall and Horowitz, 2007; Du and Wang, 2014; Wang et al., 2017). When the true model is the finite mixture model with at least two different components, the standard functional linear regression will provide a poor result. There are few papers on the development of numerical algorithm for functional finite mixture regression models. Yao et al. (2011) proposed a class of functional regression models that allow the regression structure to vary for different subpopulations. By projecting the functional predictor process onto its eigenspace, the new functional finite mixture regression model is simplified to a framework that is similar to classical mixture regression models. However, none of them considered the reproducing kernel Hilbert space (RKHS) and investigated the theoretical properties of the RKHS estimates, particularly the minimax rate.

Consider a functional finite mixture regression model such that the conditional distribution of a scalar response Y given a functional predictor $\{X(t) : t \in \mathcal{I}\}$ belongs to the class of convex combination of q^* densities

given by

$$\begin{aligned} \mathcal{M}_{q^*} = \Big\{ f^*(y|x) = \sum_{k=1}^{q^*} \pi_k^* f_0(y - \langle x, \beta_k^* \rangle) : \\ \pi_k^* \geq 0, \sum_{k=1}^{q^*} \pi_k^* = 1, \beta_k^* \in \mathcal{F} \Big\}, \end{aligned} \quad (1.1)$$

where f_0 is fixed probability density (e.g., Gaussian) on $\mathbb{R}$ and $\langle x, \beta \rangle = \int_{\mathcal{I}} x(t)\beta(t)dt$. The intercept terms can be incorporated into the model by writing each component as $f_0(y - \beta_{0k}^* - \langle x, \beta_k^* \rangle)$, where the β_{0k}^* are intercepts. We ignore them in the following analysis only for ease of presentation. Here $\mathcal{F}$ is assumed to be a reproducing kernel Hilbert space (RKHS) with the reproducing kernel K . The RKHS $\mathcal{F}$ is a linear functional space endowed with an inner product $\langle \cdot, \cdot \rangle_K$ such that for any $t \in \mathcal{I}$, $K(t, \cdot) \in \mathcal{F}$, and $f(t) = \langle K(t, \cdot), f \rangle_K$ holds for any $f \in \mathcal{F}$. For more details on the RKHS, please see Wahba (1990); Steinwart and Christmann (2008); Schölkopf (2001) and references therein. The $\mathcal{M}_{q^*}$ is parametrized by parameters $\Pi_{q^*}^* = (\pi_1^*, \dots, \pi_{q^*}^*) \in \Delta_{q^*-1}$ and $\Theta_{q^*}^* = (\beta_1^*, \dots, \beta_{q^*}^*) \in \mathcal{F}^{q^*}$, where Δ_{q^*-1} is the q^* -simplex. We call q^* the *number of mixture components* or the *model order*, $\Pi_{q^*}^*$ the *mixing probabilities*, and $\Theta_{q^*}^*$ the *coefficient functions*.

Suppose that we observe n independently and identically distributed copies of (Y, X) , denoted as $\{(Y_i, X_i) : i = 1, \dots, n\}$. Let $\mathcal{M} = \cup_q \mathcal{M}_q$. Let $f^*(y|x) \in \mathcal{M}_{q^*}$ be the true conditional distribution and $\hat{f}(y|x) \in \mathcal{M}$ be the estimated conditional density. We are interested in investigating three

important questions of interest for model (1.1):

- (a) How to construct an estimator $\hat{f}(y|x)$ that can achieve the optimal minimax rate of convergence?
- (b) How to consistently estimate the number of mixture component q^* ?
- (c) How to numerically compute all unknown parameters and functions in $\hat{f}(y|x)$?

It is well known that addressing these questions represents major challenges even for parametric mixture regression models (Chernoff, 1954; Dacunha-Castelle and Gassiat, 1999; Zhu and Zhang, 2004; Ho and Nguyen, 2016; Heinrich and Kahn, 2018). The accuracy of estimation can be naturally measured by using

$$\mathcal{R}_n(\hat{f}, f^*) = \mathbb{E}_X \left\{ \int \left(\sqrt{\hat{f}(y|X)} - \sqrt{f^*(y|X)} \right)^2 dy \right\}, \quad (1.2)$$

which is the squared Hellinger distance between $\hat{h}(y, x) = \hat{f}(y|x)f_X(x)$ and $h^*(y, x) = f^*(y|x)f_X(x)$. As the sample size n increases, the convergence rate of $\mathcal{R}_n$ reflects the difficulty of the estimation problem.

We carry out a systematic investigation of model (1.1). We make four major contributions as follows:

- (i) We construct an optimal estimate of $f^*(y|x)$ by using the following steps. We show that a minimax lower bound of $\mathcal{R}_n$ in (1.2) depends

on the reproducing kernel K , the covariance function C of the random predictor X , and the model order q^* . In particular, it depends on the decay order of the eigenvalues of the operator $K^{1/2}CK^{1/2}$. Similar phenomenon has been found in the work on the functional regression (Cai and Yuan, 2012; Du and Wang, 2014; Wang and Ruppert, 2015). Then, we establish a minimax upper bound of $\mathcal{R}_n$ based on a penalized likelihood estimator when the true coefficient functions reside in $\mathcal{M}_q$ with $q \geq q^*$. We also propose a minimal penalty that yields a consistent order estimation.

(ii) We propose a general class of penalized likelihood order estimators in order to select and estimate the model order q^* . Theoretically, we establish the strong consistency of the order estimators for model (1.1). In contrast, most existing consistency results assume a prior upper bound on the order (Csiszár and Shields, 2000; Nishii, 1988). The only exception that we are aware is the reference (Gassiat and Van Handel, 2012), which explores the consistency properties of penalized likelihood model order estimator and provides the minimal strongly consistency penalty.

(iii) We develop an Expectation-Maximization (EM) type algorithm to

estimate all unknown parameters and functions.

- (iv) We examine the finite sample performance of our methods by using simulations and a real data set collected by the Alzheimer's Disease Neuroimaging Initiative (ADNI) study.

The remainder of this paper is structured as follows. Section 2 establishes the minimax rate of convergence of $\mathcal{R}_n(\hat{f}, f^*)$ in (1.2). Section 3 presents the estimation of q^* and the estimation of the coefficient functions $\Theta_{q^*}^*$. Section 4 summarizes the numerical results of all numerical experiments and real data analysis. This paper concludes with some discussions in Section 5.

2. Methodology

In this section, we first establish the minimax rate of convergence of $\mathcal{R}_n(\hat{f}, f^*)$ in (1.2) and then introduce an estimation algorithm for $\hat{f}$.

2.1 Optimal Rate of Convergence

The optimal rate of convergence of $\mathcal{R}_n(\hat{f}, f^*)$ is established in several steps. We first derive a minimax lower bound and then show that the convergence rate of the lower bound is in fact optimal by constructing an estimator that can attain this rate of convergence.

2.1 Optimal Rate of Convergence

Minimax lower bound

We first establish the minimax lower bound of $\mathcal{R}_n$ based on an assumption given below.

A1. Let $C(t, s) = \text{cov}(X(t), X(s))$ be the covariance function of X and $\{\rho_k : k \in \mathbb{N}\}$ be the non-increasing ordered eigenvalues of the operator $K^{1/2}CK^{1/2}$. Assume that $\rho_k \asymp k^{-2r}$ with $r > 0$.

Assumption A1 specifies that the decay rate of the eigenvalues of the operator $K^{1/2}CK^{1/2}$ is of order k^{-2r} . For a concrete example, consider the univariate Sobolev space W_2^m . It is known that its reproducing kernel is $(m!)^{-2}B_m(s)B_m(t) + (-1)^{m-1}\{(2m)!\}^{-1}B_{2m}(|s - t|)$, where B_m is the m th Bernoulli polynomial (Wahba, 1990). It is known that the decay rate of the eigenvalues of this kernel is of order k^{-2m} (Micchelli and Wahba, 1981).

The minimax lower bound is given in the following theorem.

Theorem 1. *Assuming A1 holds, we have*

$$\lim_{a \rightarrow 0} \lim_{n \rightarrow \infty} \inf_{\hat{f}} \sup_{f^* \in \mathcal{M}_{q^*}} \mathbb{P}(\mathcal{R}_n(\hat{f}, f^*) \geq a(q^*/n)^{\frac{2r}{2r+1}}) = 1. \quad (2.3)$$

The result in Theorems 1 is an asymptotic result. It shows that, there exists a function $V_1(a)$ such that $\lim_{n \rightarrow \infty} \inf_{\hat{f}} \sup_{f^*} \mathbb{P}(\mathcal{R}_n(\hat{f}, f^*) \geq a(q^*/n)^{2r/(2r+1)}) \geq V_1(a)$ and $V_1(a) \rightarrow 1$ as $a \rightarrow 0$. The proof of Theorem

2.1 Optimal Rate of Convergence

1 is provided in the appendix. The main tool is adopted from Tsybakov (2009) by realizing that any lower bound for a specific case yields immediately a lower bound for the general case. Theorem 1 shows that the minimax lower bound depends on the model order q^* and how the reproducing kernel K and the covariance function C are aligned. In general, the eigenvalues of K and C alone cannot determine the decay rate of the eigenvalues of $K^{1/2}CK^{1/2}$. For functional linear regression models, Cai and Yuan (2012) used the same tool to establish the minimax lower bound for prediction.

Minimax upper bound with $q \geq q^*$

Let $f^*(y|x) \in \mathcal{M}_{q^*}$ be the true conditional distribution and $\mathcal{M} = \cup_{q=1}^{\infty} \mathcal{M}_q$. The log-likelihood function can be written as

$$\begin{aligned} \ell_n(f) &= \sum_{i=1}^n \log f(Y_i|X_i) \\ &= \sum_{i=1}^n \log \sum_{k=1}^q \pi_k f_0(Y_i - \eta(X_i, \beta_k)), \quad f \in \mathcal{M}, \end{aligned} \quad (2.4)$$

where $\eta(X, \beta) = \int_{\mathcal{I}} X(t)\beta(t)dt$. We consider a general class of penalized likelihood estimation given by

$$\hat{f} = \arg \min_{f \in \mathcal{M}_q} \left\{ -\ell_n(f) + \lambda \|\beta\|_K^2 \right\} \quad (2.5)$$

for $q \geq q^*$, where λ is a smoothing parameter that balances the trade-off between the goodness of fit to the data and the smoothness of the estimator and $\|\cdot\|_K$ is the RKHS norm.

2.1 Optimal Rate of Convergence

The following notations are used throughout:

$$\begin{aligned} H_0(y|x) &= \sup_{\eta \in \mathbb{R}} f_0(y - \eta)/f^*(y|x), H_1(y|x) &= \sup_{\eta \in \mathbb{R}} |\dot{f}_0(y - \eta)|/f^*(y|x), \\ H_2(y|x) &= \sup_{\eta \in \mathbb{R}} |\ddot{f}_0(y - \eta)|/f^*(y|x), H_3(y|x) &= \sup_{\eta \in \mathbb{R}} |f_0^{(3)}(y - \eta)|/f^*(y|x), \end{aligned}$$

where $\dot{f}_0$, $\ddot{f}_0$, and $f_0^{(3)}$ are the first-, second-, and third-order derivatives of $f_0(\cdot)$, respectively. We need two additional assumptions.

B1. $f_0 \in C^3$ and $f_0(x)$ and $\dot{f}_0(x)$ vanish as $x \rightarrow \infty$. We assume $H_k(\cdot|\cdot) \in L^4(h^*d\mu)$ for $k = 0, 1, 2$ and $H_3(\cdot|\cdot) \in L^2(h^*d\mu)$.

B2. Given the functional predictor X , there exists a disjoint partition of $\mathbb{R} = A_0 \cup \{\cup_{k=1}^{q^*} A_k\}$ such that $A_1, \dots, A_{q^*}$ are bounded intervals, each bounded interval A_j contains precisely one component $\eta_k^* = \langle X, \beta_k^* \rangle$ for $k = 1, \dots, q^*$, and the unbounded set A_0 contains no component.

Condition B1 is similar to the condition adopted in the reference (Gas-siat and van Handel, 2014). This condition is satisfied in particular when f_0 is chosen as the standard normal density. Condition B2 characterizes the identifiability issue. In general, given x , the mean components $\langle x, \beta_k^* \rangle$ should be well separated to guarantee the identifiability.

Theorem 2. Assume that B1-B2 hold. Let $\{\rho_k : k \in \mathbb{N}\}$ be the non-increasing ordered eigenvalues of the operator $K^{1/2}CK^{1/2}$. Assume that

2.1 Optimal Rate of Convergence

$\rho_k \asymp k^{-2r}$ with $r > 1/2$. For any $q \geq q^*$, we have

$$\lim_{A \rightarrow \infty} \lim_{n \rightarrow \infty} \sup_{f^* \in \mathcal{M}_{q^*}} \mathbb{P} \left(\mathcal{R}_n(\hat{f}, f^*) \leq A(q/n)^{\frac{2r}{2r+1}} \right) = 1 \quad (2.6)$$

and $\|\hat{\beta}\|_K^2 = O_p(1)\|\beta^*\|_K^2$, provided that λ is of order $q^{2r/(2r+1)}n^{1/(2r+1)}$.

The result in Theorem 2 is also an asymptotic result. It shows that there exists a function $V_2(a)$ such that $\lim_{n \rightarrow \infty} \inf_{\hat{f}} \sup_{f^*} \mathbb{P}(\mathcal{R}_n(\hat{f}, f^*) \leq A(q^*/n)^{2r/(2r+1)}) \geq V_2(A)$ and $V_2(A) \rightarrow 1$ hold as $A \rightarrow \infty$. The proof of Theorem 2 is provided in the appendix. It combines two main tools. The first one is to characterize the local geometry of finite mixtures (Gassiat and van Handel, 2014) and the second one is to use the empirical process theory with the covering numbers to establish the convergence rate (van de Geer, 2000). Instead, the penalized estimator has an explicit solution for function linear regression models in Cai and Yuan (2012) and establishing the upper bound is more straightforward. Theorem 2 establishes the upper bound on the rate of the convergence of $\mathcal{R}_n$ based on the penalized likelihood estimator when $q \geq q^*$. However, we still cannot claim the minimax optimal rate of convergence since the model order q^* is unknown. Therefore, the consistent estimation of q^* is critical for achieving the minimax optimality on the rate of convergence of $\mathcal{R}_n$.

Consistent order estimation

2.1 Optimal Rate of Convergence

The number of components q^* of the true mixture $f^* \in \mathcal{M}$ can be estimated by using a general class of penalized likelihood order estimator:

$$\hat{q}_n = \arg \max_{q \geq 1} \left\{ \sup_{f \in \mathcal{M}_q} \left(\ell_n(f) - \lambda \|\beta\|_K^2 \right) - \text{pen}_n(q) \right\}, \quad (2.7)$$

where $\text{pen}_n(q)$ is a penalty function and $\ell_n(f)$ is the likelihood function. Our goal is to understand which $\text{pen}_n(q)$ can yield the strong consistency of the order estimator, i.e., $\hat{q}_n \rightarrow q^*$ as $n \rightarrow \infty$ a.s. Achieving this goal requires a precise understanding of the difference of the penalized log-likelihood functions given by

$$\sup_{f \in \mathcal{M}_q} \left(\ell_n(f) - \lambda_{q,n} \|\beta\|_K^2 \right) - \sup_{f \in \mathcal{M}_{q^*}} \left(\ell_n(f) - \lambda_{q^*,n} \|\beta\|_K^2 \right)$$

as $n \rightarrow \infty$, uniformly in the model order $q > q^*$. In this section, we discuss the selection of $\text{pen}_n(q)$, which yields the strong consistency of $\hat{q}_n$.

Theorem 3. *Assume B1-B2 hold. Let $\{\rho_k : k \in \mathbb{N}\}$ be the nonincreasing ordered eigenvalues of the operator $K^{1/2}CK^{1/2}$. Assume that $\rho_k \asymp k^{-2r}$ with $r > 1/2$. Let $c > 0$ be a constant and*

$$\text{pen}_n(q) = cq^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}} \log(n). \quad (2.8)$$

Then, we have

(a). $\hat{q}_n \rightarrow q^*$ as $n \rightarrow \infty$ a.s.;

2.1 Optimal Rate of Convergence

$$(b). \lim_{A \rightarrow \infty} \lim_{n \rightarrow \infty} \sup_{f^* \in \mathcal{M}_{q^*}} \mathbb{P} \left(\mathcal{R}_n(\hat{f}, f^*) \geq A(q^*/n)^{\frac{2r}{2r+1}} \right) = 0.$$

The proof of Theorem 3 is provided in the appendix, which is obtained by precisely characterizing the difference of the penalized log-likelihood functions. The intuition for (2.8) is that, since we are dealing with infinite dimensional parameters like β_k , this order requires that the intrinsic dimension for each component is about $(n/q)^{1/(2r+1)}$ and the total dimension for q components is $q^{2r/(2r+1)} n^{1/(2r+1)}$. Theorem 3 shows that the penalty term with the order $q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}} \log(n)$ yields a strong consistent order estimator. This term depends on the decay rate of the eigenvalues of the operator $K^{1/2}CK^{1/2}$. We may compare this with the popular BIC penalty

$$\text{BIC}_n(q) = \frac{dq + q - 1}{2} \log(n),$$

where d is the dimension of the parameter space. However, due to the existence of the infinite dimensional parameters, it is not straightforward to choose the BIC penalty in our setting. Theorems 1-3 together show that the minimax rate of convergence for $\mathcal{R}_n$ is $(q^*/n)^{\frac{2r}{2r+1}}$, which is determined by the rate of decay of the eigenvalues of the operator $K^{1/2}CK^{1/2}$ and the model order q^* .

2.2 The Estimation Algorithm

2.2 The Estimation Algorithm

The estimation procedure for model (1.1) consists of two parts: (i) the estimation of q^* and (ii) the estimation of the coefficient functions $\Theta_{q^*}^*$. We propose a two-step estimation procedure as follows. First, for different values of q , we obtain the estimation of Θ_q for each given q . Second, based on the estimation of Θ_q , we compute the term inside the maximum in (2.7) and then determine the estimate of q^* accordingly. In this section, we fix f_0 to be a Gaussian density. By an abuse of notation, we use $f_0(Y_i|X_i, \beta_k, \sigma^2)$ to denote $f_0(Y_i - \langle X_i, \beta_k \rangle)$.

EM algorithm

For a given q , the estimate of Θ_q can be obtained via an Expectation-Maximization (EM) algorithm. Define u_{ik} as the indicator of whether X_i is from component k , i.e. $u_{ik} = 1$ if X_i comes from the k -th component, and $u_{ik} = 0$ otherwise. If the missing data u_{ik} 's could be observed, then the penalized log-likelihood for the complete data is given by

$$\log L_c(\Theta_q, \sigma^2) = \sum_{i=1}^n \sum_{k=1}^q u_{ik} \{ \log \pi_k + \log f_0(Y_i|X_i, \beta_k, \sigma^2) \} - \sum_{k=1}^q \frac{n\lambda \|\beta_k\|_K^2}{2\sigma^2},$$

where λ controls the level of the penalty.

The corresponding EM algorithm is given in the following E-step and M-step:

2.2 The Estimation Algorithm

E-step:

Denote the estimates of parameters in the m -th iteration as $\Theta_q^{(m)} = \{\beta_1^{(m)}, \dots, \beta_q^{(m)}\}$, $\Pi_q^{(m)} = \{\pi_1^{(m)}, \dots, \pi_q^{(m)}\}$, and $\sigma^{2(m)}$. We estimate $\tau_{ik} = P(u_{ik} = 1)$ as follows

$$\tau_{ik}^{(m+1)} = \frac{\pi_k^{(m)} f_0(Y_i | X_i, \beta_k^{(m)}, \sigma^{2(m)})}{\sum_{k=1}^q \pi_k^{(m)} f_0(Y_i | X_i, \beta_k^{(m)}, \sigma^{2(m)})}. \quad (2.9)$$

The mixing probabilities $\Pi^{(m+1)}$ are estimated accordingly by

$$\pi_k^{(m+1)} = \frac{1}{n} \sum_{i=1}^n \tau_{ik}^{(m)}. \quad (2.10)$$

M-step:

We maximize the following Q function with respect to Θ_q and σ^2 :

$$\begin{aligned} & Q(\Theta_q, \sigma^2) \\ &= \sum_{i=1}^n \sum_{k=1}^q \tau_{ik}^{(m)} (\log \pi_k + \log f_0(Y_i; X_i, \beta_k, \sigma^2)) - \sum_{k=1}^q \frac{n\lambda \|\beta_k\|_K^2}{2\sigma^2}. \end{aligned} \quad (2.11)$$

By the representer theorem (Wahba, 1990), for each β_k , there exists a vector $C_k = (c_{1k}, \dots, c_{nk})^T \in R^n$ such that the quantity that maximizes the Q function (2.11) can be expressed as:

$$\beta_k(t)^{(m+1)} = \sum_{i=1}^n c_{ik} \int_{\mathcal{I}} K(t, s) X_i(s) ds \quad (2.12)$$

and $\|\beta_k\|_K^2 = C_k^T W C_k$, where $W = (W_{ij})$ is an n by n Gram matrix with

$$W_{ij} = \iint_{\mathcal{I} \times \mathcal{I}} X_i(s) K(s, t) X_j(t) ds dt \quad \text{for } i, j \in \{1, \dots, n\}. \quad (2.13)$$

2.2 The Estimation Algorithm

Therefore, the maximization of the Q function (2.11) can be solved component-wisely by solving the optimization with respect to C_k .

We consider the case when f is the normal distribution, then the conditional distribution of Y_i , is given by

$$Y_i|X_i \sim N\left(\int_{\mathcal{I}} X_i(t)\beta_k(t)dt, \sigma^2\right) = N\left(C_k^T W_{\cdot,i}, \sigma^2\right),$$

where $W_{\cdot,i}$ is the i -th column of the Gram matrix (2.13).

The Q function (2.11) then reduces to (up to a constant)

$$\begin{aligned} & Q(\Theta_q, \sigma^2) \\ &= \sum_{i=1}^n \sum_{k=1}^q \tau_{ik}^{(m)} \left(\log \pi_k - \frac{1}{2} \log \sigma^2 - \frac{(Y_i - C_k^T W_{\cdot,i})^2}{2\sigma^2} \right) - \sum_{k=1}^q \frac{n\lambda C_k^T W C_k}{2\sigma^2}. \end{aligned} \quad (2.14)$$

The estimate of C_k in the above equation can be expressed as a Tikhonov regularized weighted least square problem. The solution is given by

$$C_k^{(m+1)} = \left(W^T T_k^{(m)} W + n\lambda W \right)^{-1} W^T T_k^{(m)} Y, \quad (2.15)$$

where $T_k^{(m)} = \text{diag}\{\tau_{1k}^{(m)}, \dots, \tau_{nk}^{(m)}\}$ and $Y = (Y_1, \dots, Y_n)^T$.

We then construct the coefficient functions β_k 's by plugging $c_{ik}^{(m+1)}$'s into (2.12), i.e.

$$\beta_k(t)^{(m+1)} = \sum_{i=1}^n c_{ik}^{(m+1)} \int_{\mathcal{I}} K(t, s) X_i(s) ds. \quad (2.16)$$

2.2 The Estimation Algorithm

The estimation of σ^2 is achieved by solving the penalized MLE in (2.14), leading to

$$\sigma^{2(m+1)} = \frac{\sum_{i=1}^n \sum_{k=1}^q \tau_{ik}^{(m)} \left(Y_i - C_k^{T(m+1)} W_{\cdot, i} \right)^2}{\sum_{i=1}^n \sum_{k=1}^q \tau_{ik}^{(m)}} + \frac{n\lambda \sum_{k=1}^q C_k^T W C_k}{\sum_{i=1}^n \sum_{k=1}^q \tau_{ik}^{(m)}}. \quad (2.17)$$

We iteratively proceed the updates of (2.9) and (2.10) in E-step and the updates of (2.15), (2.16) and (2.17) in M-step until the convergence is reached.

We are using the Gaussian kernel throughout the paper. The bandwidth, denoted by ϱ , of the reproducing kernel $K(\cdot, \cdot)$ and the ridge penalty λ are treated as hyper-parameters. They are tuned based on cross validation. Other kernels can be easily incorporated into our algorithm. Learning optimal kernels is definitely a non-trivial question and deserves further investigation. A good method of learning optimal kernels is to combine multiple candidate kernels.

Order estimation

The optimal order of the mixture model can be estimated through the optimization in (2.7). This is a mixed integer programming (MIP), whose solution may not be directly obtained in practice. We denote the negative of Equation (2.7) inside the maximum as the order objective function, i.e.

$$\text{Order}(q) = \left(-\ell_n(f^{(q)}) + \lambda \|\beta^{(q)}\|_K^2 \right) + \text{pen}_n(q), \quad (2.18)$$

where $f^{(q)}$ and $\beta^{(q)}$ are the estimates calculated from the EM algorithm with the model order being q . The first part of $\text{Order}(q)$ is essentially the penalized loss and the second part is the penalty (2.8) on q . Thus we conduct a sequential search for the optimal order q^* . Specifically, we start from $q = 1$ and increase its value by 1 each time, and then compute the $\text{Order}(q)$ according to (2.18). As the model order increases, the penalized loss part in the $\text{Order}(q)$ will decrease, and the penalty on the model order will increase. Once $\text{Order}(q)$ no longer decreases, we select the q value that minimizes $\text{Order}(q)$ as the optimal estimate.

3. Numerical Results

We conduct simulations to evaluate the accuracy and efficiency of our methods and then apply them to the analysis of a real data set obtained from the ADNI study.

3.1 Synthetic experiments

We perform simulations in two different scenarios including one with two mixing components ($q^* = 2$) and another with three ($q^* = 3$). The true coefficient images are generated from a Gaussian function with different centers. The covariate images $X_i(t)$'s are simulated from a Gaussian random

3.1 Synthetic experiments

Figure 1: The first row of images includes the true coefficients β_1 and β_2 in the first scenario, and the bottom row includes the true coefficients β_1 , β_2 , and β_3 in the second scenario.

field. Figure 1 displays the true coefficients for these two scenarios.

The responses Y_i 's follow a mixture of functional linear models given by

$$Y_i = \sum_{k=1}^q \delta_{ik} \left(\beta_{k0} + \int_{t \in \mathcal{T}} X_i(t) \beta_k(t) dt \right) + \epsilon_i, \quad (3.19)$$

where $\delta_{ik} = 1$ if the subject i comes from the k -th component, and 0 otherwise. The noise term ϵ_i follows a standard normal distribution and

3.1 Synthetic experiments

Figure 2: The top row of images includes the estimates of β_1 and β_2 in scenario 1 from one replication, and the bottom row is the estimates of β_1 , β_2 and β_3 in scenarios 2.

is independent of $X_i(t)$. In each scenario, we set the sample size in each components to be 80, i.e., $\sum_{i=1}^n \delta_{ik} = 80$, and the total number of samples are $n = 160$ and 240 in scenarios 1 and 2, respectively.

The initial tuning range for the bandwidth ϱ of the kernel K and the ridge penalty level λ is from a 2-dimensional grid, i.e., $\sigma \otimes \lambda = \{2^{-5}, 2^{-4}, \dots, 2^5\}^{\otimes 2}$.

We start with the functional linear model with one component and increase

3.1 Synthetic experiments

the value q by 1 each time. For each q , the stopping criteria of the EM algorithm is determined by either $\sum_{k=1}^q \|C_k^{(m+1)} - C_k^{(m)}\|^2 / \{\sum_{k=1}^q \|C_k^{(m)}\|^2\} \leq 10^{-5}$ or the total number of iteration is over 500. To evaluate the estimation performance, we first check the estimation of q^* . If q^* is correctly estimated, we further compute the relative mean squared error (RMSE) for each β_k , i.e. $\text{RMSE} = \|\hat{\beta}_k - \beta_k\|^2 / \|\beta_k\|^2$. For each sample, we denote $\hat{u}_{ik} = 1$, if $k = \arg \max_j \{\hat{\tau}_{ij}\}$, and compute the assignment accuracy as $\text{ACC} = n^{-1} \sum_{i=1}^n \sum_{k=1}^{q^*} \delta(\hat{u}_{ik}, u_{ik})$, where $\delta(\cdot, \cdot)$ is the indicator function. The empirical prediction risk is quantified as the root mean square prediction error, i.e. $\text{RMSPE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$. We also conduct the regression analysis using just the functional linear model (FLM) (without the mixing components identification) as a baseline for the RMSPE comparison. Note that the basic FLM only has one component, so the RMSE and ACC comparisons are not applicable.

We present the estimation results in each scenario in Table 1. In both scenarios, we can correctly estimate the order of the mixing components q^* in all 100 repetitions. In scenario 1, the assignment accuracy is 86.5%, whereas in scenario 2, it is 65.1%. This decrease of accuracy is mainly due to the increase of the number of components.

We achieve desirable relative mean square errors in both scenarios with

3.2 MMSE score prediction in ADNI study

Table 1: The empirical mean and standard error in the parenthesis of relative mean squared error (RMSE), the assignment accuracy (ACC), and the root mean square prediction error (RMSPE) in scenarios 1 and 2, labeled as S1 and S2, respectively. FFMRM denotes the functional finite mixture regression model; FLM denotes the functional linear model. For each case, 100 simulated data sets were used.

	RMSE			ACC	RMSPE	
	β_1	β_2	β_3		FFMRM	FLM
S1	1.80(0.38)	1.84(0.39)	N/A	0.86(0.06)	1.01(0.47)	3.65(0.35)
S2	1.99(0.39)	2.04(0.37)	2.10(0.28)	0.65(0.23)	1.02(0.34)	3.53(0.32)

a slightly better performance in scenario 1. To graphically demonstrate the estimated coefficient, we randomly pick up one iteration for each scenario and plot the estimated coefficients in Figure 2. The estimated coefficients can correctly capture the non-zeros regions and recover the patterns in the true coefficients.

3.2 MMSE score prediction in ADNI study

To further demonstrate the usefulness of model (1.1), we apply our methods to a real data set obtained from the Alzheimer’s Disease Neuroimaging

3.2 MMSE score prediction in ADNI study

Table 2: The demographical information of all participants in ADNI. The means are reported with the standard deviations included in the parentheses.

Diagnosis	Gender(F/M)	Age (years)	MMSE
CN	164/167	74.46 (5.58)	28.99 (1.23)
SMC	61/42	72.01 (5.46)	29.01 (1.96)
EMCI	127/161	71.26 (7.51)	28.35 (1.55)
LMCI	152/245	73.66 (7.41)	26.97 (2.70)
AD	99/142	74.96 (7.88)	23.25 (2.10)

Initiative (ADNI) study. The ADNI study as a large scale multi-site study has collected g magnetic resonance imaging (MRI), positron emission tomography (PET) images, Cerebrospinal fluid (CSF), and blood biomarkers, among many others. More information about this study can be found at the ADNI website (<http://adni.loni.usc.edu/>).

We study the Positron Emission Tomography (PET) data, and use them as imaging predictors to predict the Mini-Mental State Examination (MMSE) scores. The PET images measure the metabolic processes of the patients, such as flows of blood to different parts of the brain, via detect-

3.2 MMSE score prediction in ADNI study

ing the radioactivity of the injected tracer. We analyze the PET images collected at the baseline of the ANDI study. Among a total number of 1,360 participants, there are five diagnostic groups, including Normal Control (CN), Significant Memory Concern (SMC), Early Mild Cognitive Impairment (EMCI), Late Mild Cognitive Impairment (LMCI) and diagnosed Alzheimer’s Disease (AD). The demographical information of the participants is summarized in Table 2 and a sample image from each type of participants is provided in Figure 3.

We remove the age and gender factors by fitting a linear model in each voxel and use the residual maps as the covariate images of model (1.1). The same configuration of the EM algorithm in the simulation studies is used to train the model and the adaptive tuning procedure is utilized for tuning parameter selection. Finally, three mixing components are determined by the EM algorithm with their corresponding coefficients images displayed in Figure 4. The overall proportional probability π_k ’s are estimated as 19.8%, 41.0%, and 39.2%, respectively. We conduct a hierarchical clustering on the patients according to their estimated proportional probabilities to each component τ_{ik} and illustrate the corresponding similarity matrix in Figure 5. These clusters indicate potential heterogeneous disease patterns of AD among the population, which is a fact that has been proved by existing

3.2 MMSE score prediction in ADNI study

Figure 3: The five rows of images are the PET images of different types of participants. We randomly pick one image from each group for illustration. The types of the participants are AD, CN, EMCI, LMCI and SMC, from top to bottom respectively. Eight transverse slices located at $Z = 8$ to 78 with equal increment of 10 , are displayed from left to right, respectively.

studies (Latta et al., 2015; Dong et al., 2016). We overlay the coefficient images on the MNI-152 ROI template (Fonov et al., 2011), and are able to identify several regions of interest: $\hat{\beta}_1$ mainly represents the impairment in sup frontal and parietal lobe; $\hat{\beta}_2$ highlights corpus callosum and occipital

3.2 MMSE score prediction in ADNI study

Figure 4: The three rows of images are the estimated coefficients, $\hat{\beta}_1$, $\hat{\beta}_2$ and $\hat{\beta}_3$ from top to bottom, respectively. Eight transverse slices located at $Z = 8$ to 78 with equal increment of 10, are displayed from left to right, respectively.

lobe; and $\hat{\beta}_3$ mostly covers the middle frontal gyrus. Many studies in literature have shown that the reduced glucose metabolic activities and structural impairment in frontal lobe, parietal lobe and occipital lobe of the cerebrum are associated with the degradation in cognition and the progression to Alzheimer's Disease (Lin et al., 2017; Heneka et al., 2015).

Figure 5: The similarity matrix of the estimation of τ_k 's. The value indicates the pairwise Euclidean distance of the proportional probabilities.

4. Conclusion

We have developed a functional finite mixture regression model with functional predictors in the reproducing kernel Hilbert space. This is a challenging problem because of the unknown model order and the existence of infinite dimensional unknown parameters. Our theoretical developments discover a strong consistent estimator of the model order using a penalized likelihood estimation and establish the minimax rate of convergence

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for the estimation risk. It is shown that the optimal rate is jointly determined by the alignment of the reproducing kernel, covariance kernel, and the model order. An efficient EM algorithm is also proposed, and empirical experimental results demonstrate the merits of our method.

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Appendix: Technical Lemmas and Proofs of Theorems

A1. Technical Lemmas

Lemma 1. Assume B1 and B2 hold. Define $H_q(\epsilon) = \{\sqrt{f/f^*} : f \in \mathcal{M}_q, \mathcal{H}(h, h^*) \leq \epsilon\}$. Then

$$N_{[\cdot]}(H_q(\epsilon), \delta) \leq \left(\frac{C_1 \epsilon}{\delta}\right)^{10(C_2 \delta^{-\frac{1}{r}+1})_{q+1}} \quad (4.20)$$

for all $q \geq q^*$ and $\delta/\epsilon \leq 1$.

Proof. We prove the lemma by extending the arguments in Gassiat and van Handel (2014).

Note that $f/f^* = h/h^*$. We denote by $\|\cdot\|_p$ the $L^p(h^*d\mu)$ -norm, i.e., $\|g\|_p^0 = \int |g|^p h^* d\mu$.

Denote $\eta_i^* = \langle x, \beta_i^* \rangle$ and $\eta_j = \langle x, \beta_j \rangle$, $i = 1, \dots, q^*$, $j = 1, \dots, q$. It follows from B2 that we can

find a partition of $\mathbb{R}$, $A_0, A_1, \dots, A_{q^*}$, such that each bounded set A_i , $i = 1, \dots, q^*$, contains

precisely one component $\eta_i^* = \langle X, \beta_i^* \rangle$ and the unbounded set $A_0 = \mathbb{R}^M \setminus (A_1 \cup \dots \cup A_{q^*})$

contains no component. Let $f \in \mathcal{M}_q$, so that we can write $f = \sum_{i=1}^q \pi_i f_0(y - \eta_i)$. Then,

$$\begin{aligned} \frac{f - f^*}{f^*} &= \sum_{j: \eta_j \in A_0} \pi_j \frac{f_0(y - \eta_j)}{f^*} \\ &\quad + \sum_{i=1}^{q^*} \left\{ \left(\sum_{j: \eta_j \in A_i} \pi_j - \pi_i^* \right) \frac{f_0(y - \eta_i^*)}{f^*} + \sum_{j: \eta_j \in A_i} \frac{f_0(y - \eta_j) - f_0(y - \eta_i^*)}{f^*} \right\}. \end{aligned}$$

Taylor expansion gives

$$f_0(y - \eta_j) - f_0(y - \eta_i^*) = \dot{f}_0(y - \eta_i^*)(\eta_j - \eta_i^*) + \frac{1}{2} \ddot{f}_0(y - \bar{\eta})(\eta_j - \eta_i^*)^2.$$

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Using Assumption B2, we find that

$$\left| \frac{f - f^*}{f^*} \right| \leq \left[\sum_{j: \eta_j \in A_0} \pi_j + \sum_{i=1}^{q^*} \left\{ \left| \sum_{j: \eta_j \in A_i} \pi_j - \pi_i^* \right| + \left| \sum_{j: \eta_j \in A_i} \pi_j (\eta_j - \eta_i^*) \right| + \frac{1}{2} \sum_{j: \eta_j \in A_i} \pi_j (\eta_j - \eta_i^*)^2 \right\} \right] (H_0 + H_1 + H_2).$$

On the other hand, it follows from Theorem 3.10 of Gassiat and van Handel (2014) that there exists a constant c^* such that

$$\left\| \frac{f - f^*}{f^*} \right\|_1 \geq c^* \left[\sum_{j: \eta_j \in A_0} \pi_j + \sum_{i=1}^{q^*} \left\{ \left| \sum_{j: \eta_j \in A_i} \pi_j - \pi_i^* \right| + \left| \sum_{j: \eta_j \in A_i} \pi_j (\eta_j - \eta_i^*) \right| + \frac{1}{2} \sum_{j: \eta_j \in A_i} \pi_j (\eta_j - \eta_i^*)^2 \right\} \right].$$

Hence, for all $f \in \mathcal{M}$,

$$\frac{|f/f^* - 1|}{\|f/f^* - 1\|_1} \leq S := \frac{1}{c^*} (H_0 + H_1 + H_2).$$

In addition, using $|\sqrt{x} - 1| \leq |x - 1|$, we find

$$\frac{|\sqrt{h/h^*} - 1|}{\mathcal{H}(h, h^*)} \leq \frac{|h/h^* - 1|}{\frac{1}{2} \|h/h^* - 1\|_1} = \frac{|f/f^* - 1|}{\frac{1}{2} \|f/f^* - 1\|_1} \leq 2S.$$

Similar to Lemma 3.15 of [1], for and $f \in \mathcal{M}$, we have

$$\frac{|\sqrt{h/h^*} - 1|}{H(h, h^*)} - \frac{h/h^* - 1}{\sqrt{\chi^2(h||h^*)}} \leq (4\|S\|_4^2 S + 2S^2) H(h, h^*),$$

where the chi-square divergence is defined as $\chi^2(h||h^*) = \int (h/h^* - 1)^2 h^* d\mu$. This allows us to

make further approximation based on Lemma 3.16 of [1]. Let $\alpha > 0$, and for every $f \in \mathcal{M}_q$

such that $H(h, h^*) \leq \alpha$. Define

$$\tilde{\ell} = \sum_{i=1}^{q^*} \left\{ a_i \frac{f_0(y - \eta_i^*)}{f^*} + b_i \frac{\dot{f}_0(y - \eta_i^*)}{f^*} + e_i^2 \frac{\ddot{f}_0(y - \eta_i^*)}{f^*} \right\} + \sum_{j=1}^q \gamma_j \frac{f_0(y - \eta_j)}{f^*},$$

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where

$$\begin{aligned} \sum_{i=1}^{q^*} |a_i| &\leq \frac{1}{c^*} + \frac{1}{\sqrt{c^* \alpha}}, \quad \sum_{i=1}^{q^*} |b_i| \leq \frac{1}{c^*} + 2 \frac{c}{\sqrt{c^* \alpha}}, \\ \sum_{i=1}^{q^*} e_i^2 &\leq \frac{1}{c^*}, \quad \sum_{j=1}^q \gamma_j \leq \frac{1}{\sqrt{c^* \alpha} \wedge c^*}. \end{aligned} \quad (4.21)$$

We have

$$\left| \frac{h/h^* - 1}{\sqrt{\chi^2(h \| h^*)}} - \tilde{\ell} \right| \leq \frac{\sqrt{2}}{2(c^*)^{5/4}} (\|H_3\|_2 S + H_3) \alpha^{1/4}.$$

Define

$$d_f = \frac{\sqrt{f/f^*} - 1}{\|\sqrt{f/f^*} - 1\|_2},$$

and

$$\mathcal{D}_q = \{d_f : f \in \mathcal{M}_q, f \neq f^*\}, \quad \mathcal{D}_{q,\alpha} = \{d_f : f \in \mathcal{M}_q, f \neq f^*, \mathcal{H}(h, h^*) \leq \alpha\}.$$

Then,

$$N_{[\cdot]}(\mathcal{D}_q, \delta) \leq N_{[\cdot]}(\mathcal{D}_{q,\alpha}, \delta) + N_{[\cdot]}(\mathcal{D}_q \setminus \mathcal{D}_{q,\alpha}, \delta).$$

We estimate both bracketing numbers separately. Define a family of functions

$$\tilde{\mathcal{L}}_{q,\alpha} = \left\{ \sum_{i=1}^{q^*} \left\{ a_i \frac{f_0(y - \eta_i^*)}{f^*} + b_i \frac{\dot{f}_0(y - \eta_i^*)}{f^*} + e_i^2 \frac{\ddot{f}_0(y - \eta_i^*)}{f^*} \right\} + \sum_{j=1}^q \gamma_j \frac{f_0(y - \eta_j)}{f^*} \right\},$$

where $(a, b, e, \gamma) \in \mathbb{R}^{q^*} \times \mathbb{R}^{q^*} \times \mathbb{R}^{q^*} \times \mathbb{R}^q$ satisfies the constraint (4.21). For $\tilde{l}, \tilde{l}' \in \tilde{\mathcal{L}}_{q,\alpha}$,

$$\begin{aligned} |\tilde{l} - \tilde{l}'| &\leq H_0 \sum_{i=1}^{q^*} |a_i - a'_i| + H_1 \sum_{i=1}^{q^*} |b_i - b'_i| + H_0 \sum_{i=1}^q |\gamma_i - \gamma'_i| \\ &\quad + \frac{1}{\sqrt{c^* \alpha} \wedge c^*} H_1 \sum_{i=1}^q |\langle x, \beta_i - \beta'_i \rangle| + \frac{2H_2}{\sqrt{c^*}} \sum_{i=1}^{q^*} |e_i - e'_i|. \end{aligned}$$

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Note that

$$\begin{aligned} \mathbb{E}_X \left(\sum_{i=1}^q |\langle x, \beta_i - \beta'_i \rangle| \right)^2 &\leq q \sum_{i=1}^q \mathbb{E}_X |\langle x, \beta_i - \beta'_i \rangle|^2 = q \sum_{i=1}^q \sum_{k=1}^{\infty} \rho_k (g_{ik} - g'_{ik})^2 \\ &\leq q \sum_{i=1}^q \sum_{k=1}^M \rho_k (g_{ik} - g'_{ik})^2 + M^{-2r} o_M(1). \end{aligned}$$

We may choose $M = c_1 \delta^{-1/r}$, so that

$$|\tilde{l} - \tilde{l}'| \leq V \|(a, b, \gamma, g, e) - (a', b', \gamma', g', e')\|_{\text{norm}} + o(\delta),$$

where $V = 3(H_0 + H_1 + H_2)$ and $\|\cdot\|_{\text{norm}}$ is the norm on $\mathbb{R}^{3q^* + c_2 q(\delta^{-1/r} + 1)}$ defined by

$$\|(a, b, \gamma, g, e)\|_{\text{norm}} = \sum_{i=1}^{q^*} |a_i| + \sum_{i=1}^{q^*} |b_i| + \sum_{i=1}^q |\gamma_i| + \frac{q}{\sqrt{c^* \alpha} \wedge c^*} \sum_{i=1}^q \sum_{k=1}^M \rho_k g_{ik}^2 + \frac{2}{\sqrt{c^*}} \sum_{i=1}^{q^*} |e_i|.$$

Using the standard fact of the covering number for the Euclidean ball we obtain

$$N_{[\cdot]}(\tilde{L}_{q,\alpha}, \delta) = \left(\frac{c_3 + \delta}{\delta} \right)^{3q^* + c_2 q(\delta^{-1/r} + 1)}.$$

Since $q \geq q^*$ and $\delta \leq 1$, we therefore obtain

$$N_{[\cdot]}(\mathcal{D}_{q,\alpha}, \delta) \leq \left(\frac{c_4}{\delta} \right)^{c_5 q(\delta^{-1/r} + 1)}.$$

□

Lemma 2. Assume B1 and B2 hold.

(a).

$$\mathbb{P} \left[\sup_{f \in \mathcal{M}_q} \sum_{i=1}^n \log \frac{f(Y_i | X_i)}{f^*(Y_i | X_i)} \geq \alpha \right] \leq C_3 e^{-\alpha/C_3}$$

for all $\alpha \geq C_4 q^{2r/(2r+1)} n^{1/(2r+1)}$.

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(b).

$$\overline{\lim}_{n \rightarrow \infty} \sup_{f \in \mathcal{M}_q} \frac{1}{n} \sum_{i=1}^n \log \frac{f(Y_i|X_i)}{f^*(Y_i|X_i)} < 0, \text{ a.s.}$$

Proof. Let $h(y, x) = f(y|x)f_X(x)$ and $h^*(y, x) = f^*(y|x)f_X(x)$ for $f \in \mathcal{M}_q$ and $f^* \in \mathcal{M}_{q^*}$.

Denote by $\bar{h} = (h + h^*)/2$. We first have the inequalities $\mathcal{K}(h, h^*) \geq \mathcal{H}^2(h, h^*)$, and

$$\sum_{i=1}^n \log \frac{h}{h^*} \leq 2\sqrt{n}\nu_n(\log \frac{\bar{h}}{h^*}) - 2n\mathcal{K}(\bar{h}, h^*). \quad (4.22)$$

Therefore,

$$\begin{aligned} \mathbb{P}\left[\sup_h \sum_{i=1}^n \log \frac{h}{h^*} \geq \alpha\right] &\leq \mathbb{P}\left[\sup_h \sqrt{n}\nu_n(\log \frac{\bar{h}}{h^*}) - n\mathcal{H}^2(\bar{h}, h^*) \geq \frac{\alpha}{2}\right] \\ &\leq \sum_{s=0}^S \mathbb{P}\left[\sup_{h \in \mathcal{G}_s} \nu_n(\log \frac{\bar{h}}{h^*}) \geq \frac{\alpha 2^{s-1}}{\sqrt{n}}\right] \\ &= \sum_{s=0}^S \mathbb{P}\left[\sup_{h \in \mathcal{G}_s} \nu_n(\log \sqrt{\frac{\bar{h}}{h^*}}) \geq \frac{\alpha 2^{s-2}}{\sqrt{n}}\right], \end{aligned}$$

where $\mathcal{G}_0 = \{\bar{h} : n\mathcal{H}^2(\bar{h}, h^*) \leq \alpha\}$, $\mathcal{G}_s = \{\bar{h} : \alpha 2^{s-1} < n\mathcal{H}^2(\bar{h}, h^*) \leq \alpha 2^s\}$, $1 \leq s \leq S$, $S =$

$\min\{s : \alpha 2^s > 2n\}$. We need to find the bracketing number for $\bar{H}_q(\epsilon) = \{\sqrt{h/h^*} : \mathcal{H}(\bar{h}, h^*) \leq \epsilon\}$.

This can be easily deduced from Lemma 1 such that

$$N_{[\cdot]}(\bar{H}_q(\epsilon), \delta) \leq \left(\frac{2\sqrt{2}C_1}{\delta} \epsilon\right)^{10(C_2\delta^{-\frac{1}{r}} + 1)q+1}. \quad (4.23)$$

Note that $\int_0^\epsilon \sqrt{\log N_{[\cdot]}(\bar{H}_q(\epsilon), \delta)} d\delta \leq c\sqrt{q}\epsilon^{1-1/(2r)}$. It requires that $c\sqrt{q}\epsilon^{1-1/(2r)} \leq \sqrt{n}\epsilon^2$

such as $\epsilon \geq c_1(q/n)^{r/(2r+1)}$. Next, apply Theorem 7.4 of van de Geer (2000), together with

$\sqrt{\alpha 2^{s/2+2}}/\sqrt{n} \geq c_1(q/n)^{r/(2r+1)}$, i.e., $\alpha \geq c_2 q^{2r/(2r+1)} n^{1/(2r+1)}$. We obtain

$$\sum_{s=0}^S \mathbb{P}\left[\sup_{h \in \mathcal{G}_s} \nu_n(\log \sqrt{\frac{\bar{h}}{h^*}}) \geq \frac{\alpha 2^{s-2}}{\sqrt{n}}\right] \leq \sum_{s=0}^S c_3 e^{-\frac{\alpha 2^s}{c_3 2^s}} \leq C_3 e^{-\alpha/C_3}.$$

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This finishes the proof of Part (a).

To prove Part (b), it follows from (4.22) that it is enough to show that

$$\lim_{n \rightarrow \infty} \sup_{f \in \mathcal{M}_q} n^{-1/2} \nu_n(\log \sqrt{\frac{\bar{h}}{h^*}}) = 0, \quad \text{a.s.}$$

As in the proof of Part (a), we have

$$\mathbb{P} \left[\sup_{f \in \mathcal{M}_q} n^{-1/2} \nu_n(\log \sqrt{\frac{\bar{h}}{h^*}}) \geq \alpha \right] \leq c_4 e^{-n\alpha^2/c_4}$$

for every $\alpha > 0$ such that $c_2 q^{2r/(2r+1)} n^{1/(2r+1)} \leq \alpha \sqrt{n} \leq 32\sqrt{n}$. Hence,

$$\sum_{n=1}^{\infty} \mathbb{P} \left[\sup_{f \in \mathcal{M}_q} n^{-1/2} \nu_n(\log \sqrt{\frac{\bar{h}}{h^*}}) \geq \alpha \right] \leq \infty$$

for $0 < \alpha \leq 32$. Part b follows from Borel-Cantelli. $\square$

Lemma 3. Assume B1 and B2 hold. Define

$$\Delta_n(q, q^*) = \sup_{f \in \mathcal{M}_q} \left(\ell_n(f) - \lambda_{q,n} \|\beta\|_K^2 \right) - \sup_{f \in \mathcal{M}_{q^*}} \left(\ell_n(f) - \lambda_{q^*,n} \|\beta\|_K^2 \right),$$

where $\lambda_{q,n} = C_5 q^{2r/(2r+1)} n^{1/(2r+1)}$ and $\lambda_{q^*,n} = \tilde{C}_5 (q^*)^{2r/(2r+1)} n^{1/(2r+1)}$. Then,

$$\overline{\lim}_{n \rightarrow \infty} \sup_{q > q^*} \frac{\Delta_n(q, q^*)}{q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}}} \leq C_6, \quad \text{a.s.} \quad (4.24)$$

Proof. Using the fact that

$$\sup_{f \in \mathcal{M}_{q^*}} \left(\ell_n(f) - \lambda_{q^*,n} \|\beta\|_K^2 \right) \geq \ell_n(f^*) - \lambda_{q^*,n} \|\beta^*\|_K^2$$

yield

$$\Delta_n(q, q^*) \leq \sup_{f \in \mathcal{M}_q} \sum_{i=1}^n \log \frac{f(Y_i|X_i)}{f^*(Y_i|X_i)} + \lambda_{q^*,n} \|\beta^*\|_K^2.$$

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Furthermore, from Part (a) of Lemma 2, for $\alpha \geq C_4$,

$$\mathbb{P}\left[\sup_{q \geq q^*} \frac{1}{q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}}} \sup_{f \in \mathcal{M}_q} \sum_{i=1}^n \log \frac{f(Y_i|X_i)}{f^*(Y_i|X_i)} \geq \alpha\right] \leq \sum_{q=q^*}^{\infty} C_3 e^{-\alpha q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}} / C_3} \leq \frac{c_1}{n^2}.$$

The lemma follows easily using the Borel-Cantelli. $\square$

A2: Proof of Theorem 1

The constants c_i used in the proof are all generic positive constants. First realize that any lower bound for a specific case yields immediately a lower bound for the general case. In the following, consider a special case where q^* and $(\pi_1^*, \dots, \pi_{q^*}^*)$ are known. f_0 is a fixed known density function.

Direct calculation of the Kullback-Leibler divergence between $h^* = f^*(y|x)f_X(x)$ and $h = f(y|x)f_X(x)$ where $f^*(y|x), f(y|x) \in \mathcal{M}_{q^*}$ yields

$$\begin{aligned} \mathcal{K}(h, h^*) &= \mathbb{E}_{h^*} \left\{ \log \frac{h^*}{h} \right\} = \mathbb{E}_{h^*} \left\{ \log \frac{\sum_{k=1}^{q^*} \pi_k^* h_k^*}{\sum_{k=1}^{q^*} \pi_k^* h_k} \right\} = \mathbb{E}_{h^*} \left\{ \log \sum_{k=1}^{q^*} \tau_k \frac{h_k^*}{h_k} \right\} \\ &\geq \mathbb{E}_{h^*} \left\{ \sum_{k=1}^{q^*} \tau_k \log \frac{h_k^*}{h_k} \right\} = \sum_{k=1}^{q^*} \pi_k^* \mathbb{E}_{h_k^*} \left\{ \frac{h_k/h}{h_k^*/h^*} \log \frac{h_k^*}{h_k} \right\}, \end{aligned} \quad (4.25)$$

where $\tau_k = \pi_k^* h_k^*/h$ for $k = 1, \dots, q^*$ and the inequality is due to the Jensen's Inequality. Note that $\pi_k^* h_k/h = \pi_k^* f_0(y - \eta_k) / \sum_{i=1}^{q^*} \pi_i^* f_0(y - \eta_i)$ is the probability of a data point coming from the k -th component. We assume this probability bound below away from zero. Therefore, h_k/h

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is bounded below away from zero and above by a positive constant. Hence,

$$\begin{aligned}
 \mathcal{K}(h, h^*) &= \sum_{k=1}^{q^*} \pi_k^* \mathbb{E}_{h_k^*} \left\{ \frac{h_k/h}{h_k^*/h^*} \log \frac{h_k^*}{h_k} \right\} \\
 &= \sum_{k=1}^{q^*} \pi_k^* \int_{h_k^* > h_k} \frac{h_k/h}{h_k^*/h^*} h_k^* \log \frac{h_k^*}{h_k} d\mu + \sum_{k=1}^{q^*} \pi_k^* \int_{h_k^* \leq h_k} \frac{h_k/h}{h_k^*/h^*} h_k^* \log \frac{h_k^*}{h_k} d\mu, \\
 &\geq c_3 \sum_{k=1}^{q^*} \pi_k^* \int_{h_k^* > h_k} h_k^* \log \frac{h_k^*}{h_k} d\mu + c_4 \sum_{k=1}^{q^*} \pi_k^* \int_{h_k^* \leq h_k} h_k^* \log \frac{h_k^*}{h_k} d\mu \\
 &\geq c_5 \sum_{k=1}^{q^*} \pi_k^* \mathcal{K}(h_k, h_k^*).
 \end{aligned}$$

Using the fact $\log y - \log x - \frac{1}{x}(y-x) + \frac{1}{2c_6}(y-x)^2 \leq 0$ for $0 \leq y \leq \sqrt{c_6}$,

$$\begin{aligned}
 \mathcal{K}(h_k, h_k^*) &= \mathbb{E}_{h_k^*} \left\{ \log \frac{h_k^*}{h_k} \right\} \\
 &\geq \frac{1}{2c_6} \mathbb{E}_{h_k^*} \left\{ f_0(Y - \eta(X, \beta_k)) - f_0(Y - \eta(X, \beta_k^*)) \right\}^2 \\
 &= \frac{1}{2c_6} \mathbb{E}_{h_k^*} \left\{ f_0^2(Y - \tilde{\eta}_k)(\eta(X, \beta_k - \beta_k^*))^2 \right\} \\
 &= \frac{1}{2c_6} \mathbb{E}_X \left\{ \mathbb{E}_{f_0(Y|X)} (f_0^2(Y - \tilde{\eta}_k)|X)(\eta(X, \beta_k - \beta_k^*))^2 \right\} \\
 &\geq c_7 \mathbb{E}_X \left\{ (\eta(X, \beta_k - \beta_k^*))^2 \right\} \\
 &= c_7 \|\beta_k - \beta_k^*\|_C^2,
 \end{aligned}$$

where $\tilde{\eta}_k$ is a point between $\eta(X, \beta_k^*)$ and $\eta(X, \beta_k)$. Therefore, $\mathcal{K}(h, h^*)$ is bounded below by

$\|\beta - \beta^*\|_C^2$ up to a constant, where $\|\beta - \beta^*\|_C^2 = \sum_{k=1}^{q^*} \|\beta_k - \beta_k^*\|_C^2$. A similar calculation also

yields that $\mathcal{K}(h, h^*)$ is bounded above by $\|\beta - \beta^*\|_C^2$ up to a constant.

In the following, we adopt the results from Tsybakov (2009) to establish the lower bound,

which is based upon testing multiple hypotheses. In particular, we can find a subset $\{\beta^{(0)}, \dots, \beta^{(N)}\} \subset$

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$\mathcal{F}^{q^*}$ with N increasing with n , such that for some positive constant c and all $0 \leq i < j \leq N$,

$$\|\beta^{(i)} - \beta^{(j)}\|_C^2 \geq 2c\gamma^{\frac{2r}{2r+1}} (n/q^*)^{-\frac{2r}{2r+1}}, \quad (4.26)$$

and

$$\frac{1}{N} \sum_{j=1}^N \mathcal{K}(h^{(j)}, h^{(0)}) \leq \gamma \log N, \quad (4.27)$$

then we can conclude according to Theorem 2.5 of Tsybakov (2009) that,

$$\inf_{\hat{\beta}} \sup_{\beta^* \in \mathcal{F}^{q^*}} \mathbb{P}\left(\|\beta^{(i)} - \beta^{(j)}\|_C^2 \geq c\gamma^{\frac{2r}{2r+1}} (n/q^*)^{-\frac{2r}{2r+1}}\right) \geq \frac{\sqrt{N}}{1 + \sqrt{N}} (1 - 2\gamma - \sqrt{\frac{2\gamma}{\log N}}),$$

which yields

$$\lim_{a \rightarrow 0} \lim_{n \rightarrow \infty} \inf_{\hat{\beta}} \sup_{\beta^* \in \mathcal{F}^{q^*}} \mathbb{P}\left(\|\hat{\beta} - \beta^*\|_C \geq a(n/q^*)^{-\frac{r}{2r+1}}\right) \geq 1.$$

Hence Theorem 1 will be proved.

Next, we construct the subset $\{\beta^{(0)}, \dots, \beta^{(N)}\} \subset \mathcal{F}^{q^*}$, $k = 1, \dots, q^*$. Let $\beta^{(j)} = (\beta_1^{(j)}, \beta_2^{(j)}, \dots, \beta_{q^*}^{(j)})$,

$j = 1, \dots, N$. We show that both (4.26) and (4.27) are satisfied. Let $\widetilde{M} = \lfloor M/q^* \rfloor$ for some

large number M to be decided later. Consider the function space

$$\mathcal{H}^* = \left\{ \beta = \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} b_k M^{-1/2} L_{K^{1/2}} \varphi_k : (b_{M+1}, \dots, b_{2M}) \in \{0, 1\}^M \right\}, \quad (4.28)$$

where $\{\varphi_k : k \geq 1\}$ are the orthonormal eigenfunctions of $K^{1/2}CK^{1/2}$. For any $\beta \in \mathcal{H}^*$, observe

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that

$$\begin{aligned} \|\beta\|_K^2 &= \left\| \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} b_k M^{-1/2} L_{K^{1/2}} \varphi_k \right\|_K^2 \\ &= \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} b_k^2 M^{-1} \|L_{K^{1/2}} \varphi_k\|_K^2 \\ &\leq \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} M^{-1} \|L_{K^{1/2}} \varphi_k\|_K^2 \leq 1, \end{aligned}$$

which shows that $\mathcal{H}^* \subset \mathcal{F}$. The Varshamov-Gilbert bound shows that for any $M \geq 8$, there

exists a set $\mathcal{B} = \{b^{(0)}, b^{(1)}, \dots, b^{(N)}\} \subset \{0, 1\}^M$ such that

1. $b^{(0)} = (0, \dots, 0)'$;
2. $H(b, b') > M/8$ for any $b \neq b' \in \mathcal{B}$, where $H(\cdot, \cdot) = \frac{1}{4} \sum_{i=1}^M (b_i - b'_i)^2$ is the Hamming distance;
3. $N \geq 2^{M/8}$.

The subset $\{\beta^{(0)}, \dots, \beta^{(N)}\} \subset \mathcal{F}^{q^*}$ is chosen as $\beta_j^{(i)} = \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} b_{j,k-\widetilde{M}}^{(i)} M^{-1/2} L_{K^{1/2}} \varphi_k$, $i = 0, \dots, N$, $j = 1, \dots, q^*$. For any $0 \leq i < j \leq N$, observe that

$$\|\beta^{(i)} - \beta^{(j)}\|_C^2 = \sum_{l=1}^{q^*} \mathbb{E}_X (\langle \beta_l^{(i)} - \beta_l^{(j)}, X \rangle)^2 = \sum_{l=1}^{q^*} \sum_{k=\widetilde{M}+1}^{2\widetilde{M}} (b_{l,k-\widetilde{M}}^{(i)} - b_{l,k-\widetilde{M}}^{(j)})^2 M^{-1} \rho_k.$$

Therefore,

$$\|\beta^{(i)} - \beta^{(j)}\|_C^2 \geq s_{2\widetilde{M}} M^{-1} \sum_{l=1}^{q^*} \sum_{k=1}^{\widetilde{M}} (b_{l,k}^{(i)} - b_{l,k}^{(j)})^2 \geq \rho_{2\widetilde{M}}/2 \asymp (M/q^*)^{-2r},$$

and

$$\|\beta^{(i)} - \beta^{(j)}\|_C^2 \leq s_{\widetilde{M}} M^{-1} \sum_{l=1}^{q^*} \sum_{k=1}^{\widetilde{M}} (b_{l,k}^{(i)} - b_{l,k}^{(j)})^2 \leq \rho_{\widetilde{M}} \asymp (M/q^*)^{-2r}.$$

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By taking M to be the smallest integer greater than $c_2 \gamma^{-\frac{1}{2r+1}} (q^*)^{2r/(2r+1)} n^{\frac{1}{2r+1}}$ with $c_2 = (c_1 \cdot 8 \log 2)^{1/(1+2r)}$, the theorem is proved.

A3: Proof of Theorem 2

For any $q \geq q^*$, since $\hat{f}$ is the maximum, we have

$$-\ell(\hat{f}) + \lambda \|\hat{\beta}\|_K^2 \leq -\ell(f^*) + \lambda \|\beta^*\|_K^2,$$

which gives

$$-(\ell(\hat{f}) - \ell(f^*)) + \lambda \|\hat{\beta}\|_K^2 \leq \lambda \|\beta^*\|_K^2. \quad (4.29)$$

Define

$$d_h = \frac{\sqrt{\frac{h}{h^*}} - 1}{\mathcal{H}(h, h^*)}.$$

Using $\log(1+x) \leq x$,

$$\begin{aligned} \ell(f) - \ell(f^*) &= \sum_{i=1}^n 2 \log(1 + \mathcal{H}(h, h^*) d_h(Y, X_i)) \\ &\leq \sum_{i=1}^n 2 \mathcal{H}(h, h^*) d_h(Y, X_i) \\ &= 2\sqrt{n} \nu_n(d_h) \mathcal{H}(h, h^*) - n \mathcal{H}^2(h, h^*), \end{aligned}$$

where $\nu_n(g) = n^{-1/2} \sum_{i=1}^n (g(Y_i, X_i) - \mathbb{E}g(Y_i, X_i))$. So,

$$-(\ell(f) - \ell(f^*)) \geq n \mathcal{H}^2(h, h^*) - 2\sqrt{n} \nu_n(d_h) \mathcal{H}(h, h^*).$$

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Combining this with (4.29),

$$\begin{aligned} n \mathcal{H}^2(\hat{h}, h^*) + \lambda \|\hat{\beta}\|_K^2 &\leq \lambda \|\beta^*\|_K^2 + 2\sqrt{n} \nu_n(d_{\hat{h}}) \mathcal{H}(\hat{h}, h^*) \\ &= \lambda \|\beta^*\|_K^2 + 2\sqrt{n} (\nu_n(g_{\hat{h}}) - \nu_n(g_{h^*})), \end{aligned} \quad (4.30)$$

where $g_h = \sqrt{h/h^*} = \sqrt{f/f^*}$. It is critical to investigate the behavior of $|\nu_n(g_h) - \nu_n(g_{h^*})|$ as a function of $\mathcal{H}(h, h^*)$.

It follows from Lemma 1 that the bracketing entropy of $H_q(\epsilon)$ is

$$H_{[\cdot]}(\delta) = \log N_{[\cdot]}(H_q(\epsilon), \delta) \leq (10(C_2\delta^{-\frac{1}{r}} + 1)q + 1) \log\left(\frac{C_1\epsilon}{\delta}\right).$$

Then,

$$\int_0^\epsilon H_{[\cdot]}^{1/2}(\delta) d\delta \leq c \sqrt{q} \epsilon^{1-\frac{1}{2r}}.$$

The reminder of proof is identical to that in Section 5.6 of van de Geer (2001). We obtain

$$\sup_{f \in \mathcal{M}_q} \frac{|\nu_n(g_h) - \nu_n(g_{h^*})|}{\sqrt{q} \mathcal{H}(h, h^*)^{1-\frac{1}{2r}} \vee n^{-\frac{r-1/2}{2r+1}}} = O_p(1). \quad (4.31)$$

This allows us to conclude that

$$\sqrt{n} |\nu_n(g_{\hat{h}}) - \nu_n(g_{h^*})| = \sqrt{n} \frac{|\nu_n(g_{\hat{h}}) - \nu_n(g_{h^*})|}{\sqrt{q} \mathcal{H}(\hat{h}, h^*)^{1-1/2r}} \sqrt{q} \mathcal{H}(\hat{h}, h^*)^{1-1/2r} = O_p(\sqrt{n}) \sqrt{q} \mathcal{H}(\hat{h}, h^*)^{1-1/2r}.$$

Combining this with (4.30) yields that $\mathcal{H}(\hat{h}, h^*) = O_p(n^{-r/(2r+1)})$ provided that λ is of order

$n^{1/(2r+1)}$. This finishes the proof of Theorem.

4.1 Proof of Theorem 3

4.1 Proof of Theorem 3

First note that

$$\overline{\lim}_{n \rightarrow \infty} \sup_{q > q^*} \frac{\Delta_n(q, q^*)}{\text{pen}_n(q) - \text{pen}_n(q^*)} \leq \lim_{n \rightarrow \infty} \sup_{q > q^*} \frac{q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}}}{\text{pen}_n(q) - \text{pen}_n(q^*)} \overline{\lim}_{n \rightarrow \infty} \sup_{q > q^*} \frac{\Delta_n(q, q^*)}{q^{\frac{2r}{2r+1}} n^{\frac{1}{2r+1}}} = 0.$$

Therefore, for all $q > q^*$.

$$\sup_{f \in \mathcal{M}_q} \left(\ell_n(f) - \lambda_{q,n} \|\beta\|_K^2 \right) - \text{pen}_n(q) < \sup_{f \in \mathcal{M}_{q^*}} \left(\ell_n(f) - \lambda_{q^*,n} \|\beta\|_K^2 \right) - \text{pen}_n(q^*).$$

This shows that $\overline{\lim}_{n \rightarrow \infty} \hat{q}_n \leq q^*$ a.s., which means that we do not asymptotically overestimate the order.

On the other hand, for any $q < q^*$,

$$\overline{\lim}_{n \rightarrow \infty} \frac{1}{n} \Delta_n(q, q^*) \leq \overline{\lim}_{n \rightarrow \infty} \sup_{f \in \mathcal{M}_q} \frac{1}{n} \sum_{j=1}^n \log \frac{f(Y_i|X_i)}{f^*(Y_i|X_i)} + \lim_{n \rightarrow \infty} \frac{\lambda_{q^*,n}}{n} \|\beta^*\|_K^2$$

which is strictly negative based on Part (b) of Lemma 2. Since $\text{pen}_n(q)/n \rightarrow 0$ as $n \rightarrow \infty$ for $q < q^*$, we have

$$\overline{\lim}_{n \rightarrow \infty} \frac{1}{n} \left\{ \Delta_n(q, q^*) - \text{pen}_n(q) + \text{pen}_n(q^*) \right\} < 0, \quad a.s.$$

We obtain, for all $q < q^*$,

$$\sup_{f \in \mathcal{M}_q} \left(\ell_n(f) - \lambda_{q,n} \|\beta\|_K^2 \right) - \text{pen}_n(q) < \sup_{f \in \mathcal{M}_{q^*}} \left(\ell_n(f) - \lambda_{q^*,n} \|\beta\|_K^2 \right) - \text{pen}_n(q^*).$$

This shows that $\overline{\lim}_{n \rightarrow \infty} \hat{q}_n \geq q^*$ a.s., which means that we do not asymptotically underestimate the order.