

## PROPORTIONAL ODDS MODEL WITH LOG-CONCAVE DENSITY ESTIMATION

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*Abstract:* We add a log-concave qualitative constraint on the baseline distribution of the proportional odds model. A full maximum likelihood method is developed for the joint estimation of the regression parameters and densities. The asymptotic properties of the estimates are established. A likelihood ratio test is constructed to test the significance of the regression parameter. We also propose a Kolmogorov-Smirnov type test to assess the log-concavity of the baseline distribution. A simulation study and an application to data from the Chicago Healthy Aging Study show the usefulness of our method.

*Key words and phrases:* Density ratio model, exponential tilting, semiparametric method, shape constrained estimation, survival analysis.

### 1. Introduction

The density ratio model, or exponential tilt model, is useful for modeling treatment effects, the biased-sampling problem, and the distribution of a mix of discrete and continuous variables (Cheng, Qin and Zhang (2009); Qin (1998); Terrell (2003); Zou, Fine and Yandell (2002); Chen (2007)), among many other applications. Cheng and Chu (2004) and Fokianos (2004) show that a density estimation based on data from all samples under the density ratio model is more efficient than a traditional estimation based on separate samples. Luo and Tsai (2012), and Diao, Ning and Qin (2012) generalize the density ratio model to a proportional likelihood ratio model by incorporating covariates:

$$f(y|\mathbf{x}) = \frac{dF_0(y) \exp(y\mathbf{x}^T\boldsymbol{\beta})}{\int \exp(y\mathbf{x}^T\boldsymbol{\beta})dF_0(y)}, \quad (1.1)$$

where  $F_0(\cdot)$  is the baseline distribution of response  $y$ , and  $\mathbf{x}$  and  $\boldsymbol{\beta}$  are linear covariates and coefficient vectors, respectively. For example, density estimations for the above models can be used to describe the distributional difference of an outcome between groups. To the best of our knowledge, the current literature on model (1.1) treats the baseline distribution as a nuisance, estimated only em-

pirically. We generalize the functional form of the regression part of model (1.1), and propose a joint estimation of the baseline density and regression parameters.

Moreover, we impose a log-concave qualitative constraint on the baseline density for model (1.1). Therefore the baseline density is  $p(y) = \exp \varphi(y)$ , for some concave function  $\varphi : \mathbb{R} \rightarrow [-\infty, \infty)$ . Density estimations without any constraint are known to be inefficient, because the parameter space is too large. A popular approach is to use smoothing methods, such as a kernel density estimation, or an estimation based on a roughness penalization. Estimating model (1.1) involves iteratively updating the estimate of the nonparametric or parametric components, while conditioning on the others. Smoothing methods cause an intensive computational burden, because the optimal smoothing parameter needs to be selected at each iteration. As a useful alternative, the log-concave density estimation is an automatic nonparametric estimation that avoids the problem of selecting tuning parameters. The univariate log-concave density estimation has the same minimax rate of order  $n^{-4/5}$  as that of a density estimation with two bounded derivatives (Ibragimov and Khas'minskii (1983); Seregin and Wellner (2010); Kim and Samworth (2016)). Thus, compared with traditional approaches that include tuning parameter selection, the proposed approach offers computational advantages without loss of asymptotic efficiency.

The well-studied log-concave densities include most of the commonly used parametric distributions (Walther (2009)), such as the uniform, normal, logistic, chi-square, chi, gamma, beta, and Weibull distributions. Estimations with log-concave constraints have practical applications in econometric modeling, reliability theory, and estimations of monotonic hazard rates (Bagnoli and Bergstrom (2005); Barlow and Proschan (1975); Hall et al. (2001)). Although there is no nonparametric maximum likelihood estimation for a unimodal density (Birge (1997)), such an estimation does exist for a log-concave density, and may be used instead of the larger class of unimodal densities (Dumbgen and Rufibach (2009)).

A maximum likelihood estimation of a multidimensional log-concave density is shown to have a smaller mean integrated squared error than those of kernel-based methods, for moderate to large sample sizes (Cule and Samworth (2010)). In addition, we obtain finite-sample efficiency for the regression parameter estimates by imposing a correct log-concavity constraint on the baseline density estimation for model (1.1). Now how confident can we be that the shape constraint is correct in practical applications when we do not know the true distribution, a priori? In other words, it is critical that we determine the log-concavity of

the baseline distribution. For example, Walther’s (2002) method is equivalent to testing whether a parameter  $c$  is equal to zero. However, it is computationally expensive because it requires many bootstrap estimates based on a set of values of  $c$ . Cule and Samworth (2010) introduce a permutation test, and Hazelton (2010) proposes a test using a kernel density estimation. However, theoretical support is still lacking for these two methods. Chen and Samworth (2013) develop a test based on smoothed log-concave density estimates. Nevertheless, while these methods test the log-concavity of the marginal density estimation, they do not incorporate covariates. Thus, we propose a Kolmogorov-Smirnov type test to assess the log-concavity of the baseline distribution, which is shown to be consistent.

The rest of the paper is organized as follows. The model and estimation method are introduced in Section 2. Section 3 describes the asymptotic properties of the estimates and a test of the log-concavity of the baseline distribution. The results of simulation studies and an application to data from the Chicago Healthy Aging Study are presented in Section 4. Section 5 concludes the paper.

**2. Models and Methods**

Let the random vector  $Y$  follow distribution  $P_Y$  on a given set  $\mathcal{Y} \subseteq \mathbb{R}$ ,  $P_Y$  have a density  $p_Y$  in  $\mathcal{Y}$ , and  $p_Y \in \mathcal{P}_c$  for a log-concave class of probability densities  $\mathcal{P}_c$ . The random vector  $\mathbf{X}$  follows distribution  $P_X$  on a given set  $\mathcal{X} \subseteq \mathbb{R}^k$ . Our conditional model of interest is

$$f(y; \mathbf{x}, \boldsymbol{\beta}, p) = \frac{p(y)e^{\eta(y, \mathbf{x}|\boldsymbol{\beta})}}{\int p(y)e^{\eta(y, \mathbf{x}|\boldsymbol{\beta})} dy}, \tag{2.1}$$

where  $\eta(y, \mathbf{x}|\boldsymbol{\theta})$  is a parametric regression function that depends on parameters  $\boldsymbol{\beta} \in \boldsymbol{\Theta}$ , for  $\boldsymbol{\Theta} \subseteq \mathbb{R}^{1 \times k}$ , and the baseline density  $p$  is log-concave. A simple form for  $\eta(y, \mathbf{x}|\boldsymbol{\theta})$  is linear  $y\mathbf{x}^T\boldsymbol{\beta}$ , as in model (1.1). However, it can be specified using other parametric forms to accommodate various applications, for example, the transformed linear form  $H_Y(y)H_X(\mathbf{x})^T\boldsymbol{\beta}$  for known functions  $H_X$  and  $H_Y$ . We call model (2.1) the proportional odds model with a log-concave distribution (POML), because the proportionality between conditional odds  $\{f(y_1|\mathbf{x}_1)/f(y_1|\mathbf{x}_2)\}/\{f(y_2|\mathbf{x}_1)/f(y_2|\mathbf{x}_2)\} = \exp\{\eta(y_1, \mathbf{x}_1|\boldsymbol{\beta}) - \eta(y_1, \mathbf{x}_2|\boldsymbol{\beta}) + \eta(y_2, \mathbf{x}_2|\boldsymbol{\beta}) - \eta(y_2, \mathbf{x}_1|\boldsymbol{\beta})\}$ .

In addition to the nice properties of model (2.1) described in the literature (Rathouz and Gao (2009); Luo and Tsai (2012)), we examine the relationships between model (2.1) and a shape-constrained survival analysis, and generalized

models with a random component under a shape constraint. Distributions under a shape constraint on the hazard rate are of considerable practical interest (Hall et al. (2001); Qin et al. (2011)). Because it imposes a log-concave constraint, the POML might be utilized to model the monotonic hazard rate (Dumbgen and Rufibach (2009)) for complete data using  $h(y; \mathbf{x}, \boldsymbol{\beta}) = f(y; \mathbf{x}, \boldsymbol{\beta}) / \{1 - F(y; \mathbf{x}, \boldsymbol{\beta})\}$ . Although challenging, the POML for censored data can be estimated using a EM type algorithm (Cheng, Qin and Zhang (2009); Shen, Jing and Qin (2012)). Rathouz and Gao (2009) extended the generalized linear model with density estimations for categorical responses using exponential tilting. POML can be represented as a generalized model with a canonical link function and an additional log-concave constraint on a random component.

Denote  $P_{X,Y}$  as the joint distribution of  $(Y, \mathbf{X})$ . The likelihood function for  $(\boldsymbol{\beta}, p)$  is

$$L_P(\boldsymbol{\beta}, p) = \int \log p(y) dP_Y + \int \eta(y, \mathbf{x} | \boldsymbol{\beta}) dP_{X,Y} - \int \left[ \log \int \exp\{\eta(y, \mathbf{x} | \boldsymbol{\beta})\} p(\mathbf{y}) d\mathbf{y} \right] dP_X. \quad (2.2)$$

The maximum likelihood estimators (MLEs) satisfy  $(\hat{\boldsymbol{\beta}}_n, \hat{p}_n) = \arg \max_{\boldsymbol{\beta}, p \in \mathcal{P}_e} L_{\mathbb{P}}(\boldsymbol{\beta}, p)$ , where  $\mathbb{P}$  denotes the empirical distribution.

Let  $(y_{(1)}, \dots, y_{(k)})$  be the observed ordered distinct response with corresponding observed frequencies  $(m_1, \dots, m_k)$ , and vector  $\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_k)$ , for  $\varphi_i = \log p(y_{(i)})$ . We propose an iterative procedure for the simultaneous estimation of the parametric and nonparametric components of the POML as follows:

*Initialization:* set initial values for  $\hat{\boldsymbol{\beta}}$ , which may be the result of an educated guess in a practical application. In our study, we choose the initial values from the null space,  $\hat{\boldsymbol{\beta}} = \mathbf{0}$ .

*Density Estimation:* update  $\boldsymbol{\varphi}$  using

$$\hat{\boldsymbol{\varphi}} = \arg \max_{\boldsymbol{\varphi} \in \mathcal{P}_e} \left[ \sum_{i=1}^n \eta(y_i, \mathbf{x}_i | \hat{\boldsymbol{\beta}}) + \sum_{l=1}^k m_l \varphi_l - \sum_{i=1}^n \log \int \exp\{\varphi(y) + \eta(y, \mathbf{x}_i | \hat{\boldsymbol{\beta}})\} dy \right]. \quad (2.3)$$

*Regression Parameter Estimation:* update  $\boldsymbol{\beta}$  using

$$\hat{\boldsymbol{\beta}} = \arg \max_{\boldsymbol{\beta}} \left[ \sum_{i=1}^n \eta(y_i, \mathbf{x}_i | \boldsymbol{\beta}) + \sum_{l=1}^k m_l \hat{\varphi}_l - \sum_{i=1}^n \log \int \exp\{\hat{\varphi}(y) + \eta(y, \mathbf{x}_i | \boldsymbol{\beta})\} dy \right].$$

*Iteration:* iterate for the density and regression parameter estimations until convergence.

The estimation of the conditional density is an optimization problem with a nonlinear objective function and a concave constraint on the result. We aim to estimate the baseline density function  $f(\cdot) = dF(\cdot)/d\mu$  nonparametrically for a Lebesgue measure  $\mu$ , or equivalently,  $\varphi(\cdot) = \log(f)$ , and parameters  $\beta$ . Estimating the vector  $\varphi$  is sufficient because the nonparametric maximum likelihood estimate of the log-concave density exists and is a piecewise linear continuous function, with knots on the observation points (Dumbgen and Rufibach (2009)). The iterative convex minorant algorithm (Groeneboom and Wellner (1992)) and active set algorithm (Fletcher (1987)) have been used to estimate the marginal log-concave density. As discussed by Dumbgen, Husler and Rufibach (2011), the likelihood function in expression (2.3) is infinitely often differentiable and strictly concave on  $\mathbb{R}^k$ . We extend the active set algorithm of Dumbgen, Husler and Rufibach (2011) to maximize (2.3) for a conditional density estimation. The term “active set” refers to the set of knots where the slope changes in a continuous piecewise linear function. Essentially, the active set algorithm incorporates two iterative procedures: updating the active set, and updating the density estimate within the active set. We also tried a gradient method for the conditional log-concave density estimation, and found it to be computationally inefficient for large sample sizes. The estimation of the regression parameters is a nonlinear optimization problem, and can be maximized using a Newton-Raphson type algorithm.

Our MLE approach differs from the empirical likelihood approach in the literature (Luo and Tsai (2012); Diao, Ning and Qin (2012)) in terms of estimating the baseline distribution. The empirical likelihood approach only provides an empirical estimate for the distribution function, that is, a stepwise function with jumps at data points. The likelihood approach for the POML provides an estimated density function with a log-concave shape constraint. Qin and Zhang (2005) develop a useful kernel density estimation under a density ratio model. However, the kernel density estimation relies on empirical likelihood estimates. That is, they first estimate the regression parameters and the empirical estimate  $\tilde{F}_0$  of the baseline distribution function  $F_0$ . Then, they obtain the kernel estimator of density  $\hat{f}_0$  by smoothing the increment in  $\tilde{F}_0$ .

### 3. Inferential Results

In this section, we consider the asymptotic properties of the estimates of the regression parameters and the baseline distribution. We also propose a log-

likelihood ratio test for the hypothesis related to the regression parameters  $\beta$ , and a Kolmogorov-Smirnov type test for assessing the log-concavity of the baseline density.

To build the theoretical results, we make the followed assumptions:

A. The true parameters  $(\beta_0, p_0)$  maximize  $L_P(\beta, p)$ , and the Kullback-Leibler information exists and is finite; that is,

$$E_0 \left\{ \left| \log \frac{f(y; \mathbf{x}, \beta, p)}{f(y; \mathbf{x}, \beta_0, p_0)} \right| \right\} < \infty,$$

where  $E_0$  denotes the expectation under  $P_{X,Y}$ ;

B. The domains of  $P_Y$  and  $P_X$  are compact in the Euclidean space;

C. The parameter space  $\Theta$  is convex compact. The function  $\eta(y, \mathbf{x}|\beta)$  is a parametric continuous differentiable function in terms of  $\beta$ . The parameter  $\beta \in \Theta$  is identifiable from  $\eta(\mathbf{y}, \mathbf{x}|\beta)$ ;

D. The information matrix  $-(\partial^2 E[L_P(\beta, p)])/(\partial \beta^2)|_{\beta=\beta_0}$  is positive-definite;

E. The true log-concave density function  $p_0$  is continuously differentiable.

Assumption A is required for consistency. Condition B is a general regularity condition, used to apply the asymptotic theorem to large samples. The identification condition Assumption C is a basic criterion. The theoretical results might not succeed if this condition is weak. Conditions D and E are needed to derive the  $\sqrt{n}$ -consistency and asymptotic normality of the regression parameter estimates  $\hat{\beta}$ .

### 3.1. Consistency: Multi-dimensional log-concave distribution

In this paper, we focus on the case  $Y \subseteq \mathbb{R}$ . The estimation for a POML with a multivariate log-concave baseline distribution is challenging, and is addressed elsewhere (Cule and Samworth (2010)). However, we find that the MLE of the POML with  $\mathbf{Y} \subseteq \mathbb{R}^d$  is theoretically consistent, and show it here for generality.

Let the random vector  $\mathbf{Y}$  follow distribution  $P_Y$  on a given set  $\mathcal{Y} \subseteq \mathbb{R}^d$ , and let  $P_Y$  have density  $p_Y$  in a log-concave class  $\mathcal{P}_c$  of the probability density on  $\mathcal{Y}$ . Let  $h(p, q)$  denote the Hellinger distance between two probability measures with densities  $p$  and  $q$  with respect to the Lebesgue measure on  $\mathbb{R}^d$ :  $h^2(p, q) = 1/2 \int (\sqrt{p} - \sqrt{q})^2 d\mu = 1 - \int \sqrt{p \cdot q} d\mu$ . Denote the joint density:

$$g_{\beta, p} = \frac{p(\mathbf{y}) e^{\eta(\mathbf{y}, \mathbf{x}|\beta)}}{\int p(\mathbf{y}) e^{\eta(\mathbf{y}, \mathbf{x}|\beta)} d\mathbf{y}} p_x(\mathbf{x}).$$

It can be seen that the likelihood (2.2) is  $\log g_{\beta, p}$ , with  $p_x(\mathbf{x})$  omitted because it does not involve  $(\beta, p)$ .

**Lemma 1.** *The Hellinger distance satisfies  $h^2(g_{\beta,p}, g_{\beta_0,p_0}) \geq ah^2(p, p_0)$  for a positive constant  $a$ .*

*Proof.* see Appendix.

The consistency of the MLE of a log-concave density on  $\mathbb{R}$  with respect to the Hellinger metric is established by Pal, Woodroffe and Meyer (2007), and the uniform consistency is shown by Dumbgen and Rufibach (2009). Both the Hellinger consistency (Seregin and Wellner (2010)) and the uniform consistency (Cule and Samworth (2010); Schuhmacher, Husler and Duumbgen (2011)) of the MLE for the multivariate log-concave density on  $\mathbb{R}^d$  are established. Dumbgen, Samworth and Schuhmacher (2011) present the consistency of the MLE for multivariate log-concave distributions in terms of the total variation distance in the regression model. We first establish the connection between the joint and baseline densities in terms of the Hellinger distance under the POML in Lemma 1. This implies that  $h^2(p, p_0) = 0$  if  $h^2(g_{\beta,p}, g_{\beta_0,p_0}) = 0$ . Then, in the following Theorem, we show that the estimates of the baseline density and regression parameters are both consistent. Specifically, the estimate of the baseline density is Hellinger consistent.

**Theorem 1.** *Under Assumptions A-C, the sequence of MLEs  $(\hat{\beta}_n, \hat{p}_n) = \arg \max_{\beta,p \in \mathcal{P}_c} L_{\mathbb{P}}(\beta, p)$  satisfy:  $\hat{\beta}_n \rightarrow \beta_0$  and  $h(\hat{p}_n, p_0) \rightarrow 0$  as  $n \rightarrow \infty$ . Moreover,  $\hat{p}_n \rightarrow p_0$  pointwise and the convergence is uniform on a compact space.*

*Proof.* see Appendix.

### 3.2. Asymptotic normality: One-dimensional log-concave distribution

In this section, we establish the asymptotic normality for the estimates of  $\beta$  for the case  $Y \subseteq \mathbb{R}$ . First, let us introduce the concept of a bracketing number with a Hellinger metric specific to our problem (van der Vaart and Wellner (1996)). An  $\varepsilon$ -bracket is a bracket  $[g^L, g^U]$ , with  $h(g^L, g^U) < \varepsilon$ , where the bracket  $[g^L, g^U]$  is the set of all functions  $g$  with  $g^L \leq g \leq g^U$  and  $g \in \mathcal{G}$ . The bracketing number  $N_{[\cdot]}(\varepsilon, \mathcal{G}, h)$  is the minimum number of  $\varepsilon$ -brackets needed to cover  $\mathcal{G}$ . The logarithm of the bracketing number is generally referred to entropy with bracketing.

**Lemma 2.** *Let  $\mathcal{G}_\delta = \{g_{\beta,p} : h(p, p_0) < \delta, \|\beta - \beta_0\| < \delta\}$ , and  $h_0^2(p, q) = h^2(p + p_0, q + p_0)$  for  $\delta > 0$ . There is a constant  $C > 0$ , such that*

$$\log N_{[\cdot]}(\varepsilon, \mathcal{G}_\delta, h_0) \leq c(\varepsilon^{-1/2}),$$

*for  $\varepsilon$  small enough, and a constant  $c$ .*

*Proof.* see Appendix.

The bounds for the metric entropy with bracketing for the class of log-concave densities determine the global rate of convergence of the MLE. Doss and Wellner (2016) obtain that the bound of entropy with respect to a Hellinger metric is of order  $O(\varepsilon^{-1/2})$  for MLEs of univariate log-concave densities, and that the rate of convergence is  $O(n^{-2/5})$ . Similarly, we establish the entropy of the joint density of interest in Lemma 2. In the following lemma, we establish the rate of convergence of the baseline density, conditioning on the convergence rate of the regression parameters. This implies that the baseline density estimation achieves an optimal rate if the estimates of the regression parameters behave reasonably well.

**Lemma 3.** *Let  $\hat{p}_{\tilde{\beta}} = \operatorname{argmax}_{p \in \mathcal{P}_c} L_{\mathbb{P}}(\tilde{\beta}, p)$ , and let Assumptions C and D hold. Then*

$$h(\hat{p}_{\tilde{\beta}}, p_0) \leq O(n^{-2/5} + \|\tilde{\beta} - \beta_0\|).$$

*Proof.* see Appendix.

Utilizing the profile likelihood (Murphy and van der Vaart (2000)) method and the results of Lemma 3, we can prove the asymptotic normality of the estimates of  $\beta$ .

**Theorem 2.** *Under Assumptions A-E,  $\sqrt{n}(\hat{\beta} - \beta_0)$  is asymptotic normal with mean zero and covariance matrix  $\tilde{I}_0$ .*

*Proof.* see Appendix for proof and details of  $\tilde{I}_0$ .

Establishing the asymptotic normality when  $\mathbf{Y} \subseteq \mathbb{R}^d$  presents nontrivial technical challenges, and thus is left to future research. The convergence rate shown in Lemma 3 is used to establish the  $\sqrt{n}$ -asymptotic normality in Theorem 2. If the baseline density is multivariate for the POML (i.e.,  $\mathbf{Y} \subseteq \mathbb{R}^d$ ), the derivation of the convergence rate includes additional technique difficulties. A first step might be to extend Lemma 2 to an entropy bound for the multivariate case. Kim and Samworth (2016) show that the minimax lower bound rate for a Hellinger loss is  $n^{-1/(d+1)}$ , for  $d \geq 2$ , for log-concave density estimations without covariates. If these convergence rates can be established for the baseline density estimation in the POML, we conjecture that asymptotic normality for  $\sqrt{n}(\hat{\beta} - \beta_0)$  can be achieved for  $d = 2, 3$ . However, for  $d > 4$ ,  $\sqrt{n}$ -asymptotic normality might not be satisfied; thus, we may need to find alternative estimators to achieve optimal rates of convergence.

### 3.3. Inference for regression parameters

Because the estimates are obtained using the maximum likelihood estimation procedure, it is natural to use the log-likelihood ratio test to test the regression parameters. A likelihood ratio inference proceeds by fitting a series of reduced and nested models. Thus each reduced model in the sequence is contained within the previous one. Denote the hypothesis of interest as  $H_0 : \beta = \beta_\phi$ . The testing technique employs the profile likelihood because we are interested in testing the low-dimensional parameter  $\beta$ , rather than the high-dimensional parameter  $p$ . Define the profile likelihood as  $pL(\beta) = L\{\beta, p(\beta)\}$ , where  $p(\beta) = \operatorname{argmax}_p L(\beta, p)$  and  $L(\beta, p)$  is the full likelihood. The difference between the reduced model and the full model with no restriction on  $\beta$  can be examined by calculating the profile likelihood ratio test statistic  $G = 2\{pL(\hat{\beta}) - pL(\beta_\phi)\}$ . The asymptotic distribution of this test statistic is presented in the following lemma.

**Lemma 4.** *Under Assumptions A-E and the null hypothesis  $H_0 : \beta = \beta_\phi$ ,*

$$2\{pL(\hat{\beta}) - pL(\beta_\phi)\} \rightarrow \chi_u^2 \quad \text{in distribution,}$$

where  $\chi_u^2$  is a chi-squared distribution with  $u$  degrees of freedom, equal to the difference between the number of parameters specified under the reduced model and that under the full model.

*Proof.* The proof follows immediately from Corollary 2 in Murphy and van der Vaart (2000).

Substituting the estimator  $\hat{\beta}$  into the respective score vector and information matrix of  $\beta$ , the covariance matrix of  $\hat{\beta}$  can be obtained from the sandwich estimator:

$$\left\{ -\frac{\partial^2 pL_n(\beta)}{\partial \beta \partial \beta^T} \Big|_{\hat{\beta}} \right\}^{-1} \left[ \sum_{i=1}^n \left\{ \frac{\partial pL(y_i, \mathbf{x}_i, \beta)}{\partial \beta} \Big|_{\hat{\beta}} \right\} \left\{ \frac{\partial pL(y_i, \mathbf{x}_i, \beta)}{\partial \beta} \Big|_{\hat{\beta}} \right\}^T \right] \left\{ -\frac{\partial^2 pL_n(\beta)}{\partial \beta \partial \beta^T} \Big|_{\hat{\beta}} \right\}^{-1}.$$

The explicit analytical expression for the gradient and the hessian of the profile likelihood  $pL(\beta)$  is very complicated. In practical applications, we can use numerical derivatives for the variance estimates.

### 3.4. Assess log-concavity of baseline density

An essential assumption of the POML (2.1) is the log-concave shape constraint on the baseline density, which may be violated in practical application.

It is important to have an inferential tool to diagnose the appropriateness of log-concavity. Many tests have been developed in the literature. Walther (2002) represents the mixture of log-concave densities as  $\exp\{\phi(y) + c\|y\|^2\}$ , for a concave function  $\phi$  and constant  $c \geq 0$ . The test for a log-concave distribution is equivalent to testing whether  $c = 0$ . A limitation of this approach is that it is only practical for small sample sizes, because the computation of the test statistics requires constructing many bootstrap samples. Cule and Samworth (2010) present a permutation test with an easy implementation, but with less power. The test by Hazelton (2010) is based on choosing the smallest bandwidth for the kernel density estimate, with log-concavity satisfied. An extension of this test to model (2.1) results in an excessive computational burden, because it is nontrivial to find optimal kernel estimates, as discussed in the introduction. Moreover, there is a lack of theoretical support for tests utilizing kernel densities or permutations.

Motivated by the aforementioned works, we develop a test for the log-concavity of the baseline distribution that is computationally feasible and supported theoretically. In what follows, we present a Kolmogorov-Smirnov type test to examine the log-concave assumption. The test statistic is essentially the distance between the shape-constrained and nonconstrained MLEs of the baseline distribution, in terms of a uniform metric. Denote by  $\mathcal{F}_c$  the family of distributions with log-concave densities, and the MLEs  $(\hat{\beta}_n, \hat{F}_n) = \arg \max_{\beta, F \in \mathcal{F}_c} \mathbb{P}_n\{l(\beta, F)\}$ , where

$$l(\beta, F) = dF(y) + \eta(\mathbf{y}, \mathbf{x}|\beta) - \log \int \exp(\mathbf{y}\mathbf{x}^T \beta) dF(y).$$

Let  $(\tilde{\beta}, \tilde{F}_n)$  maximize the empirical likelihood without a shape constraint. Luo and Tsai (2012) demonstrate that the empirical likelihood estimates are both computationally and asymptotically efficient. We test the log-concavity using the test statistic  $T_n = \sqrt{n} \|\hat{F}_n(y) - \tilde{F}_n(y)\|_\infty$ , where  $\|\cdot\|_\infty$  is the supnorm.

Because the distribution of  $T_n$  is difficult to derive, we propose a bootstrap testing procedure, as follows:

- 1) Obtain the shape-constraint estimates  $(\hat{\beta}_n, \hat{F}_n)$  and empirical estimates  $(\tilde{\beta}, \tilde{F}_n)$  for the data  $\{Y, \mathbf{X}\}$ , and calculate  $T_n$ ;
- 2) Use the bootstrap method to sample data  $\{Y^*, \mathbf{X}\}$  from the null distribution  $f(y; \mathbf{x}, \hat{\beta}_n, \hat{F}_n)$ , obtain the shape-constrained MLEs  $(\hat{\beta}^*, \hat{F}_n^*)$  and the empirical estimates  $(\tilde{\beta}^*, \tilde{F}_n^*)$  without a shape constraint, and calculate  $T^*$ ;
- 3) Repeat the bootstrap process  $N$  times;
- 4) Compute the upper  $\alpha$ -level critical value  $\xi_\alpha$  from  $T^*$ , and reject the null hypothesis if  $T_n > \xi_\alpha$ .

We investigate the asymptotic property of our proposed Kolmogorov-Smirnov type test under the alternative hypothesis; that is, the log-concave shape constraint is violated. The results show that test based on the proposed bootstrap procedure is consistent.

**Theorem 3.** *Under Assumptions A-C, if the true distribution  $F_0 \notin \mathcal{F}_c$ , then  $P(T_n > \xi_\alpha) \rightarrow 1$ .*

*Proof.* see Appendix.

## 4. Numerical Studies

### 4.1. Simulation

We conduct a simulation study to assess the performance of our methods. The data are generated from the following POML with a linear regression function:

$$f(y; x_1, x_2, \beta_1, \beta_2, p) = \frac{p(y)e^{y\beta_1x_1+y\beta_2x_2}}{\int p(y)e^{y\beta_1x_1+y\beta_2x_2}dy}, \tag{4.1}$$

with  $x_1 \sim \text{Binomial}(1, 0.5)$  under the following four settings: I.  $p(y) \sim N(0, 1)$ ,  $x_2 \sim N(0, 1)$ ,  $\beta_1 = 0$ , and  $\beta_2 = 0$ ; II.  $p(y) \sim N(0, 1)$ ,  $x_2 \sim N(0, 1)$ ,  $\beta_1 = 1$ , and  $\beta_2 = 0.5$ ; III.  $p(y) \sim \text{Exponential}(1)$ ,  $x_2 \sim \text{Exponential}(1)$ ,  $\beta_1 = 0$ , and  $\beta_2 = 0$ ; IV.  $p(y) \sim \text{Exponential}(1)$ ,  $x_2 \sim \text{Exponential}(1)$ ,  $\beta_1 = -1$ , and  $\beta_2 = -0.5$ .

For each setting, we generate 500 data sets, and fit the data using the POML. The bias, standard deviation, mean squared error (MSE), and coverage probability of the 95% confidence intervals of the estimated regression parameters are shown in Table 1. This table also shows the empirical rejection rates for a significance level of 0.05, using the likelihood ratio test  $G$ . The mean estimated density functions are shown in Figure 1. In summary, our method does a reasonably effective job of providing accurate estimates of the regression parameters and the density functions. The proposed likelihood ratio test is an adequate tool for testing the significance of regression parameters.

For the purpose of comparing our results with those of existing similar methods, we also fit the data using the empirical likelihood approach of Luo and Tsai (2012). Define the relative efficiency as  $RE = MSE_{POML}/MSE_{EL}$ , where  $MSE_{POML}$  is the MSE of the estimate using our method, and  $MSE_{EL}$  is the MSE using the empirical likelihood approach. Figure 2 shows the REs for the estimations of the regression parameters  $(\beta_1, \beta_2)$ . We can see that the MLE with a log-concave density constraint has a smaller MSE than those of the empirical likelihood estimates without shape constraints for moderate to large sample sizes.

Table 1. Estimates of regression parameters in the simulation studies using POML. The data are generated from the following POML:  $f(y; x_1, x_2, \beta_1, \beta_2, p) = (p(y)e^{y\beta_1 x_1 + y\beta_2 x_2}) / (\int p(y)e^{y\beta_1 x_1 + y\beta_2 x_2} dy)$ , with  $x_1 \sim \text{Binomial}(1, 0.5)$  and the following four settings: I.  $p(y) \sim N(0, 1)$ ,  $x_2 \sim N(0, 1)$ ,  $\beta_1 = 0$ , and  $\beta_2 = 0$ ; II.  $p(y) \sim N(0, 1)$ ,  $x_2 \sim N(0, 1)$ ,  $\beta_1 = 1$ , and  $\beta_2 = 0.5$ ; III.  $p(y) \sim \text{Exp.}(1)$ ,  $x_2 \sim \text{Exp.}(1)$ ,  $\beta_1 = 0$ , and  $\beta_2 = 0$ ; IV.  $p(y) \sim \text{Exp.}(1)$ ,  $x_2 \sim \text{Exp.}(1)$ ,  $\beta_1 = -1$ , and  $\beta_2 = -0.5$ . Bias: estimated regression parameters minus true values; Est.: estimates; sd: sampling standard deviation of estimates; mse: average of estimated mean squared error; CP: coverage probability of 95% confidence interval; RR: empirical rejection rate of a nominal 0.05 level using the log-likelihood ratio test.

	n	$\beta_1$					$\beta_2$				
		Bias	sd.	mse	CP	RR	Est.	sd.	mse	CP	RR
I	200	0.009	0.148	0.022	0.920	0.058	0.006	0.072	0.005	0.964	0.038
	500	0.001	0.090	0.008	0.956	0.062	-0.00005	0.043	0.002	0.940	0.046
II	200	0.013	0.186	0.035	0.960	0.992	0.021	0.090	0.009	0.960	0.966
	500	-0.005	0.111	0.012	0.944	1.000	-0.005	0.054	0.003	0.966	0.996
III	200	0.006	0.151	0.023	0.952	0.066	0.016	0.081	0.007	0.960	0.052
	500	0.005	0.085	0.007	0.952	0.044	0.009	0.047	0.002	0.954	0.046
IV	200	-0.031	0.320	0.103	0.950	0.984	-0.044	0.210	0.046	0.955	0.880
	500	-0.015	0.190	0.036	0.944	1.000	-0.001	0.122	0.015	0.958	0.994

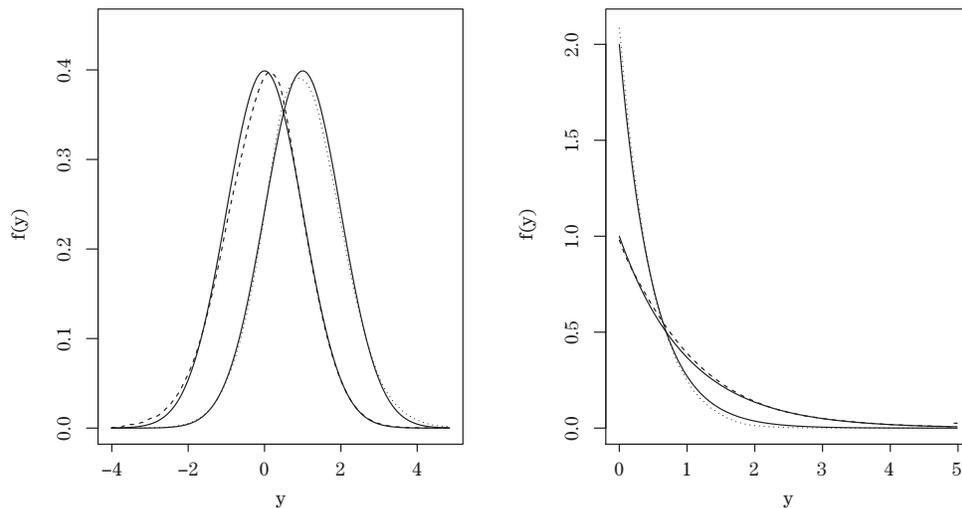


Figure 1. Plots of mean estimated densities and distributions for control and treatment groups in simulation. Left: normal distribution in setting II with  $N = 200$ ; right: exponential distribution in setting IV with  $N = 200$ . Dashed line: estimated density for control group ( $\beta_1 = 0$ ); dotted line: estimated density for treatment group ( $\beta_1 = 1$ ); solid line: true densities.

Table 2. Results of power simulation. The data are generated from model (4.1) with mixture normal baseline distribution  $0.5N(\mu_1, 1) + 0.5N(\mu_2, 1)$ . There is only a binary predictor  $x \sim \text{binomial}(1, 0.5)$ , with regression coefficient equal to one. The significance level is  $\alpha = 0.05$ .

n	Type I Error Rate		Power
	$\mu_1 = 0, \mu_2 = 0$	$\mu_1 = 0, \mu_2 = 2$	$\mu_1 = 0, \mu_2 = 4$
100	0.070	0.105	0.580
200	0.055	0.055	0.900

Intuitively, adding an appropriate shape constraint on the distribution provides some efficiency gains in terms of finite-sample performance. As discussed by Cule and Samworth (2010), the poor approximation of the convex hull of the data of the support of the underlying density results in relatively poor performance of the log-concave maximum likelihood estimator for small sample sizes. In small samples, the less desirable baseline density estimates affect the quality of the estimation of the regression parameter as well.

Another simulation is conducted to evaluate the behavior of our proposed test for the log-concave constraint. The data are generated from model (4.1), with a mixture normal baseline distribution  $0.5N(\mu_1, 1) + 0.5N(\mu_2, 1)$ . For simplicity, we only consider a binary predictor  $x \sim \text{binomial}(1, 0.5)$ , with regression coefficient  $\beta = 1$ . The baseline mixture  $p(\cdot)$  has three settings:  $(\mu_1 = 0, \mu_2 = 0)$ ,  $(\mu_1 = 0, \mu_2 = 2)$ , and  $(\mu_1 = 0, \mu_2 = 4)$ . It is well known that the log-concavity is satisfied when  $|\mu_2 - \mu_1| \leq 2$ . We generate 200 data sets for each setting and for two sample sizes ( $N = 100$  and  $N = 200$ ). Within each data set, 100 bootstrap samples are generated to obtain the critical value for the test statistics. As shown in Table 2, our proposed testing procedure performs appropriately in terms of the type-I error rate and power, even for a relatively small sample size.

#### 4.2. Chicago healthy aging study

As described in the introduction, the Chicago Healthy Aging Study (CHAS) is a re-examination of a sample of 1,395 surviving participants (ages 65-84, 28% female) from the Chicago Heart Association Detection Project in Industry 1967-1973 cohort (CHA) (Pirzada et al. (2013)). Their cardiovascular disease (CVD) risk profiles were originally ascertained at ages 25-44. This study re-examined 421 participants who were low-risk (LR) and 974 participants who were not-LR at the baseline. LR is defined as having favorable levels of five major CVD risk factors: serum total cholesterol  $< 200$  mg/dL and not taking cholesterol-lowering

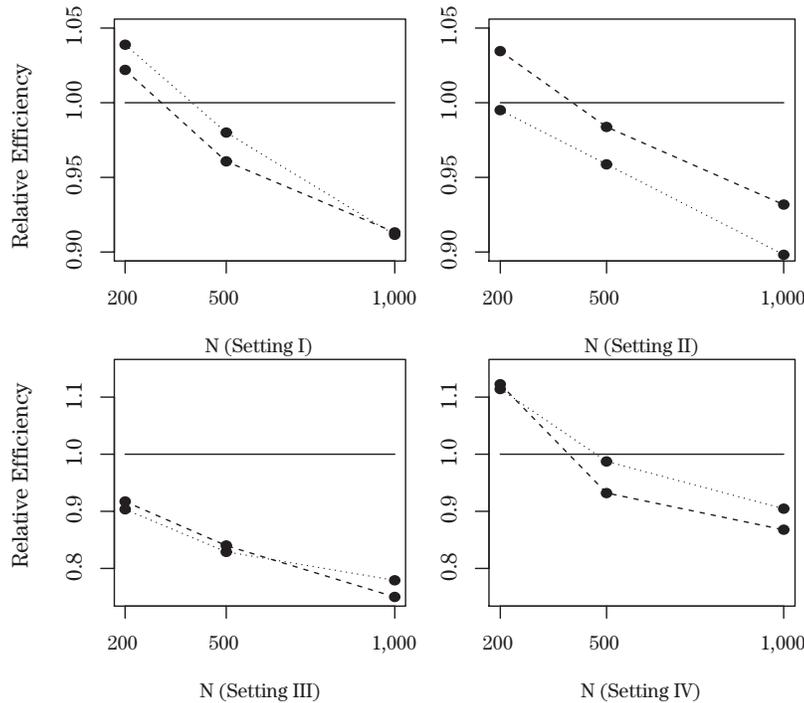


Figure 2. Relative efficiency for regression parameters  $(\beta_1, \beta_2)$  between estimates using POML and empirical likelihood (EL) estimates. Dashed line: estimated relative efficiency  $MSE_{POML}/MSE_{EL}$  for  $\hat{\beta}_1$ ; dotted line: estimated relative efficiency  $MSE_{POML}/MSE_{EL}$  for  $\hat{\beta}_2$ .

medication; blood pressures  $\leq 120/\leq 80$  mmHg and not taking antihypertensive medication; BMI  $< 25$  (mass(kg)/{height(m)}<sup>2</sup>); not smoking; and no history of diabetes or heart attack. In the CHAS study, LR and not-LR CHA participants were randomly selected from the 12,119 surviving original CHA participants, in which there are 1,034 LR and 11,085 not-LR individuals at the baseline. There is a problem with biased sampling because the baseline LR participants were oversampled to obtain adequate samples for between-group comparisons. In addition, the CHAS participants tended to be healthier than the CHA participants not selected for CHAS.

Although the importance of the LR status in overcoming the CVD epidemic is often recognized, the long-term association of LR status at a younger age with objectively measured health in older age has not been examined (Daviglius et al. (2004)). We divide the CHAS participants into four groups: LR, 0 RF, 1 RF, 2+ RF. The 0 RF, 1 RF, 2+ RF refer to having 0, 1, and  $\geq 2$  of the five

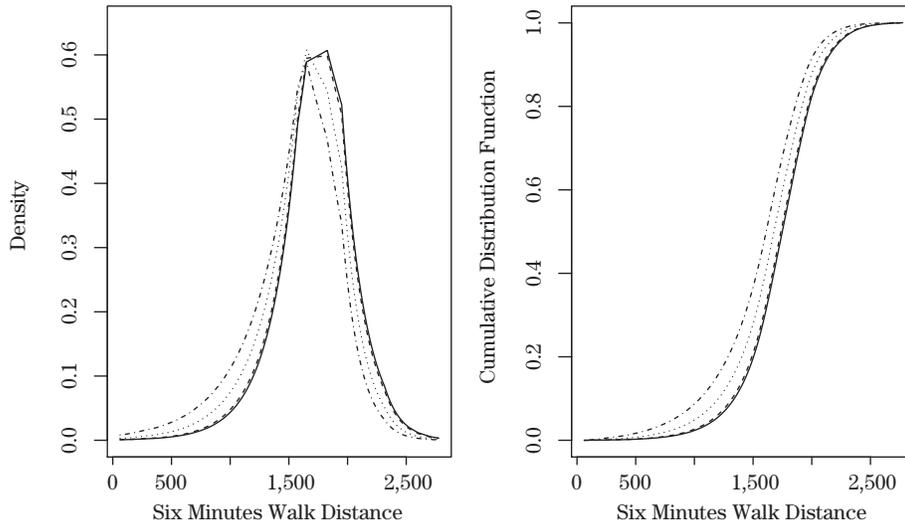


Figure 3. Estimated densities and cumulative distribution functions for six minutes walking distance of participants in CHAS study using POML by risk groups, adjusted for gender and age. Left: estimated density functions; right: estimated cumulative distribution functions. Solid Line: LR; dashed line: 0 RF; dotted line: 1 RF; dash-dotted line: 2+ RF. Waking distance is measured in foot.

adverse CVD risk factors, respectively (Daviglius et al. (2016)). The POML is applied to study the distributional difference of six minutes walking distance (measured in feet) between LR and not-LR participants, defined at the baseline. For illustration purposes, we consider four discrete predictors, binary indicators of the risk group (0 RF, 1 RF, and 2+ RF), gender, and the continuous predictor, age. The estimated regression coefficients for the 0 RF, 1 RF, and 2+ R groups are  $-0.056$  (p-value = 0.583),  $-0.339$  (p-value < 0.001), and  $-0.627$  (p-value < 0.001), respectively. The estimated coefficients for male and age are  $0.848$  (p-value < 0.001) and  $-0.368$  (p-value < 0.001), respectively. The test statistic for testing log-concavity is  $T_n = 0.088$ , with  $\#\{b : T_n > T_b^*\}/100 = 0.4$ , where  $T_b^*$  for  $b = 1, \dots, 99$  is calculated from 99 bootstrap samples, following our proposed bootstrap procedure. Consequently, we fail to reject the hull hypothesis that the baseline distribution is log-concave. The plots of the estimated densities and cumulative functions for four risk groups are shown in Figure 3. The estimated six minute walking distance of participants in the LR and 0 RF groups cluster around 1,760 feet, while those of participants in the 1 RF and 2+ RF groups cluster around 1,640 feet. The estimated densities using our proposed method clearly capture the left skewness, and provide insightful information about the

distributional difference of a six minute walking distance for the individuals in each group. Compared with individuals without risk factors at a younger age, the results imply that those who do have risk factors at a younger age, and have survived to an older age, will have shorter six minute walking distances, after adjusting for gender and age.

## 5. Conclusion

We propose a log-concave shape constraint on the baseline density function for the POML, enabling us to model a variety of distributions. We present a maximum likelihood estimation method to jointly estimate the regression parameters and densities. The asymptotic properties, including the consistency and normality of the estimates, are explored. Inference tests are also developed: a log-likelihood ratio test for the significance of a regression parameter, and a Kolmogorov-Smirnov type test to assess the log-concavity. A simulation study and an application to data from the CHAS study show the usefulness of our method.

To improve the small-sample performance, a smoothed log-concave estimate of the baseline density in the POML might help. Denote by  $s^2$  the sample variance of observed  $Y$ , and by  $\sigma_{\hat{p}}^2$  the variance of the estimated log-concave density. A smoothed version of  $\hat{p}$  can be derived via convolution, as  $\tilde{p}(z) = \int \phi_{\hat{\gamma}}(z - y)\hat{p}(y)dy$ , where  $\phi_{\hat{\gamma}}$  is the density for  $N(0, \hat{\gamma})$ . For observation  $Y$  generated from the marginal log-concave density, the nonnegativity of  $\hat{\gamma}$  is ensured by the fact  $\sigma_{\hat{p}}^2 \leq s^2$  (corollary 2.3, Dumbgen and Rufibach (2009)). If  $\sigma_{\hat{p}}^2$  is the variance of the estimated baseline density in the POML, then the criterion  $\sigma_{\hat{p}}^2 \leq s^2$  is not always satisfied, because the observed  $Y$  is generated from a distribution conditioning on various values of  $\mathbf{x}$ . Thus, it is difficult, but promising to develop smoothed baseline log-concave density estimates for the POML in future research.

Another interesting topic is to extend the POML to multi-dimensional responses that allows for the joint modeling of associations between multiple response and multiple covaraites. This is motivated by the work of Cule and Samworth (2010), who establish the existence, uniqueness, and computation of a non-parametric MLE for multi-dimensional log-concave densities; this MLE is a fully automatic nonparametric density estimator. In general, kernel estimations for multi-dimensional densities, and specifying a symmetric, positive-definite bandwidth matrix are challenging tasks.

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**Appendix: Proof of Theorems**

*Proof of Lemma 1*

Let assume that

$$h^2(g_{\beta,p}, g_{\beta_0,p_0}) < ah^2(p, p_0) \tag{A.1}$$

for any  $a > 0$ . Since  $0 \leq h^2(g_{\beta,p}, g_{\beta_0,p_0}) \leq 1$  and  $0 \leq h^2(p, p_0) \leq 1$ , both  $h^2(g_{\beta,p}, g_{\beta_0,p_0}) = 0$  and  $h^2(p, p_0) > 0$  have to be satisfied to meet the inequality (A.1).

If  $h^2(g_{\beta,p}, g_{\beta_0,p_0}) = 0$ , then  $\int \sqrt{g_{\beta,p}g_{\beta_0,p_0}} dy dx = 1$ , and  $g_{\beta,p} = g_{\beta_0,p_0}$  follows by Cauchy–Schwarz inequality. We have  $p = p_0$  and  $\beta = \beta_0$  by the identifiable property of the parameter  $(p_0, \beta_0)$  (Lemma 1 of Luo and Tsai (2012)). This contradict  $h^2(p, p_0) > 0$ .

*Proof of Theorem 1*

Denote  $\phi = \log p$ , and  $f_{\beta,p} = p(\mathbf{y}) \exp\{\eta(\mathbf{y}, \mathbf{x}|\beta)\}/Q_p(\beta)$  where  $Q_p(\beta) = \int p(\mathbf{y}) \exp\{\eta(\mathbf{y}, \mathbf{x}|\beta)\} d\mathbf{y}$ . For  $\varepsilon > 0$ , we have

$$\begin{aligned} 0 \leq L_{\mathbb{P}}(\hat{\beta}_n, \hat{p}_n) - L_{\mathbb{P}}(\beta_0, p_0) &= \int \log g_{\hat{\beta}_n, \hat{p}_n} d\mathbb{P} - \int \log g_{\beta_0, p_0} d\mathbb{P} \\ &\leq \int \log(\varepsilon + g_{\hat{\beta}_n, \hat{p}_n}) d\mathbb{P} - \int \log g_{\beta_0, p_0} d\mathbb{P} = \int \log\{\varepsilon + g_{\hat{\beta}_n, \hat{p}_n}\} d(\mathbb{P} - P_{X,Y}) \\ &\quad + \int \log \left\{ \frac{\varepsilon + g_{\hat{\beta}_n, \hat{p}_n}}{\varepsilon + g_{\beta_0, p_0}} \right\} dP_{X,Y} + \int \log\{\varepsilon + g_{\beta_0, p_0}\} dP_{X,Y} - \int \log g_{\beta_0, p_0} d\mathbb{P}. \end{aligned}$$

By assumption B and Lemma 3.2 in Seregin and Wellner (2010), it is not difficulty to show that  $\int \log\{\varepsilon + g_{\hat{\beta}_n, \hat{p}_n}\} d(\mathbb{P} - P_{X,Y}) \rightarrow 0$  almost surely for  $\varepsilon$  small enough. Following Lemma 1 in Pal, Woodrooffe and Meyer (2007), it can be derived:

$$\int \log \left( \frac{\varepsilon + g_{\hat{\beta}_n, \hat{p}_n}}{\varepsilon + g_{\beta_0, p_0}} \right) dP_{X,Y} \leq 2 \int \sqrt{\frac{\varepsilon}{\varepsilon + g_{\beta_0, p_0}}} dP_{X,Y} - 2h^2(g_{\hat{\beta}_n, \hat{p}_n}, g_{\beta_0, p_0}).$$

By the strong law of large numbers:

$$\int \log\{\varepsilon + g_{\beta_0,p_0}\}dP_{X,Y} - \int \log g_{\beta_0,p_0}d\mathbb{P} \rightarrow \int \log \left\{ \frac{\varepsilon + g_{\beta_0,p_0}}{g_{\beta_0,p_0}} \right\} dP_{X,Y} \rightarrow 0$$

as  $\varepsilon \rightarrow 0$ .

Consequently, we have

$$\begin{aligned} 0 &\leq \liminf \left[ \int \log\{\varepsilon + g_{\hat{\beta}_n,\hat{p}_n}\}d(\mathbb{P} - P_{X,Y}) + \int \log \left\{ \frac{\varepsilon + g_{\hat{\beta}_n,\hat{p}_n}}{\varepsilon + g_{\beta_0,p_0}} \right\} dP_{X,Y} \right. \\ &\quad \left. + \int \log\{\varepsilon + g_{\beta_0,p_0}\}dP_{X,Y} - \int \log g_{\beta_0,p_0}d\mathbb{P} \right] \\ &\leq 2 \int \sqrt{\frac{\varepsilon}{\varepsilon + g_{\beta_0,p_0}}}dP_{X,Y} - 2\limsup\{h^2(\hat{p}_n, p_0)\}. \end{aligned}$$

As  $\varepsilon \rightarrow 0$ , we have  $\limsup\{h^2(g_{\hat{\beta}_n,\hat{p}_n}, g_{\beta_0,p_0})\} \rightarrow 0$ , and  $\limsup\{h^2(\hat{p}_n, p_0)\} \rightarrow 0$  follows from Lemma 1. Following the same arguments of Lemma 3.14 in Seregin and Wellner (2010),  $\hat{p}_n \rightarrow p_0$  pointwise and the convergence is uniform on compact space.

The  $\lim_{n \rightarrow \infty} \{\int \log g_{\hat{\beta}_n,\hat{p}_n}d\mathbb{P} - \int \log g_{\beta_0,p_0}d\mathbb{P}\} \geq 0$  yields

$$\int \log g_{\hat{\beta}_n,\hat{p}_n}dP_{X,Y} - \int \log g_{\beta_0,p_0}dP_{X,Y} \geq 0,$$

and

$$\begin{aligned} &\int (\hat{\phi}_n - \phi_0)dP_Y + \int \{\eta(\mathbf{y}, \mathbf{x}|\hat{\beta}_n) - \eta(\mathbf{y}, \mathbf{x}|\beta_0)\}dP_{X,Y} \\ &\geq \int \{\log Q_{\hat{p}_n}(\hat{\beta}_n) - \log Q_p(\beta_0)\}dP_X. \end{aligned} \tag{A.2}$$

Let  $\hat{\phi}(\mathbf{y}) - \phi_0(\mathbf{y}) = c(\mathbf{y})$  and  $\eta(\mathbf{y}, \mathbf{x}|\hat{\beta}_n) - \eta(\mathbf{y}, \mathbf{x}|\beta_0) = b(\mathbf{y}, \mathbf{x}|\hat{\beta}_n, \beta_0)$ , we have

$$\frac{Q_{\hat{p}_n}(\hat{\beta}_n)}{Q_{p_0}(\beta_0)} = \int e^{c(\mathbf{y})+b(\mathbf{y},\mathbf{x}|\hat{\beta}_n,\beta_0)} f_{\beta_0,p_0} d\mathbf{y} \geq e^{\int \{c(\mathbf{y})+b(\mathbf{y},\mathbf{x}|\hat{\beta}_n,\beta_0)\} f_{\beta_0,p_0} d\mathbf{y}}$$

with the equality hold when  $c(\mathbf{y}) + b(\mathbf{y}, \mathbf{x}|\hat{\beta}_n, \beta_0) = c_0$  for a constant  $c_0$  by Jensen's inequality. Furthermore,

$$\begin{aligned} \int \log \left\{ \frac{Q_{\hat{p}_n}(\hat{\beta}_n)}{Q_{p_0}(\beta_0)} \right\} dP_X &\geq \int \int \{c(\mathbf{y}) + b(\mathbf{y}, \mathbf{x}|\hat{\beta}_n, \beta_0)\} f_{\beta_0,p_0} d\mathbf{y} dP_X \\ &= \int c(\mathbf{y})dP_Y + \int b(\mathbf{y}, \mathbf{x}|\hat{\beta}_n, \beta_0)dP_{X,Y}, \end{aligned}$$

by the law of total expectation. Combining with (A.2), we have

$$\begin{aligned} &\int (\hat{\phi}_n - \phi_0)dP_Y + \int \{\eta(\mathbf{y}, \mathbf{x}|\hat{\beta}_n) - \eta(\mathbf{y}, \mathbf{x}|\beta_0)\}dP_{X,Y} \\ &= \int \{\log Q_{\hat{p}_n}(\hat{\beta}_n) - \log Q_p(\beta_0)\}dP_X, \end{aligned}$$

and it has to be  $c(\mathbf{y}) + b(\mathbf{y}, \mathbf{x}|\hat{\beta}_n, \beta_0) = c_0$ . Based on the facts that both  $\exp(\hat{\phi}_n)$  and  $\exp(\phi_0)$  need to be a density function, and both  $\mathbf{Y}$  and  $\mathbf{X}$  are not degenerate, we can deduce  $c_0 = 0$ . Furthermore, it implies  $\eta(\mathbf{y}, \mathbf{x}|\hat{\beta}_n) \rightarrow \eta(\mathbf{y}, \mathbf{x}|\beta_0)$  because again both  $Y$  and  $\mathbf{X}$  are not degenerate, followed by  $\hat{\beta}_n \rightarrow \beta_0$  based on assumption C.

*Proof of Lemma 2*

By Theorem 4.2 of Doss and Wellner (2016), we know that  $N_{[\cdot]}(\varepsilon, \sqrt{\mathcal{P}_c}, L_2) \lesssim \exp\{\varepsilon^{-1/2}\}$  for  $L_2(p, q) = (\int |p - q|^2 d\lambda)^{1/2}$ , where  $\lesssim$  means the left side bounded by a constant times the right side. It imply that there is a set of functions  $\{(p_1^l, p_1^u, \dots, p_s^l, p_s^u) : L_2(\sqrt{p_i^l}, \sqrt{p_i^u}) < \varepsilon, i \in (1, \dots, s)\}$  such that, for each  $p \in \mathcal{P}$ ,  $p_i^l \leq p \leq p_i^u$  for some  $i$ . Furthermore, let  $p_i^L = p_i^l - \varepsilon$  and  $p_i^U = p_i^u + \varepsilon$ , which satisfy  $p_i^L + \varepsilon \leq p \leq p_i^U - \varepsilon$ .

Consider  $t$  points  $\beta_1, \dots, \beta_t$  in the neighborhood  $B(\beta_0, \delta)$ . By our model assumptions B and C, the  $\exp\{\eta(y, \mathbf{x}|\beta)\}$  is bounded for  $\beta \in B(\beta_0, \delta)$ . Following the arguments in the proof of Lemma 3.1 by Huang (1996), by choosing appropriate  $\delta$  and  $t \lesssim 1/\varepsilon$ , we have

$$\exp\{y, \mathbf{x}|\beta_j\} p_i^L(y) \leq \exp\{\eta(y, \mathbf{x}|\beta)\} p(y) \leq \exp\{\eta(y, \mathbf{x}|\beta_j)\} p_i^U(y), \tag{A.3}$$

for  $j \in (1, \dots, t)$ .

For each  $(\beta, p) \in B(\beta_0, \delta) \times \mathcal{P}_c$ ,  $i \in (1, \dots, s)$ , and  $j \in (1, \dots, t)$ , inequalities (A.3) imply

$$g_{ij}^L \leq g_{\beta,p} \leq g_{ij}^U,$$

where

$$g_{ij}^L = \frac{p_i^L(y) e^{\eta(y, \mathbf{x}|\beta_j)}}{\int p_i^U(y) e^{\eta(y, \mathbf{x}|\beta_j)} dy} p_x(\mathbf{x}) \quad \text{and} \quad g_{ij}^U = \frac{p_i^U(y) e^{\eta(y, \mathbf{x}|\beta_j)}}{\int p_i^L(y) e^{\eta(y, \mathbf{x}|\beta_j)} dy} p_x(\mathbf{x}).$$

By Assumption B, we can see that  $L_2(g_{ij}^L, g_{ij}^U) \lesssim L_2(p_i^L, p_i^U)$ . It implies, there exist  $\{g_{ij}^L, g_{ij}^U : i = 1, \dots, s, j = 1, \dots, t\}$  such that  $g_{ij}^L \leq g \leq g_{ij}^U$  for any  $g \in \mathcal{G}_\delta$  and some  $i \in (1, \dots, s), j \in (1, \dots, t)$ . That is,  $N_{[\cdot]}(\varepsilon, \sqrt{\mathcal{G}_\delta}, L_2) \lesssim \varepsilon^{-1} \exp(\varepsilon^{-1/2})$ . For small enough  $\varepsilon$ , the claim of the theorem is followed since  $N_{[\cdot]}(\varepsilon, \mathcal{G}_\delta, h_0) \leq N_{[\cdot]}(\varepsilon, \mathcal{G}_{4\delta}, h) \leq N_{[\cdot]}(\varepsilon/\sqrt{2}, \sqrt{\mathcal{G}_\delta}, L_2)$ .

*Proof of Lemma 3*

Define  $m_{\beta,p} = \log\{(g_{\beta,p} + g_{\beta_0,p_0})/2g_{\beta_0,p_0}\}$ . Utilizing the relation  $P\{\log(p/q)\} \lesssim -h^2(p, q)$  and the arguments in Theorem 3.4.4 of van der Vaart and Wellner (1996), it can be shown that  $P_0(m_{\beta,p} - m_{\beta_0,p_0}) \lesssim -h^2(g_{\beta,p}, g_{\beta_0,p_0})$ . Lemma 1 leads to  $P_0(m_{\beta,p} - m_{\beta_0,p_0}) \lesssim -h^2(p, p_0)$ . By Taylor series expansion in  $\beta$ , we have  $P_0(m_{\beta,p_0} - m_{\beta_0,p_0}) \gtrsim -\|\beta - \beta_0\|^2$ . Thus decomposing  $P_0(m_{\beta,p} - m_{\beta_0,p_0})$  as

$P_0(m_{\beta,p} - m_{\beta_0,p_0}) - P_0(m_{\beta,p_0} - m_{\beta_0,p_0})$  yields

$$P_0(m_{\beta,p} - m_{\beta,p_0}) \lesssim -h^2(p, p_0) + \|\beta - \beta_0\|^2. \tag{A.4}$$

Denote the empirical process  $\mathbb{G}_n f = \sqrt{n}(\mathbb{P} - P)f$ . Following Lemma 3.4.2 and Theorem 3.4.4 of van der Vaart and Wellner (1996), we have

$$E_{\mathcal{G}_\delta}^* |\mathbb{G}(m_{\beta,p} - m_{\beta,p_0})| \lesssim \zeta(\delta) = J_{[\cdot]}(\delta, \mathcal{G}_\delta, h_0) \left\{ 1 + \frac{J_{[\cdot]}(\delta, \mathcal{G}_\delta, h_0)}{\delta^2 \sqrt{n}} \right\}, \tag{A.5}$$

where  $J_{[\cdot]}(\delta, \mathcal{G}_\delta, h_0) = \int_0^\delta \sqrt{1 + \log N_{[\cdot]}(\varepsilon, \mathcal{G}_\delta, h_0)} d\varepsilon$ .

The inequalities (A.4) and (A.5) correspond to expressions (3.5) and (3.6) of Murphy and van der Vaart (1999). The entropy in Lemma 2 imply  $J_{[\cdot]}(\delta, \mathcal{G}_\delta, h_0) \lesssim \delta^{3/4}$ . If a sequence  $\delta_n$  satisfy  $\delta_n \lesssim n^{-2/5}$ , we have  $\delta_n^{-2} J_{[\cdot]}(\delta_n, \mathcal{G}_\delta, h_0) \lesssim \sqrt{n}$ , which is equivalent to  $\zeta_n(\delta_n) \leq \sqrt{n} \delta_n^2$ . Then  $h(\hat{p}_{\tilde{\beta}}, p_0) \leq O(n^{-2/5} + \|\tilde{\beta} - \beta_0\|)$  follows from Theorem 3.2 of Murphy and van der Vaart (1999) and Theorem 3.4.1 van der Vaart and Wellner (1996).

*Proof of Theorem 2*

In the context of least favorable model, we assume that for each  $(\beta, p)$ , there exist a map  $\mathbf{t} \rightarrow p_{\mathbf{t}}(\beta, p) = p + (\beta - \mathbf{t})h_0 p$ , where  $h_0$  is the least favorable direction at the true parameter  $(\beta_0, p_0)$ . We then form the map  $\mathbf{t} \rightarrow l(\mathbf{t}, \beta, p)(y)$  by  $l(\mathbf{t}, \beta, p)(y) = l\{\mathbf{t}, p_{\mathbf{t}}(\beta, p)\}(y)$ , where  $l(\beta, p) = \log p(y) + \eta(y, \mathbf{x}|\beta) - \log \int \exp(\eta(y, \mathbf{x}|\beta))p(y)dy$  is twice continuously differentiable for all  $y$ . The corresponding derivatives are denoted as  $\dot{l}(\mathbf{t}, \beta, p)(y)$  and  $\ddot{l}(\mathbf{t}, \beta, p)(y)$ .

In the followed, we will establish four conditions.

*Condition 1.*  $p_{\beta}(\beta, p) = p$  for every  $(\beta, p)$ .

It is satisfied for  $p_{\mathbf{t}}(\beta, p) = p + (\beta - \mathbf{t})h_0 p$ .

*Condition 2.*  $\dot{l}(\beta_0, \beta_0, p_0) = \dot{l}_{\beta_0, p_0}$ .

The score function for  $\beta$  is  $l'_{\beta, p} = \eta' - \int \eta' e^{\eta(y, \mathbf{x}|\beta)} p(y) dy / \int e^{\eta(y, \mathbf{x}|\beta)} p(y) dy$ . Let  $\mathcal{H}$  be the set of measurable function  $h : \mathcal{Y} \rightarrow [0, 1]$ , given a fixed  $p$ , let  $p_{\mathbf{t}}(\beta, p) = p + thp$ . When  $p$  is log-concave,  $p_{\mathbf{t}}$  is log-concave for  $th > 0$ . Differentiating at  $t = 0$ , we have the score for  $p$  as  $A_{\beta, p} h = h - B_{\beta, p} h = h - \int h e^{\eta(y, \mathbf{x}|\beta)} p(y) dy / \int e^{\eta(y, \mathbf{x}|\beta)} p(y) dy$ . The efficient score function for  $\beta$  at  $(\beta_0, p_0)$  is defined as  $\dot{l}_{\beta_0, p_0} = l'_{\beta_0, p_0} + A_{\beta_0, p_0} h_{\beta_0, p_0}$ . Substituting  $\beta = \mathbf{t}$  and  $p_{\mathbf{t}} = p$  in  $l(\beta, p)$  and differentiating with respect to  $\mathbf{t}$ , it is straight forward to show that  $\dot{l}(\beta_0, \beta_0, p_0) = \dot{l}_{\beta_0, p_0}$ .

*Condition 3.* For any  $\tilde{\beta}_n \xrightarrow{P} \beta_0, \hat{p}_{\tilde{\beta}_n} \xrightarrow{P} p_0$ .

It is followed by Lemma 3.

*Condition 4.* For any  $\tilde{\beta}_n \xrightarrow{P} \beta_0, P_0 \dot{l}(\beta_0, \tilde{\beta}_n, \hat{p}_{\tilde{\beta}_n}) = o_P(\|\tilde{\beta}_n - \beta_0\| + n^{-1/2})$ .

As shown in expression (17) of Murphy and van der Vaart (2000),  $P_0 \dot{l}(\beta_0, \beta_0, p)$  is of order  $O_p\{h^2(p, p_0)\}$  since  $p \rightarrow f_{\beta,p}$  is twice differentiable and  $p \rightarrow \dot{l}(\beta_0, \beta_0, p)$  is differentiable at  $p_0$ . By Lemma 3, we can see that  $P_0 \dot{l}(\beta_0, \beta_0, \hat{p}_{\tilde{\beta}_n}) = o_P(\|\tilde{\beta}_n - \beta_0\| + n^{-1/2})$  is satisfied, which is equivalent to Condition 4.

The conditions 1-4 correspond to conditions (8)-(11) in Murphy and van der Vaart (2000), in addition, we need to prove the invertibility of the information matrix to build the asymptotic property. Let  $\mathbf{D}_n(\beta, p) = \{\mathbf{D}_n1(\beta, p), \mathbf{D}_n2(\beta, p)\}$  be the element of  $\mathbb{R}^g \times l^\infty(\mathcal{H})$  given by

$$\mathbf{D}_n1(\beta, p) = \mathbb{P}l'_{\beta,p}, \quad \mathbf{D}_n2(\beta, p) = \mathbb{P}A_{\beta,p}h - P_{\beta,p}A_{\beta,p}h.$$

The expectation of  $\mathbf{D}_n(\beta, p)$  under the true distribution  $P_0 = P_{\beta_0,p_0}$  is the element  $\mathbf{D}(\beta, p) = \{\mathbf{D}_1(\beta, p), \mathbf{D}_2(\beta, p)\}$  of  $\mathbb{R}^k \times l^\infty(\mathcal{H})$  given by

$$\mathbf{D}_1(\beta, p) = \mathbb{P}_0l'_{\beta,p}, \quad \mathbf{D}_2(\beta, p) = P_0A_{\beta,p}h - P_{\beta,p}A_{\beta,p}h.$$

A Hilbert-space adjoint  $B_{\beta,p}^*$  of  $B_{\beta,p}$  is given by  $B_{\beta,p}^*q = \int q(\mathbf{x})e^{\eta(y,\mathbf{x}|\beta)}dP_X(\mathbf{x})$ . The least favourable direction,  $h_0$ , for the estimation of  $\beta$  in the presence of  $p$  is given by  $(A_{\beta_0,p_0}^*A_{\beta_0,p_0})^{-1}A_{\beta_0,p_0}^*l'_{\beta_0,p_0}$ , and it can be shown that  $A_{\beta_0,p_0}^*l'_{\beta_0,p_0} = -B_{\beta_0,p_0}^*l'_{\beta_0,p_0}$  and  $A_{\beta_0,p_0}^*A_{\beta_0,p_0} = I - B_{\beta_0,p_0}^*B_{\beta_0,p_0}$ .

The derivative of  $D$  at  $(\beta_0, p_0)$  is given by the map:

$$\dot{\mathbf{D}} : (\beta - \beta_0, p - p_0) \rightarrow \begin{pmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{pmatrix} \begin{pmatrix} \beta - \beta_0 \\ p - p_0 \end{pmatrix},$$

where  $\mathbf{H}_{11}(\beta - \beta_0) = P_0l''_0(\beta - \beta_0) = -I_0(\beta - \beta_0)$ ,  $\mathbf{H}_{12}(p - p_0) = \int B_0^*l'_0(p - p_0)dy$ ,  $\mathbf{H}_{21}(\beta - \beta_0)h = P_0A_0h(l'_0 - \eta'_0)(\beta - \beta_0)$ , and  $\mathbf{H}_{22}(p - p_0)h = -\int (I - B_0^*B_0)h(p - p_0)dy$ . Since

$$\dot{\mathbf{D}}^{-1} = \begin{pmatrix} \mathbf{H}_{11}^{-1}(\mathbf{H}_{11} + \mathbf{H}_{12}\Lambda^{-1}\mathbf{H}_{21})\mathbf{H}_{11}^{-1} & -\mathbf{H}_{11}^{-1}\mathbf{H}_{12}\Lambda^{-1} \\ -\Lambda^{-1}\mathbf{H}_{21}\mathbf{H}_{11}^{-1} & \Lambda^{-1} \end{pmatrix},$$

the continuous invertibility of  $\dot{\mathbf{D}}$  can be verified by continuous invertibility of  $\mathbf{H}_{11}$  and  $\Lambda = \mathbf{H}_{22} - \mathbf{H}_{21}\mathbf{H}_{11}^{-1}\mathbf{H}_{12}$ . By Assumption D, the matrix  $\mathbf{H}_{11}$  is continuous invertible. The operator

$$\Lambda = -\int \{I + P_0A_0(l'_0 - \eta'_0)I_0^{-1}B_0^*l'_0 - B_0^*B_0\}h(p - p_0)dy = -\int (I + K)h(p - p_0)dy$$

is continuous invertible if  $K$  is compact and  $I + K$  is one-to-one using the theory of Fredholm operator. Since  $e^{\eta(y,\mathbf{x}|\beta)}$  is sufficiently smooth, the operator  $B_0^*$  is compact by Arzelà-Ascoli theorem. The operator  $P_0A_0(l'_0 - \eta'_0)I_0^{-1}B_0^*l'_0$  is compact because it has a one-dimensional range. Thus  $K$  is compact. Now it suffices to show that  $I + K$  is one-to-one. The spectrum of the self-adjoint

operator  $I - B_0^* B_0 : L_2(p_0) \rightarrow L_2(p_0)$  is contained in  $[1, \infty)$ . Finally, this operator is continuously invertible in the Hilbert-space sense.

Following Corollary 1 and Theorem 1 in Murphy and van der Vaart (2000), the conditions 1-4, the invertibility of information matrix, and the consistence of estimators imply  $\sqrt{n}(\hat{\beta} - \beta_0)$  is asymptotic normal with mean 0 and covariance matrix  $\tilde{I}_0 = \mathbf{H}_{11} - \mathbf{H}_{12}\mathbf{H}_{22}^{-1}\mathbf{H}_{21}$ .

*Proof of Theorem 3*

Let

$$(\beta_1, F_1) = \arg \max_{\beta, F \in \mathcal{F}_c} E_0 \left\{ \log \frac{f(\mathbf{y}; \mathbf{x}, \beta, F)}{f(\mathbf{y}; \mathbf{x}, \beta_0, F_0)} \right\},$$

where  $E_0$  denote the expectation under  $P_{X,Y}$ .

Helly's lemma (van der Vaart (1998)) implies that, there exist a subsequence of  $\hat{F}_n$  which converges to a distribution  $F_2$  on the continuous points of  $F_2$ . There is also a subsequence of  $\hat{\beta}_n$  converging to  $\beta_2$  because  $\Theta$  is a compact set. It follows that

$$0 \leq \mathbb{P}_n \{l(\hat{\beta}_n, \hat{F}_n) - l(\beta_0, F_0)\} \rightarrow E_0 \{l(\beta_2, F_2) - l(\beta_0, F_0)\}.$$

Since  $(\beta_1, F_1)$  is the unique maximizer of the Kullback-Leibler information by assumption A, we conclude that  $(\beta_2, F_2) = (\beta_1, F_1)$ . That is,  $\hat{F}_n$  converge weakly to  $F_1$  whose density is log-concave when  $F_0 \notin \mathcal{F}_c$ . Since both  $\hat{F}_n$  and  $F_1$  are continuous probability distribution function, the weak convergence of  $\hat{F}_n$  implies its uniform convergence, i.e.,  $\|\hat{F}_n(y) - F_1(y)\|_\infty \rightarrow 0$  (Chow and Teicher (1978)).

Based on  $\|\hat{F}_n(y) - \tilde{F}_n(y)\|_\infty \geq \|\hat{F}_n(y) - F_0(y)\|_\infty - \|\tilde{F}_n(y) - F_0(y)\|_\infty$  and  $\|F_1(y) - F_0(y)\|_\infty \geq C$  for a positive constant  $C$ , we have

$$\lim_{n \rightarrow \infty} \inf_{\hat{F}_n(y) \in \mathcal{F}_c, F_0 \notin \mathcal{F}_c} \|\hat{F}_n(y) - \tilde{F}_n(y)\|_\infty \geq C$$

because  $\|\tilde{F}_n(y) - F_0(y)\|_\infty \rightarrow 0$  by Luo and Tsai (2012). Consequently, we have

$$\lim_{\epsilon \rightarrow 0} \lim_{n \rightarrow \infty} \inf_{\hat{F}_n(y) \in \mathcal{F}_c, F_0 \notin \mathcal{F}_c} P(T_n \geq \sqrt{n}\epsilon) = 1. \quad (\text{A.6})$$

When the true distribution satisfy the shape constraint, we have

$\lim_{n \rightarrow \infty} P(T_n \leq \sqrt{n}\epsilon) = 1$  for all  $\epsilon > 0$  since  $\|\hat{F}_n(y) - F_0(y)\|_\infty \rightarrow 0$  by Theorem 1. It follows that  $\lim_{n \rightarrow \infty} P(T^* \leq \sqrt{n}\epsilon) = 1$  because the shape constraint estimate  $(\beta^*, F^*)$  is based on data sampled from the null distribution  $\mathcal{F}_c$  in the bootstrap procedure. It implies that

$$\lim_{n \rightarrow \infty} P(\xi_\alpha \leq \sqrt{n}\epsilon) = 1 \text{ for all } \epsilon > 0, \quad (\text{A.7})$$

where  $\xi_\alpha$  is the critical values in the bootstrap procedure. Combining (A.6) and

(A.7) together, we complete the proof.

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