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Friederike Greb, Tatyana Krivobokova, Axel Munk, Stephan von Cramon-Taubadel

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Wilhelm-Weber-Str. 2 · 37073 Goettingen · Germany
Phone: +49-(0)551-3914066 · Fax: +49-(0)551-3914059

Email: crc-peg@uni-goettingen.de Web: http://www.uni-goettingen.de/crc-peg

Regularized Bayesian estimation in generalized threshold regression models

Friederike Greb [1] Tatyana Krivobokova[1, 2] Axel Munk[2, 3]
Stephan von Cramon-Taubadel [4]
Georg-August-Universität Göttingen

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Abstract

Estimation of threshold parameters in (generalized) threshold regression models is typically performed by maximizing the corresponding profile likelihood function. Certain Bayesian techniques based on non-informative priors have also been developed and are widely used. This article draws attention to finite-sample settings (not rare in practice) in which these standard estimators perform poorly or even fail. In particular, if estimation of the regression coefficients is associated with high uncertainty, the profile likelihood for the threshold parameters and thus the corresponding estimators can be strongly affected. We suggest an alternative regularized Bayesian estimator that circumvents the deficiencies of standard estimators in small samples. The new estimator can be obtained employing the empirical Bayes paradigm and, hence, requires little additional numerical effort compared with commonly used estimators. Simulations confirm excellent finite sample properties of the suggested estimator, especially in the critical settings. The practical relevance of our approach is illustrated by two real-data examples already analyzed in the literature.

Key words and phrases: empirical Bayes, nuisance parameter, threshold estimation.

1 Introduction

Modeling a response variable as a linear combination of some covariates with regression coefficients that vary between (possibly several) regimes is known as threshold regression. The choice of regime is determined by a transition function which depends on a transition variable as well as a threshold parameter. Transition functions can be either

[1]Courant Research Centre "Poverty, Equity and Growth in Developing Countries", Georg-August-Universität Göttingen, Wilhelm-Weber-Str. 2, 37073 Göttingen, Germany
[2]Institute for Mathematical Stochastics, Georg-August-Universität Göttingen, Goldschmidstrasse 7, 37077 Göttingen, Germany
[3]Max Planck Institute for Biophysical Chemistry, Am Faberg 11, 37077 Göttingen, Germany
[4]Department of Agricultural Economics and Rural Development, Georg-August-Universität Göttingen, Platz der Göttinger Sieben 5, 37073 Göttingen, Germany

smooth (Van Dijk et al., 2002, provide a comprehensive overview) or step functions. In the following, we restrict attention to the latter. In principle, the response variable can follow any distribution from the exponential family. However, such generalized threshold regression models have only recently been formally introduced by Samia and Chan (2011) and most of the literature on threshold regression deals with models with piecewise linear mean. In this article we concentrate on generalized regression models with regimes controlled by a step transition function and refer to such models as generalized threshold regression models. Generalized threshold regression models are employed in a wide range of different fields of application. Hansen (2011) provides an overview of the extensive use of generalized threshold regression models in economic applications including e.g. models of output growth, forecasting, and the term structure of interest rates or stock returns. Samia et al. (2007) employ a generalized threshold regression model to analyze plague outbreaks and Lee et al. (2011) complement these applications with examples in finance, sociology, and biostatistics among others.

Threshold estimation in generalized threshold regression models is typically performed in two stages: the estimation of the regression coefficients is followed by the maximization of the profile likelihood for the threshold parameters using a grid search, as the likelihood function is not differentiable with respect to the threshold parameter. This estimation procedure has two intrinsic problems. First, the profile likelihood is not defined for thresholds that leave fewer observations in one of the regimes than are necessary to estimate the regression coefficients. Hence, in practice it is unavoidable to restrict the domain of the threshold parameters depending on the dimension of the regression coefficients. The literature offers arbitrary constraints including one observation per dimension of the regression coefficient (Samia and Chan, 2011) or 15% of the observations (Andrews, 1993) to give just two examples. This restriction can be problematic in small samples, especially if the true threshold is close to the boundary of its domain. The second problem is due

to the direct impact of the uncertainty inherent in the regression coefficients' estimates on the profile likelihood for the threshold parameters. In an unfavorable setting the profile likelihood becomes jagged with multiple extrema, increasing the uncertainty of the threshold estimator. Large variance of the regression coefficients' estimator is again likely to be found in small samples and for the true threshold at the boundary of its domain, but also if the signal-to-noise ratio is low or the residual variance is misspecified (overdispersion in the generalized regression setting). We are not aware of any work that points out these deficiencies of the common threshold estimator even though the problematic settings frequently occur in empirical applications. Macro-economic data are often only available for a small sample, e.g. if observations correspond to different countries. Spatial arbitrage modeling is another example (Greb et al., 2011).

Bayesian methods are also popular to estimate thresholds. In the literature, a Bayesian threshold estimator is typically based on non-informative priors; we refer to it as the non-informative Bayesian estimator. For the case of a threshold regression model with piecewise linear mean, Yu (2012) shows that, regardless of the choice of priors, Bayesian threshold estimators are asymptotically efficient among all estimators in the locally asymptotically minimax sense. However, in the critical small sample settings described above, the non-informative Bayesian estimator shares all the drawbacks of the profile likelihood estimator and can completely fail in certain cases, as we discuss in Section 3.2.

In this article, we suggest an alternative threshold estimator, which we call the regularized Bayesian estimator. Contrary to previous work on estimation in threshold regression (Samia and Chan, 2011; Yu, 2012), we focus on the estimator's performance in critical small sample situations. Simulations confirm that it yields good results even in settings in which profile likelihood and non-informative Bayesian estimator are highly susceptible to faults. To summarize the intuition behind this new estimator: If regression coefficients were known, none of the problems outlined above would exist. This suggests that

stabilizing their estimates might help to prevent them from distorting the threshold estimates. In addition, regularization of regression coefficient estimates allows us to obtain a posterior density which is well-defined on the entire domain of the threshold parameters. We achieve regularization by a particular specification of priors. While it proves to be beneficial in the critical small sample situations, the choice of priors does not have an impact asymptotically (as Yu, 2012, shows for a threshold regression model with piecewise linear mean and independent observations). We further derive an explicit (approximate) expression of the posterior density, which allows us to utilize existing functions for mixed models in standard software to easily compute the estimator.

The rest of this article is organized as follows. We specify the generalized threshold regression model in the second section. In the third section, we review existing threshold estimators and point out their deficiencies. The regularized Bayesian estimator is introduced in the fourth section. In the fifth section, we briefly look at inference about the threshold parameter. Simulation results are presented in the sixth section. We use the last section to discuss two empirical applications. The appendix contains some technical details.

2 Model

Observations $\left(y_i, \boldsymbol{X}_i^T, q_i\right) \in \mathbb{R} \times \mathbb{R}^p \times \mathbb{R}$, $i = 1, \ldots, n$, are assumed to be realizations of random variables that follow a generalized threshold regression model with threshold parameter $\psi \in \mathbb{R}$, regression coefficients $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2 \in \mathbb{R}^p$ and scale (or dispersion) parameter $\phi \in \mathbb{R}^+$, that is

$$\mu_i = \mathrm{E}\left(y_i | \boldsymbol{X}_i^T, q_i\right) = h(\eta_i) \tag{1}$$

where h is a known one-to-one function, the inverse of the link function $g = h^{-1}$, and

$$\eta_i = I\left(q_i \leq \psi\right) \boldsymbol{X}_i^T \boldsymbol{\beta}_1 + I\left(q_i > \psi\right) \boldsymbol{X}_i^T \boldsymbol{\beta}_2, \tag{2}$$

with $I(\cdot)$ as the indicator function. Moreover, conditional on the design vector $\boldsymbol{X}_i^T$ and the transition variable q_i, the response variables y_i are independently drawn from an exponential family distribution with density

$$f(y_i|\psi, \phi, \boldsymbol{\beta}_1, \boldsymbol{\beta}_2) = \exp\left\{\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i, \phi)\right\}, \tag{3}$$

characterized by known functions b and c together with the natural parameter $\theta_i = \theta(\mu_i)$. Above and in the following, the same symbol denotes both a random variable and its realization; the context should eliminate ambiguities. To use matrix notation, we define vectors $\boldsymbol{\mu}$, $\boldsymbol{\eta}$, $\boldsymbol{y}$, $\boldsymbol{q}$, $\boldsymbol{I}(\boldsymbol{q} \leq \psi)$ and $\boldsymbol{I}(\boldsymbol{q} > \psi)$ by stacking μ_i, η_i, y_i, q_i, $I(q_i \leq \psi)$ and $I(q_i > \psi)$, respectively, and create an $n \times p$ matrix $\boldsymbol{X}$ with rows $\boldsymbol{X}_i^T$, $i = 1, \ldots, n$. With $\text{diag}\{\boldsymbol{I}(\cdot)\}$ the diagonal matrix with entries $\boldsymbol{I}(\cdot)$ along the diagonal and $\boldsymbol{\beta} = (\boldsymbol{\beta}_1^T, \boldsymbol{\beta}_2^T)^T$, we can write

$$\boldsymbol{\eta} = \text{diag}\{\boldsymbol{I}(\boldsymbol{q} \leq \psi)\}\boldsymbol{X}\boldsymbol{\beta}_1 + \text{diag}\{\boldsymbol{I}(\boldsymbol{q} > \psi)\}\boldsymbol{X}\boldsymbol{\beta}_2 = \boldsymbol{X}_1\boldsymbol{\beta}_1 + \boldsymbol{X}_2\boldsymbol{\beta}_2 = \boldsymbol{X}_\psi\boldsymbol{\beta}.$$

We consider generalized threshold regression models with one threshold to keep the exposition simple; extension to generalized threshold regression models with more thresholds is straightforward.

Naturally, our model covers $y_i = I(q_i \leq \psi)\boldsymbol{X}_i^T\boldsymbol{\beta}_1 + I(q_i > \psi)\boldsymbol{X}_i^T\boldsymbol{\beta}_2 + \varepsilon_i$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ and $i = 1, \ldots, n$. This is by far the most frequently encountered generalized threshold regression model in the literature. It is broad enough to comprise the popular threshold autoregressive model in which the transition variable q_i is an element of $\boldsymbol{X}_i$ (Tong and Lim, 1980; Tong, 2011, for a review of the development of the model).

Depending on the assumptions on the data generating process, model (1) – (3) can have different asymptotic behavior. A first differentiation regards the transition variable q_i. Change point models are characterized by deterministic $q_i = i$, while for threshold models q_i is a random variable which follows any continuous distribution. This is reflected in distinct limit likelihood ratio processes and, hence, asymptotic behavior of the maximum

likelihood estimators for ψ in the two models. The limiting likelihood ratio process involves a functional of random walks for change point models and of compound Poisson processes for threshold models. Check Bai (1997) for more details on the asymptotic properties in the former, and Samia and Chan (2011) for the limiting behavior of the profile log-likelihood and the asymptotic distribution of the profile likelihood threshold estimator in the latter case. If the transition variable coincides with one of the covariates and the regression function is continuous at the threshold, least squares estimates are known to be normally distributed (for threshold models, see Chan and Tsay, 1998; Feder, 1975, treats change-point models), which simplifies inference. Clearly, once the data is sampled, the estimation procedure in both change point and threshold models is the same. Referring to a threshold regression model with piecewise linear mean, Hansen (2000) points out that "if the observed values of q_i are distinct, the parameters can be estimated by sorting the data based on q_i, and then applying known methods for change point problems". However, as the focus of this article is on estimation problems that arise in small samples, we do not further differentiate models. In the real-data examples, we concentrate on discontinuous threshold models since they are frequently encountered in applications and have not been studied as extensively as change point models due to their more intricate limiting behavior.

3 Commonly used threshold estimators

3.1 The profile likelihood estimator

As noted in the introduction, the prevalent threshold estimator in the literature is the profile likelihood estimator, see e.g. Samia and Chan (2011) or Hansen (2000). Splitting all model parameters into a parameter of interest and nuisance parameters, the profile likelihood function $\mathcal{L}_p$ is constructed from the likelihood function $\mathcal{L}$ by replacing nuisance parameters with their maximum likelihood estimates at given values of

the parameter of interest. In generalized threshold regression models, our parameter of interest is the threshold parameter ψ and its domain is restricted to a random set $\Psi = \left\{\psi \in \mathbb{R} | q_{(1)} \leq \psi \leq q_{(n)}\right\} \subseteq \mathbb{R}$, where $q_{(i)}$ denotes the ith order statistics. The nuisance parameters are $\boldsymbol{\beta}^T \in \mathbb{R}^{2p}$ and $\phi \in \mathbb{R}$. Hence, we work with the conditional profile likelihood function given $\boldsymbol{X}$ and $\boldsymbol{q}$,

$$\mathcal{L}_p(\psi) = \prod_{i=1}^{n} f(y_i|\psi, \hat{\phi}_\psi, \hat{\boldsymbol{\beta}}_\psi) = \exp\left[\sum_{i=1}^{n}\left\{\frac{y_i\hat{\theta}_i - b(\hat{\theta}_i)}{\hat{\phi}_\psi} + c(y_i, \hat{\phi}_\psi)\right\}\right],$$

where $\hat{\theta}_i = \theta \circ h(\hat{\eta}_i) = \theta \circ h\left\{I(q_i \leq \psi)\boldsymbol{X}_i^T\hat{\boldsymbol{\beta}}_{1_\psi} + I(q_i > \psi)\boldsymbol{X}_i^T\hat{\boldsymbol{\beta}}_{2_\psi}\right\}$ and $\hat{\boldsymbol{\beta}}_\psi$ and $\hat{\phi}_\psi$ are maximum likelihood estimators at a fixed ψ. In the following, we assume a canonical link, that is, $\theta_i = \eta_i$. All developments still hold approximately if this assumption is not given. We denote the profile log-likelihood with $\ell_p(\psi) = \log \mathcal{L}_p(\psi)$.

To measure the proximity of a threshold ψ to the boundary of its domain Ψ, we introduce $\mathrm{d}(\psi) = \min(j, n-j)/p$ with j such that $q_{(j)} \leq \psi < q_{(j+1)}$. $\mathrm{d}(\psi)$ quantifies the distance between ψ and Ψ's boundary in terms of the number of observations between them relative to the dimension of the regression coefficients, $p = \dim(\boldsymbol{\beta}_k)$, $k = 1, 2$. When $\mathrm{d}(\psi) = 1$, ψ assigns at least p observations to each of the regimes. The allocation of 5% of the observations into one of the regimes can be expressed as $\mathrm{d}(\psi) = 0.05\, n/p$. Clearly, $\mathcal{L}_p(\psi)$ is not defined for $\mathrm{d}(\psi) < 1$, since in this case ψ does not leave enough observations for the estimation of $\boldsymbol{\beta}_k$ in one of the regimes. Hence, in practice it is inevitable to restrict Ψ to $\Psi^*(c) = \{\Psi |\ \mathrm{d}(\psi) > c\}$ for some $c \geq 1$. In the literature different heuristic suggestions for the choice of c have been proposed. For example, Hansen and Seo (2002) propose $c = 0.05\, n/p$, we find $c = 0.15\, n/p$ in Andrews (1993) and Samia and Chan (2011) even use $c = 0.25\, n/p$ for their application.

The profile likelihood threshold estimator is then given by

$$\hat{\psi}_{pL} = \underset{\psi \in \Psi^*(c)}{\operatorname{argmax}}\ \mathcal{L}_p(\psi).$$

This definition based on the restricted domain $\Psi^*(c)$ immediately suggests that in settings

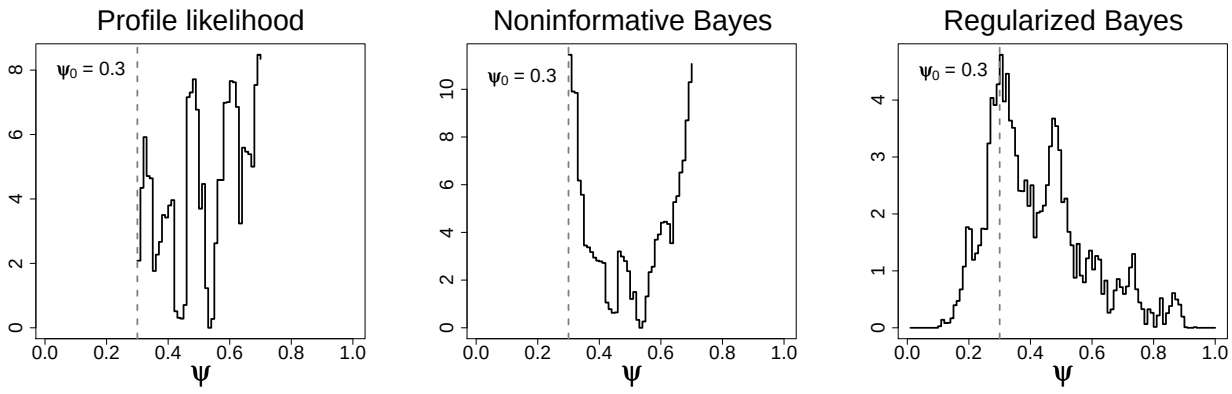

Figure 1: For a sample run corresponding to setting 1C of Section 6, $\ell_p(\psi)$ is shown on the left, $\log p_{nB}(\psi|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ in the middle and $\log p_{rB}(\psi|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ on the right.

in which $\mathrm{d}(\psi_0) < c$ for a true threshold ψ_0, $\hat{\psi}_{pL}$ is inconsistent. The left panel of Fig. 1 illustrates this showing the profile log-likelihood for a sample run of a generalized threshold regression model corresponding to the simulation setting 1C detailed in Section 6. If $\Psi^*(1) = [0.3, 0.7]$ would be restricted any further, e.g. to be $[0.31, 0.69]$, then the true threshold $\psi_0 = 0.3$ would be excluded from the threshold domain and $\hat{\psi}_{pL}$ would move to the next extremum. For small n, large p and ψ_0 close to the boundary of Ψ, $\mathrm{d}(\psi_0) < c$ is likely to be the case. Altogether, subjective restriction of the threshold domain is an undesirable property of threshold estimation based on the profile likelihood.

The same plot in Fig. 1 also exemplifies that in certain small-sample settings the profile (log-)likelihood can be jagged and have multiple extrema, leading to a very variable threshold estimator. To shed light on this behavior of $\ell_p(\psi)$, we contrast it with its analogue for known $\boldsymbol{\beta}$. Accordingly, we compare

$$-\ell_p(\psi) \propto -\frac{2}{\hat{\phi}_\psi} \sum_{i=1}^{n} \{y_i \hat{\theta}_i - b(\hat{\theta}_i)\} \approx (\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi \hat{\boldsymbol{\beta}}_\psi)^T \boldsymbol{W} (\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi \hat{\boldsymbol{\beta}}_\psi)$$

with its analogue for known $\boldsymbol{\beta}$. Here, $\hat{\boldsymbol{z}} = \boldsymbol{X}_\psi \hat{\boldsymbol{\beta}}_\psi + \boldsymbol{G}(\boldsymbol{y} - \hat{\boldsymbol{\mu}})$ is the working variable, $\boldsymbol{G} = \mathrm{diag}\{g'(\mu_i)\}$ and $\boldsymbol{W}^{-1} = \mathrm{diag}\{\phi b''(\theta_i) g'(\mu_i)^2\}$. The estimated $\boldsymbol{W}$ for fixed ψ is assumed to vary little or not at all as a function of the mean so we use $\boldsymbol{W}$ evaluated at the true $\boldsymbol{\beta}$ directly. This is a typical assumption in the literature on generalized linear models. The same applies to $\boldsymbol{G}$. We focus on the case of $\psi \leq \psi_0$, but the same arguments

hold for $\psi > \psi_0$. Denoting $\boldsymbol{z} = \boldsymbol{X}_\psi\boldsymbol{\beta} + \boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu})$, $\boldsymbol{X}_{[\psi,\psi_0]} = \text{diag}\{\boldsymbol{I}(\psi < \boldsymbol{q} \leq \psi_0)\}\boldsymbol{X}$ and $\boldsymbol{H} = \boldsymbol{W}^{1/2}\boldsymbol{X}_2(\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_{[\psi,\psi_0]}$, both of which disappear for $\psi = \psi_0$, we find

$$\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)^T\boldsymbol{W}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right) = (\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta}) + \mathcal{O}_p(2p) \tag{4}$$

$$+\left\{(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)^T\boldsymbol{H}^T - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}^{1/2}\right\}\boldsymbol{H}(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2) \tag{5}$$

$$+\left\{2(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)^T\boldsymbol{H}^T - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}^{1/2}\right\}^T\mathcal{O}_p\left(\boldsymbol{W}^{1/2}\sqrt{\text{var}\,\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right) \tag{6}$$

where $\mathcal{O}_p(2p)$ is bounded in probability for fixed p and $n \to \infty$; $\text{var}(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi)$ is a row vector containing the diagonal elements of $\boldsymbol{X}_\psi(\boldsymbol{X}_\psi^T\boldsymbol{W}\boldsymbol{X}_\psi)^{-1}\boldsymbol{X}_\psi^T$. Taking a closer look at $(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi)^T\boldsymbol{W}(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi)$ as a function of ψ, we note that replacing the true regression coefficients $\boldsymbol{\beta}$ by their maximum likelihood estimators influences $(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})$ in several ways. The $\mathcal{O}_p$-term in (4) is independent of ψ and simply shifts the profile likelihood by a constant. The deterministic term in (5) equals zero for $\psi = \psi_0$, but starts growing as $|\psi - \psi_0|$ increases. That is, even if there is no uncertainty due to estimation of $\boldsymbol{\beta}$, that is, $\text{var}(\hat{\boldsymbol{\beta}}_\psi) = 0$, the true least squares is inflated for ψ away from ψ_0, making the extremum less pronounced. The most important term is the last one in (6). This random term depends on $\text{var}\left(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)$ and can have a strong deforming effect on the true least squares even for ψ close to ψ_0. Large variance of $\hat{\boldsymbol{\beta}}_\psi$ is associated with settings characterized by small n relative to p, but can also be due to low signal-to-noise ratio, model misspecifications (e.g. overdispersion) or if the threshold is close to the boundary of its domain. This is exposed in the left as compared with the middle plot of Fig. 2; the log-likelihoods depicted in these plots belong to models which only differ in one aspect: in the plot on the left-hand side, the residual standard deviation is 0.75, while in the middle plot it is 1.5. Clearly, the log-likelihood in the middle plot is highly distorted over the whole range of Ψ, triggering multiple extrema and a highly variable estimator for ψ. Moving the true threshold closer to the boundary, as shown in the right plot of Fig. 2, leads to an even stronger deformation of the log-likelihood. In summary, in small samples and particular settings exemplified above, the profile likelihood threshold estimator can

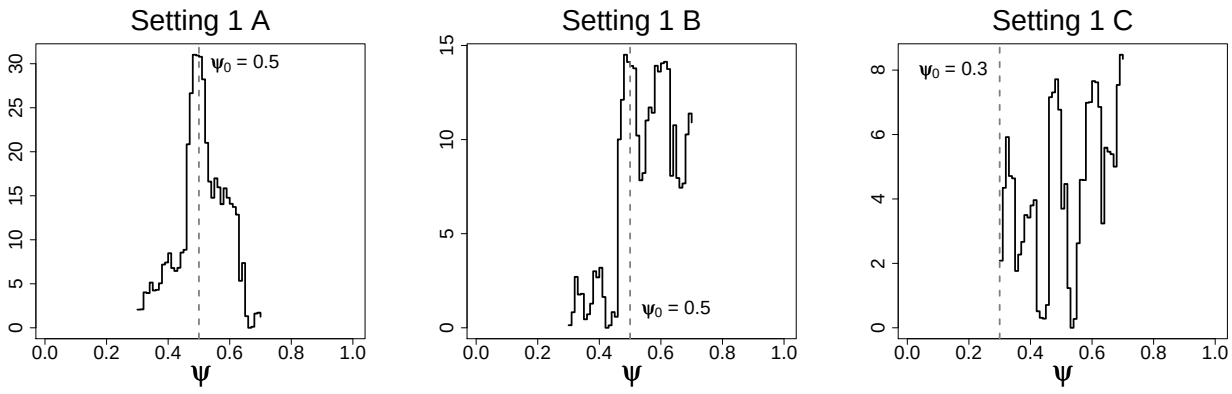

Figure 2: Sample (log) profile likelihood functions $\ell_p(\psi)$ for different settings.

perform poorly, being very sensitive to inappropriate estimates of the nuisance parameters and relying on a subjective restriction of its domain.

3.2 The Bayesian estimator

For threshold estimation in regression models with piecewise linear mean, there is a long tradition of using Bayesian techniques in applied work beginning with Bacon and Watts (1971) and including Geweke and Terui (1993) among many others. This popularity can be at least partially attributed to practical advantages, since the Bayesian approach offers a natural framework for inference and accounts for the variability of the nuisance parameters. The theoretical properties of Bayesian threshold estimators in certain generalized threshold regression models have been investigated by Yu (2012). He shows that for independently and identically distributed observations Bayesian threshold estimators are asymptotically efficient among all estimators in the locally asymptotically minimax sense and strictly more efficient than the maximum likelihood estimator. In a related paper, Chan and Kutoyants (2010) examine asymptotic properties of Bayesian estimators in threshold autoregression models. They note that the limit variance of the Bayesian estimator is smaller than that of the maximum likelihood estimator.

Without any prior knowledge of possible parameter values, it is natural to assume a uniform prior for the threshold parameter and non-informative priors for the regression

coefficients; these choices are (almost) omnipresent in the Bayesian literature on generalized threshold regression models with piecewise linear mean. While the priors do not have an impact asymptotically, it turns out that they do affect the performance of the Bayesian threshold estimator in finite samples. We show that non-informative priors can distort estimates, especially in small samples. It is straightforward to obtain an approximation of a generalized threshold regression model's posterior density $p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ associated with non-informative (improper) priors $p(\boldsymbol{\beta}) \propto 1$ and $p(\psi|\boldsymbol{q}) \propto I(\psi \in \Psi)$ based on a Laplace approximation (Shun and McCullagh, 1995; Severini, 2000) of the integral for fixed $p \ll n$

$$\int\limits_{\mathbb{R}^{2p}} p(y|\psi, \phi, \boldsymbol{\beta}, \boldsymbol{X}, \boldsymbol{q}) d\boldsymbol{\beta} = \mathcal{L}_p(\psi)(2\pi)^p \left| -\frac{\partial^2 \ell}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^T} \left(\psi, \phi, \hat{\boldsymbol{\beta}}_\psi\right) \right|^{-1/2} + \mathcal{O}\left(n^{-1}\right),$$

with $\ell(\psi, \phi, \boldsymbol{\beta}) = \log \mathcal{L}(\psi, \phi, \boldsymbol{\beta})$. As $\left| -\partial^2 \ell / \partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^T \left(\psi, \phi, \hat{\boldsymbol{\beta}}_\psi\right) \right| = \left| \boldsymbol{X}_\psi^T \boldsymbol{W} \boldsymbol{X}_\psi \right|$, we get

$$p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}) = \mathcal{L}_p(\psi)(2\pi)^p \left| \boldsymbol{X}_\psi^T \boldsymbol{W} \boldsymbol{X}_\psi \right|^{-1/2} I(\psi \in \Psi)/p(\boldsymbol{y}) + \mathcal{O}\left(n^{-1}\right).$$

With this, the prevalent Bayesian threshold estimator in the literature is the posterior mean $\hat{\psi}_{nB} = \int\limits_{\Psi^*} \psi p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}) d\psi$. Comparing $p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ with $\mathcal{L}_p(\psi)$, we note that they differ by a term proportional to $\left| \boldsymbol{X}_\psi^T \boldsymbol{W} \boldsymbol{X}_\psi \right|^{-1/2}$. In the case of Gaussian observations, $\boldsymbol{W} = \boldsymbol{I}_n/\sigma^2$. Since $\left| \boldsymbol{X}_\psi^T \boldsymbol{W} \boldsymbol{X}_\psi \right| = \left| \boldsymbol{X}_1^T \boldsymbol{W} \boldsymbol{X}_1 \right| \cdot \left| \boldsymbol{X}_2^T \boldsymbol{W} \boldsymbol{X}_2 \right| \to 0$ for $\mathrm{d}(\psi) \to 0$, $p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ becomes very large for ψ close to the boundary of Ψ. Moreover, as the profile likelihood function requires $\mathrm{d}(\psi) \geq 1$ to be well-defined, so does the calculation of the posterior density. Again, the only solution in the literature is to restrict the parameter space Ψ (which in our Bayesian framework is equivalent to working with a uniform prior $\psi \sim U[\Psi^*]$ instead of $\psi \sim U[\Psi]$). In this case, however, $p_{nB}(\psi|\phi, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$ becomes largest exactly for values of ψ which are arbitrarily included or excluded from Ψ^* by varying c. Consequently, expanding or reducing Ψ^* critically affects the Bayesian threshold estimate, whether it is calculated as the posterior mode, mean or median. The middle plot in Fig. 1 illustrates this problem.

4 The regularized Bayesian estimator

When rethinking the threshold estimator, there are good arguments for continuing to pursue Bayesian options. In general, Bayesian estimators naturally incorporate the variability of nuisance parameters and there are reasons to expect them to be (at least asymptotically) the most efficient estimators, as discussed in Section 3.2. Our idea now is to exploit understanding of when reliable estimation becomes particularly difficult in order to regularize the posterior density. We observe that both profile likelihood and posterior density become increasingly distorted as ψ approaches the boundary of Ψ (or the farther it is away from the true threshold ψ_0). Using the notation introduced in Section 2, we define

$$\boldsymbol{\eta} = \boldsymbol{X}_1\boldsymbol{\beta}_1 + \boldsymbol{X}_2\boldsymbol{\beta}_2 = (\boldsymbol{X}_1 + \boldsymbol{X}_2)\boldsymbol{\beta}_1 + \boldsymbol{X}_2(\boldsymbol{\beta}_2 - \boldsymbol{\beta}_1) = \boldsymbol{X}\boldsymbol{\beta}_1 + \boldsymbol{X}_2\boldsymbol{\delta}. \tag{7}$$

While maintaining a non-informative constant prior for $\boldsymbol{\beta}_1$, we pick a normal prior with zero mean for $\boldsymbol{\delta}$, $\boldsymbol{\delta} \sim \mathcal{N}(0, \sigma_\delta^2 \boldsymbol{I}_p)$. When σ_δ^2 tends towards infinity, this prior becomes non-informative. However, for small values σ_δ^2, we introduce prior knowledge suggesting that $\boldsymbol{\delta}$ takes values close to zero. The most important characteristic of this new choice of priors is that it regularizes the posterior density for ψ close to the boundary of Ψ. Putting priors on σ_δ^2 (e.g. an inverse Gamma distribution) and ψ specifies a full Bayesian model and allows for estimation with Markov chain Monte Carlo techniques.

Alternatively, we suggest to use a Laplace approximation to get the approximate posterior $p(\psi|\phi, \sigma_\delta^2, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q})$. This accelerates estimation and enables us to illustrate the regularizing effect. To evaluate the posterior density

$$p(\psi|\phi, \sigma_\delta^2, \boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}) = \frac{p(\psi|\boldsymbol{q})}{p(\boldsymbol{y}|\phi, \sigma_\delta^2, \boldsymbol{X}, \boldsymbol{q})} \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} p(\boldsymbol{y}|\boldsymbol{\beta}_1, \boldsymbol{\delta}, \psi, \phi, \sigma_\delta^2, \boldsymbol{X}, \boldsymbol{q}) p(\boldsymbol{\delta}|\sigma_\delta^2) d\boldsymbol{\delta} d\boldsymbol{\beta}_1,$$

we use a Laplace approximation and follow a line of reasoning closely resembling Breslow

and Clayton (1993) to obtain

$$\begin{aligned}
&\int_{\mathbb{R}^p}\int_{\mathbb{R}^p} p(\boldsymbol{y}|\boldsymbol{\beta}_1,\boldsymbol{\delta},\psi,\phi,\sigma_\delta^2,\boldsymbol{X},\boldsymbol{q})p(\boldsymbol{\delta}|\sigma_\delta^2)d\boldsymbol{\delta}d\boldsymbol{\beta}_1 \\
&\qquad = (2\pi)^{p/2}\exp\left\{-\frac{1}{2}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)^T\boldsymbol{V}^{-1}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)+\sum_{i=1}^n c(y_i,\phi)\right\} \\
&\qquad\qquad \cdot\left|\sigma_\delta^2\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2+\boldsymbol{I}_p\right|^{-1/2}\left|\boldsymbol{X}^T\boldsymbol{V}^{-1}\boldsymbol{X}\right|^{-1/2}+\mathcal{O}\left(n^{-1}\right),
\end{aligned} \tag{8}$$

with the working variable $\tilde{\boldsymbol{z}}$ defined as $\tilde{\boldsymbol{z}}=\boldsymbol{X}\hat{\boldsymbol{\beta}}_1+\boldsymbol{X}_2\hat{\boldsymbol{\delta}}+\boldsymbol{G}(\boldsymbol{y}-\boldsymbol{\mu})$, $\boldsymbol{G}=\operatorname{diag}\{g'(\mu_i)\}$, and $\boldsymbol{V}=\boldsymbol{W}^{-1}+\sigma_\delta^2\boldsymbol{X}_2\boldsymbol{X}_2^T$ for $\boldsymbol{W}^{-1}=\operatorname{diag}\{\phi b''(\theta_i)g'(\mu_i)^2\}$. Here, $\boldsymbol{\mu}$, $\boldsymbol{G}$, $\boldsymbol{W}$ and $\boldsymbol{V}$ are evaluated at the (approximate) posterior mode $(\hat{\boldsymbol{\beta}}_1,\hat{\boldsymbol{\delta}})=\arg\max_{(\boldsymbol{\beta}_1,\boldsymbol{\delta})\in\mathbb{R}^{2p}} p(\boldsymbol{\beta}_1,\boldsymbol{\delta}|\psi,\phi,\sigma_\delta^2,\boldsymbol{y},\boldsymbol{X},\boldsymbol{q})$, that is, $\hat{\boldsymbol{\beta}}_1=(\boldsymbol{X}^T\boldsymbol{V}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{V}^{-1}\tilde{\boldsymbol{z}}$ and $\hat{\boldsymbol{\delta}}=\sigma_\delta^2\boldsymbol{X}_2^T\boldsymbol{V}^{-1}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)$. Details on the derivation of (8) are provided in the appendix. In contrast to the posterior based on non-informative priors, the term $|\boldsymbol{X}_\psi^T\boldsymbol{W}\boldsymbol{X}_\psi|$ disappears, and with it the deteriorations near the boundary of Ψ observed for $p_{nB}(\psi|\phi,\boldsymbol{y},\boldsymbol{X},\boldsymbol{q})$. Moreover, $p(\psi|\phi,\sigma_\delta^2,\boldsymbol{y},\boldsymbol{X},\boldsymbol{q})$ is well-defined for all $\psi\in\Psi$, independent of $\mathrm{d}(\psi)$. It is easy to see that $\hat{\boldsymbol{\delta}}\to 0$ and $\hat{\boldsymbol{\beta}}_1\to(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}\tilde{\boldsymbol{z}}$ at the boundary of Ψ, for $\boldsymbol{X}_2=0$ or $\boldsymbol{X}_2=\boldsymbol{X}$. We do not encounter the ill-posed problem of estimating p nuisance parameters from $m<p$ observations, or calculating $\hat{\boldsymbol{\beta}}_\psi$ when $\mathrm{d}(\psi)<1$, as in profile likelihood or non-informative Bayesian estimation. Consequently, there is no need to subjectively restrict the parameter space. Considering

$$\hat{\boldsymbol{\delta}}=\sigma_\delta^2\boldsymbol{X}_2^T\boldsymbol{V}^{-1}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)=\arg\min_{\boldsymbol{\delta}\in\mathbb{R}^p}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1-\boldsymbol{X}_2\boldsymbol{\delta})^T\boldsymbol{W}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1-\boldsymbol{X}_2\boldsymbol{\delta})+\frac{1}{\sigma_\delta^2}\boldsymbol{\delta}^T\boldsymbol{\delta}, \tag{9}$$

it becomes evident that the proposed prior leads to the strategy of turning an ill-posed into a well-posed problem tracing back to Tikhonov et al. (1977). For small values of the regularization parameter $1/\sigma_\delta^2$, the first term of the functional to be minimized in (9) will drive the resulting $\hat{\boldsymbol{\delta}}$, for large values it is the latter. For the nuisance parameter estimates $\hat{\boldsymbol{\beta}}_1$ and $\hat{\boldsymbol{\beta}}_2=\hat{\boldsymbol{\beta}}_1+\hat{\boldsymbol{\delta}}$, basic matrix algebra reveals that $\hat{\boldsymbol{\beta}}_1\to(\boldsymbol{X}_1^T\boldsymbol{W}\boldsymbol{X}_1)^{-1}\boldsymbol{X}_1^T\boldsymbol{W}\tilde{\boldsymbol{z}}$ and $\hat{\boldsymbol{\beta}}_2\to(\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^T\boldsymbol{W}\tilde{\boldsymbol{z}}$ for $\sigma_\delta^2\to\infty$, while for $\sigma_\delta^2\to 0$, both $\hat{\boldsymbol{\beta}}_1$ and $\hat{\boldsymbol{\beta}}_2$ converge to

$(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}\tilde{\boldsymbol{z}}$.

Clearly, the choice of the regularization parameter σ_δ^2 is essential to any estimate based on $p(\psi|\phi,\sigma_\delta^2,\boldsymbol{y},\boldsymbol{X},\boldsymbol{q})$. It can naturally be estimated in the full Bayesian framework. However, pursuing our approximate approach further we rather make use of the empirical Bayes paradigm. In general, the empirical Bayes approach to modeling observations $\boldsymbol{y}$ differs from the usual Bayesian setup in that the hyperparameters for the highest level in the model's hierarchy are replaced by their maximum likelihood estimates. In our case, we obtain $\hat{\sigma}_\delta^2$ for fixed $\boldsymbol{X}$, $\boldsymbol{q}$ and ψ by maximizing

$$p(\boldsymbol{y}|\psi,\phi,\sigma_\delta^2,\boldsymbol{X},\boldsymbol{q}) = \int\limits_{\mathbb{R}^p}\int\limits_{\mathbb{R}^p} p(\boldsymbol{y}|\boldsymbol{\beta}_1,\boldsymbol{\delta},\psi,\phi,\sigma_\delta^2,\boldsymbol{X},\boldsymbol{q})p(\boldsymbol{\delta}|\sigma_\delta^2)d\boldsymbol{\delta}d\boldsymbol{\beta}_1,$$

so as to base threshold estimation on

$$p_{rB}(\psi|\boldsymbol{y},\boldsymbol{X},\boldsymbol{q}) = p(\psi|\boldsymbol{y},\boldsymbol{X},\boldsymbol{q},\hat{\phi}_\psi,\hat{\sigma}_\delta^2) \propto \left|\hat{\sigma}_\delta^2\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2+\boldsymbol{I}_p\right|^{-1/2}\left|\boldsymbol{X}^T\hat{\boldsymbol{V}}^{-1}\boldsymbol{X}\right|^{-1/2}$$
$$\cdot\exp\left\{-\frac{1}{2}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)^T\hat{\boldsymbol{V}}^{-1}(\tilde{\boldsymbol{z}}-\boldsymbol{X}\hat{\boldsymbol{\beta}}_1)+\sum_{i=1}^n c\left(y_i,\hat{\phi}_\psi\right)\right\} I(\psi\in\Psi),$$

with $\hat{\boldsymbol{V}}$ evaluated at $\hat{\sigma}_\delta^2$. The right plot in Fig. 1 shows log of this posterior density for a sample run corresponding to the simulation setting 1 C of Section 6. It is clearly well-defined over the whole domain of the threshold and its values are regularized at the boundary regions, making the extremum more pronounced.

Once the posterior density is obtained, one can calculate $\hat{\psi}_{rB}$. We observed that in the critical small-sample settings the posterior density is often characterized by multiple modes. Thus, an estimate based on maximization (the posterior mode) is likely to suffer from this. The posterior mean presents a more robust alternative. However, when the true threshold is located close to the boundary of Ψ, the posterior distribution is skewed towards this boundary. As a result, the posterior mean tends to be drawn towards the middle of Ψ (Doodson, 1917; Kendall, 1943, page 35). Hence, we opt for the posterior median as a compromise between the latter two. Accordingly, we suggest to calculate a

regularized Bayesian threshold estimator $\hat{\psi}_{rB}$ as

$$\int_{q_{(1)}}^{\hat{\psi}_{rB}} p_{rB}(\psi|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}, \phi)d\psi = 0.5$$

assuming a prior $p(\psi|\boldsymbol{q}) \propto I(\psi \in \Psi)$ for ψ.

By definition, the restricted (or residual) likelihood function (Harville, 1977) of a generalized linear mixed model is the approximate posterior (8). Hence, the function `glmmPQL` in the R-package *MASS* readily provides us with the desired estimate $\hat{\sigma}^2_\delta$. Moreover, the function simultaneously produces an estimate $\hat{\phi}_\psi$. For the Gaussian case, we can employ the function `lme` directly (with its parameter `method` left at the default value `REML`). It is part of the R-package *nlme*. This possibility to take advantage of existing functions implemented for mixed models greatly facilitates computation of our proposed estimator, which can be performed in seconds.

5 Inference about the threshold parameter

In our Bayesian framework it is natural to form confidence regions for ψ as credible sets; an equi-tailed credible set C of level $1 - 2\alpha$ is defined as

$$C = \int_{q_p(\alpha)}^{q_p(1-\alpha)} p(\psi|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}, \phi)d\psi, \qquad q_p(\alpha) = \inf_{x \in \Psi} \left\{ x \Big| \int_{\psi \leq x} p(\psi|\boldsymbol{y}, \boldsymbol{X}, \boldsymbol{q}, \phi)d\psi \geq \alpha \right\}.$$

These credible sets are valid for change-point and threshold models, both continuous and discontinuous. In the frequentist framework it is straightforward to obtain confidence intervals for continuous models. For discontinuous models the asymptotic distribution does not readily provide a feasible way to construct confidence intervals as it depends on (a possibly large number of) nuisance parameters. As a strategy to circumvent this problem, it has been suggested to base asymptotic developments on the assumption of a diminishing difference in coefficients between regimes, that is, to work with $\boldsymbol{\delta} = \boldsymbol{\delta}(n)$ and $\boldsymbol{\delta}(n) \to 0$ as $n \to \infty$ (Hansen, 2000). However, this approach has only been applied in

the context of models with piecewise linear mean so far. To the best of our knowledge there does not exist previous work on confidence sets for the threshold parameter in discontinuous generalized threshold regression models with a non-identity link.

To test for a threshold effect, a natural approach is to take advantage of the link to generalized linear mixed models. Understanding a threshold effect as the presence of a random effect $\boldsymbol{\delta}$ allows us to draw on existing methods for mixed models, more explicitly, on tests for a zero random effect variance $\sigma_\delta^2 = 0$. For the Gaussian case of a linear mixed model, this theory has been developed by Crainiceanu and Ruppert (2004) and Scheipl et al. (2008), who also implemented the approach in the R package `RLRsim`. An extension to generalized linear mixed models might possibly provide the basis for a unified test in generalized threshold regression models. Yet, it is beyond the scope of this paper to pursue this thought further.

6 Simulations

To assess the performance of the suggested estimator $\hat{\psi}_{rB}$ we performed a simulation study. We report results for eight different settings, covering both situations in which common estimators produce reliable results and others in which they are prone to be distorted. The difference between setting 1 and setting 2 is in the conditional distribution of y_i: in the first case, $y_i|\boldsymbol{X}_i^T, q_i$ is normally distributed, in the second case it follows a Poisson distribution. The design matrix $\boldsymbol{X}$ is random, each entry $x_{ij} \sim U[0,1]$ for setting 1, $x_{ij} \sim U[0, 0.01]$ for setting 2. The transition variable follows a uniform distribution $q_i \sim U[0,1]$. As this implies $\text{pr}\{\text{d}(\psi_0) < 1\} \approx 0.46$ for setting C, we base our simulations on a fixed sample of transition variables $q_i = i/n$, $i = 1, \ldots, n$. This way, we ensure that $\text{d}(\psi_0) = 1$, hence, that $\mathcal{L}_p(\psi_0)$ is always well-defined. While settings A and B differ from setting C in the threshold ($\psi_0 = 0.5$ for A and B; $\psi_0 = 0.3$ for C), setting A is distinct from settings B and C in the signal-to-noise-ratio, which we control by the choice

	Normal response (1)			
	A	B	C	D
ψ_0	0.5	0.5	0.3	0.3
$\boldsymbol{\delta}$	$U[-0.5, 0.5]$	$U[-0.5, 0.5]$	$U[-0.5, 0.5]$	$U[-0.25, 0.25]$
$\text{var}(y_i)$	0.75^2	1.5^2	1.5^2	0.25^2
x_{ij}	$U[0, 1]$	$U[0, 1]$	$U[0, 1]$	$U[0, 1]$
p	30	30	30	10
	Poisson response (2)			
	A	B	C	D
ψ_0	0.5	0.5	0.3	0.3
$\boldsymbol{\delta}$	$U[10, 20]$	$U[0, 10]$	$U[0, 10]$	$U[10, 20]$
x_{ij}	$U[0, 0.01]$	$U[0, 0.01]$	$U[0, 0.01]$	$U[0, 0.01]$
p	30	30	30	10

Table 1: Differences between simulation settings.

of $\boldsymbol{\delta} = \boldsymbol{\beta}_2 - \boldsymbol{\beta}_1$ relative to the variance of the observations. For setting 1 A – C, the difference $\boldsymbol{\delta} \sim U[-0.5, 0.5]$ and random variables are simulated with variances $\text{var}(y_i) = 0.75^2$ (setting A) and $\text{var}(y_i) = 1.5^2$ (settings B and C). For setting 2 A the difference $\boldsymbol{\delta} \sim U[10, 20]$, whereas $\boldsymbol{\delta} \sim U[0, 10]$ for settings 2 B and C. Setting D features less nuisance parameters than A – C; $p = \dim(\boldsymbol{\beta}_1) = \dim(\boldsymbol{\beta}_2) = 10$ for D, $p = 30$ for A – C. The sample size is $n = 100$. Table 1 sums up differences between settings. Regression coefficients $\boldsymbol{\beta}_1$ are drawn from a Poisson distribution with mean 10. To be unambiguous, parameters $\boldsymbol{\delta}$ and $\boldsymbol{\beta}_1$ are fixed; we randomly generate them once at the beginning of the simulation according to the distributions specified. Our Monte Carlo sample contains 1000 replications.

All three estimators $\hat{\psi}_{pL}$, $\hat{\psi}_{nB}$ and $\hat{\psi}_{rB}$ perform well given a high signal-to-noise-ratio and ψ_0 in the middle of Ψ (setting A). Lowering the signal-to-noise-ratio (setting B) alters the results: we observe nearly unbiased estimates $\hat{\psi}_{pL}$, $\hat{\psi}_{nB}$ and $\hat{\psi}_{rB}$, but due to its very small variance the latter stands out by its small mean square error. When we shift the true threshold towards the boundary of Ψ (setting C), $\hat{\psi}_{rB}$ clearly outperforms both $\hat{\psi}_{pL}$ and

		bias			mean square error		
Setting	ψ_0	$\hat{\psi}_{pL}$	$\hat{\psi}_{nB}$	$\hat{\psi}_{rB}$	$\hat{\psi}_{pL}$	$\hat{\psi}_{nB}$	$\hat{\psi}_{rB}$
1 A	0.5	-0.002	0.001	0.000	0.002	0.009	0.000
		(0.045)	(0.095)	(0.000)			
1 B	0.5	-0.003	-0.001	-0.001	0.010	0.023	0.006
		(0.100)	(0.152)	(0.077)			
1 C	0.3	0.110	0.087	0.031	0.024	0.024	0.008
		(0.110)	(0.126)	(0.084)			
1 D	0.3	0.064	0.080	0.059	0.036	0.066	0.017
		(0.032)	(0.060)	(0.014)			
2 A	0.5	0.001	0.026	0.000	0.000	0.001	0.000
		(0.000)	(0.000)	(0.000)			
2 B	0.5	0.004	−0.111	−0.004	0.003	0.029	0.001
		(0.055)	(0.126)	(0.032)			
2 C	0.3	0.054	0.049	−0.002	0.007	0.010	0.001
		(0.071)	(0.089)	(0.032)			
2 D	0.3	0.025	-0.045	0.015	0.013	0.032	0.003
		(0.013)	(0.030)	(0.003)			

Table 2: Simulation results. Standard errors are reported in parentheses below the bias.

$\hat{\psi}_{nB}$ in terms of mean square error, bias and variance. The differences in bias, variance and mean squared error are more pronounced with a greater number of nuisance parameters p, but still visible in simulations with smaller ratio p/n (setting D). Results are summarized in Fig. 3 and Table 2. The effects of increasing the signal-to-noise-ratio and shifting ψ_0 on $\ell_p(\psi)$ are illustrated in Fig. 2. The mode of $\ell_p(\psi)$ is less pronounced in setting 1B than in 1A. Further, the number of local maxima rises and they become more distinctive as we move to setting 1B and then to 1C.

7 Applications

This work is originally motivated by the application of threshold vector error correction models in price transmission analysis. Such models are rather involved and we refer to

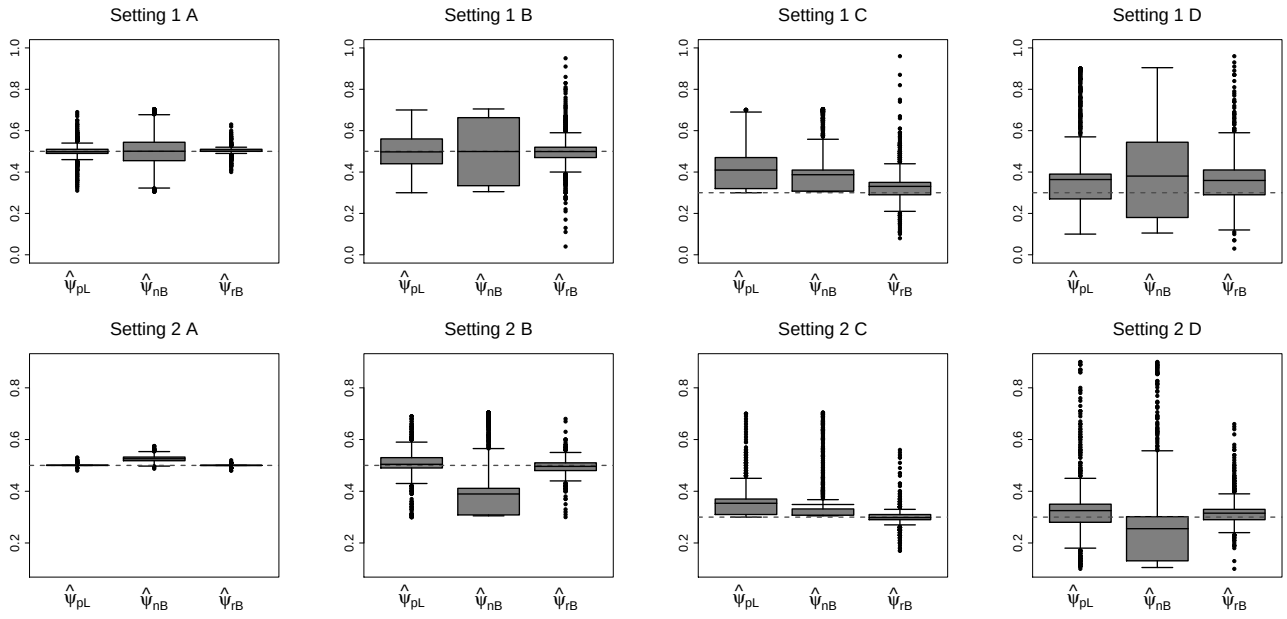

Figure 3: Boxplots for different estimators and selected simulations. Dashed lines indicate the true threshold ψ_0, black lines in the boxes are sample means.

Greb et al. (2011) for more details and two more real data examples using our regularized Bayesian estimator.

7.1 Cross-country growth behavior

As another application of the regularized Bayesian threshold estimator, we consider the case of economic growth modeling. Durlauf and Johnson (1995) estimate a standard growth model using cross-sectional data on a sample of 96 countries and investigate whether the coefficients of this model differ across sub-sets of countries depending on their initial conditions. Their analysis is based on the so-called regression tree methodology (Breiman et al., 1984), which suggests three thresholds based on two different transition variables for this application. Hansen (2000) revisits their paper. Using the Durlauf and Johnson data he estimates a regression

$$\log(GDP)_{i,1985} - \log(GDP)_{i,1960}$$
$$= \zeta + \beta \log(GDP)_{i,1960} + \pi_1 \log(INV)_i + \pi_2 \log(n_i + g + \delta) + \pi_3 \log(SCHOOL)_i + \varepsilon_i$$

which explains real GDP growth between 1960 and 1985 in country i, $\log(GDP)_{i,1985} - \log(GDP)_{i,1960}$, using real GDP in 1960 $GDP_{i,1960}$, the investment to GDP ratio INV_i, the growth rate of the working-age population n_i, the rate of technological change g, the rate of depreciation of physical and human capital stocks δ, and the fraction of working-age population enrolled in secondary school $(SCHOOL)_i$. With reference to Durlauf and Johnson (1995), he sets $g + \delta = 0.05$. He tests for a threshold effect based on either one of transition variables they propose. He only finds evidence based on the transition variable $\log(GDP)_{i,1960}$ and calculates the profile likelihood (or, equivalently, least squares) estimate as $\hat{\psi}_{pL} = 6.76$ together with an asymptotic 95% confidence interval $[6.39, 7.49]$. This corresponds to an estimate of \$863 per capita GDP in 1960 with an associated confidence interval of [\$594, \$1794]. Hansen (2000) acknowledges that while the confidence interval seems rather tight (given observations for $GDP_{i,1960}$ ranging from \$383 to \$12362), it effectively contains 40 of the 96 countries in the sample. This is in line with the number of local maxima in the profile likelihood function which hints at the uncertainty inherent in this method (Fig. 4). In addition, the fact that $\hat{\psi}_{pL}$ leaves only 18 observations in the first regime gives rise to concern that the threshold might be located close to the boundary of Ψ. We know that the profile likelihood is typically distorted if this is the case.

Hence, we reestimate the model with the regularized Bayesian estimator. The latter depends on the parameterization of the transition variable. As $\log(GDP)_{i,1960}$ is an explanatory variable, we choose the parameterization $q_i = \log(GDP)_{i,1960}$. Figure 4 shows that the resulting posterior density differs considerably from the profile likelihood function and that the location of the maximum shifts. This is not surprising given the deformations often observed for the profile likelihood function close to the boundary of the threshold parameter space. The posterior median is located at $\hat{\psi}_{rB} = 7.37$ compared with Hansen's (2000) $\hat{\psi}_{pL} = 6.76$. It implies that for the 43 poorest countries coefficients

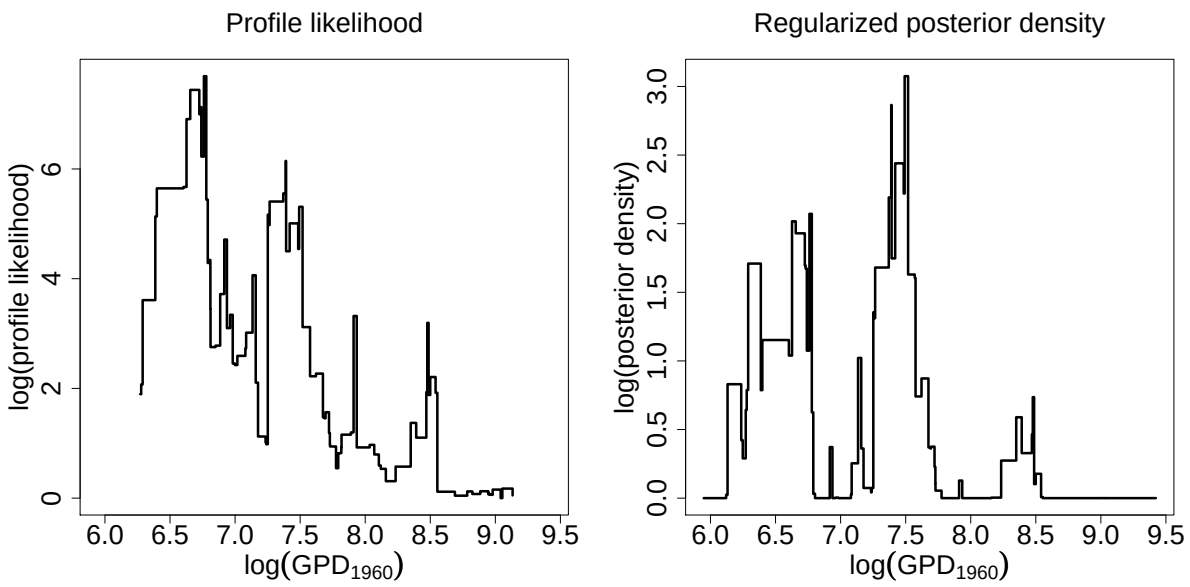

Figure 4: Profile likelihood and regularized posterior density for a threshold based on the transition variable $q_i = \log(GDP)_{i,1960}$.

for the growth model are distinct from the rest, whereas the profile likelihood estimate implicates that this is only the case for the poorest 18 countries. While it is not possible to state conclusively that the regularized Bayesian estimate is more appropriate from an economic perspective, the shapes of the likelihoods in Fig. 4 and the fact that the profile likelihood estimate is near the boundary of its domain suggests that the latter may be distorted by the weaknesses of the profile likelihood method discussed above.

Comparing profile likelihood estimates for the regression coefficients with their regularized Bayesian counterparts, we note that there is much less difference between regimes according to regularized Bayesian than profile likelihood estimates (see table 7.1). The difference between the two regimes as estimated within the regularized Bayesian framework is negligible. This is in line with Hansen's (2000) finding that the null hypothesis of no threshold is not rejected at the 5%-level (Hansen, 2000, page 587). The example demonstrates the effect of using the suggested regularized Bayesian estimator instead of the profile likelihood estimator in small samples with a multi-modal profile likelihood and high uncertainty attached to the estimate $\hat{\psi}_{pL}$ obtained by maximizing it.

	1st regime					2nd regime				
	$\hat{\zeta}$	$\hat{\beta}$	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$	$\hat{\zeta}$	$\hat{\beta}$	$\hat{\pi}_1$	$\hat{\pi}_2$	$\hat{\pi}_3$
pL	4.31	-0.66	0.23	-0.29	0.02	3.66	-0.32	0.50	-0.49	0.36
	(3.21)	(0.33)	(0.14)	(0.92)	(0.11)	(0.85)	(0.07)	(0.11)	(0.30)	(0.07)
rB	3.36	-0.41	0.47	-0.60	0.22	3.37	-0.38	0.47	-0.62	0.20
	(0.85)	(0.08)	(0.09)	(0.28)	(0.06)	(0.85)	(0.07)	(0.09)	(0.28)	(0.07)

Table 3: Regressions coefficient estimates. "pL" refers to the profile likelihood, "rB" to the regularized Bayesian framework. Standard errors in parentheses below the estimates.

7.2 Effects of climate on snowshoe hare survival

In addition, we study a famous dataset of snowshoe hare abundance in the main drainage of Hudson Bay in Canada. It consists of annual observations starting in the 19th century. A preeminent feature of the data is cyclical fluctuations in the hare population, see Fig. 5. These have been ascribed to the predator-prey relationship between lynx and snowshoe hares. Samia and Chan (2011) highlight selected references and further investigate one strand of the discussion focusing on the effect of snow conditions on hunting efficiency in different phases of the cylce. To this end, they estimate a generalized threshold regression model with the hare count y_t as a Poisson distributed response whose mean is related to the explanatory variables via a log-link,

$$\log(\mu_t) = \beta_0 + \beta_1 D_t + \begin{cases} \sum_{i=1}^{3} \beta_{1,i} \log(y_{t-i}+1) + \beta_{1,4} w_{t-1} & y_{t-d} \leq \psi, \\ \sum_{i=1}^{3} \beta_{2,i} \log(y_{t-i}+1) + \beta_{2,4} w_{t-1} & y_{t-d} > \psi \end{cases}$$

for the years $t = 1844, \ldots, 1904$. Apart from the regression coefficients and the threshold, the delay of the transition variable d is included as an additional parameter, $d \in \{1, 2, 3\}$. As the count for the year $t = 1863$ is considered an outlier, the model contains a dummy variable $D_t = I(t = 1863)$. The covariate w_t denotes the detrended annual winter climate index of the North Atlantic Oscillation. We follow them in estimating this model. Our analysis is based on the series of hare abundance initially presented graphically by MacLulich (1937) which we calibrate with data available online; it is included in the sup-

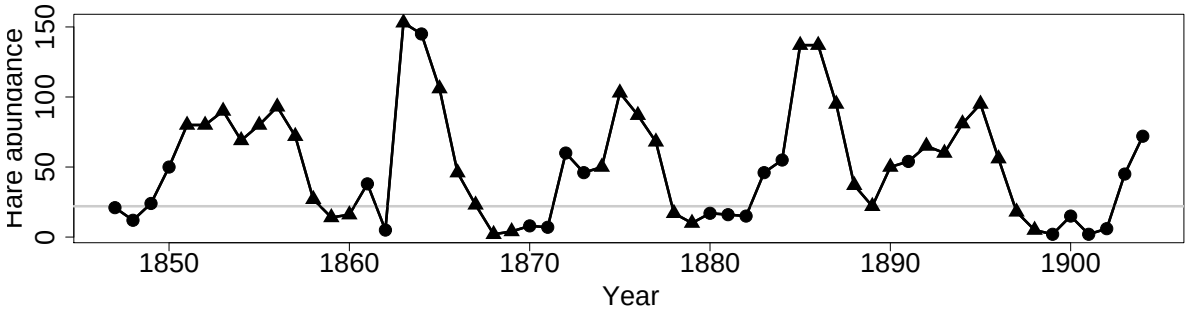

Figure 5: Annual hare abundance. Observations estimated to belong to the lower regime are plotted as dots, observations estimated to belong to the upper regime as triangles. The horizontal grey line indicates the location of the estimated threshold, $\hat{\psi}_{rB} = 22$.

plementary material to this paper. We further use the North Atlantic Oscillation index published at www.cru.uea.ac.uk/cru/data/nao.

The series of 61 observations is rather short and maximizing out regression coefficients leaves us with a profile likelihood function for (d, ψ) which is characterized by various local maxima; it is displayed in the upper row of Fig. 6 for $d = 1, 2, 3$ and $\psi \in \Psi^*(1)$. In addition, we cannot rule out overdispersion. Hence, we are confronted with a setting in which the regularized Bayesian estimate can be more reliable than the profile likelihood estimate. This becomes evident in the second row of Fig. 6, which shows the posterior densities for ψ corresponding to $d = 1, 2, 3$. While we obtain a profile likelihood estimate $(\hat{d}_{pL}, \hat{\psi}_{pL}) = (3, 55)$, the regularized Bayesian estimator yields $(\hat{d}_{rB}, \hat{\psi}_{rB}) = (2, 22)$ with $\hat{d}_{rB}$ calculated as the posterior median based on a flat prior on $\{1, 2, 3\}$.

When referring to Samia and Chan (2011) we have to keep in mind that their results diverge slightly from ours and are not directly comparable as we were not able to obtain the data they used. Yet, their profile likelihood estimate is still very close, $(\hat{d}_{pL}, \hat{\psi}_{pL}) = (3, 69)$. However, they discard this estimate in favor of $(\hat{d}, \hat{\psi}) = (2, 25)$, giving heuristic arguments based on residual analysis. The latter also allows for a very plausible interpretation. Apparently, our regularized Bayesian estimate $(\hat{d}_{rB}, \hat{\psi}_{rB}) = (2, 22)$ is close to the preferred estimate in Samia and Chan (2011). In fact, the difference in estimated thresholds only

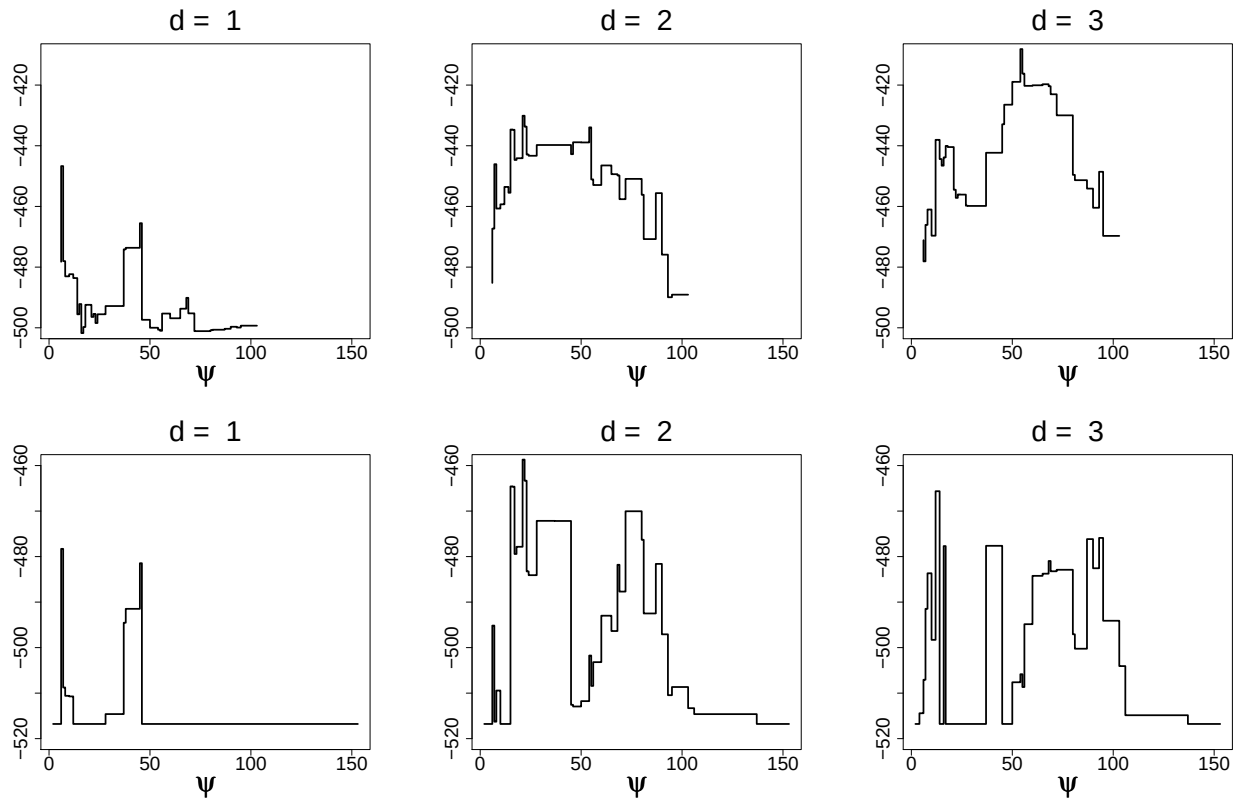

Figure 6: Log-likelihood functions (upper row) and log-posterior densities (lower row) for different delays of the transition variable.

has implications for a single observation ($t = 1869$). Except for this, thresholds induce identical allocations of observations to regimes (in the respective datasets), as is clearly visible when comparing our Fig. 5 with Fig. 1 in Samia and Chan (2011). Hence, the regularized Bayesian estimator enables us to attain a meaningful estimate directly avoiding any arbitrary modification of the suggested estimation method as done by Samia and Chan (2011). Coefficient estimates are similar in both modeling frameworks.

8 Conclusions

In this work we describe settings in which estimation of generalized threshold regression models can be problematic. We suggest a new regularized Bayesian estimator which outperforms standard estimators. In particular, the suggested threshold estimator is defined on the whole parameter space and thus circumvents the subjective and often misleading

restriction of the threshold domain which standard estimators require. Moreover, regularizing the posterior density at the boundary of its domain helps to improve estimation, especially if the true threshold is close to this boundary. Employing the empirical Bayes approach, we can use built-in functions for generalized linear mixed models in statistics software and obtain estimates with little additional numerical effort and without the use of Markov chain Monte Carlo or other sampling techniques. Inference about the estimated parameter can be carried out in the standard Bayesian manner. Simulation studies and a real-data example confirm the effectiveness and relevance of our method.

Acknowledgments

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Appendix

Derivation of equations (4) – (6)

We first approximate the profile likelihood,

$$\begin{aligned}-\ell_p(\psi) \propto -\frac{1}{\hat{\phi}_\psi}\sum_{i=1}^{n} y_i\hat{\theta}_i - b(\hat{\theta}_i) \approx \frac{1}{2}\sum_{i=1}^{n}\frac{(y_i-\hat{\mu}_i)^2}{\hat{\phi}_\psi b''(\hat{\theta}_i)} = \frac{1}{2}\sum_{i=1}^{n}\frac{\{\hat{z}_i - (\boldsymbol{X}_\psi)_i\hat{\boldsymbol{\beta}}_\psi\}^2}{\hat{\phi}_\psi g'(\hat{\mu}_i)^2 b''(\hat{\theta}_i)}\\ =\frac{1}{2}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)^T \widehat{\boldsymbol{W}}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right) \approx \frac{1}{2}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)^T \boldsymbol{W}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)\end{aligned}$$

where

$$\hat{\boldsymbol{z}} = \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi + \widehat{\boldsymbol{G}}\left(\boldsymbol{y}-\hat{\boldsymbol{\mu}}\right),\ \widehat{\boldsymbol{G}} = \operatorname{diag}\left\{g'(\hat{\mu}_i)\right\} \text{ and } \widehat{\boldsymbol{W}} = \operatorname{diag}\left\{\hat{\phi}_\psi b''(\hat{\theta}_i)g'(\hat{\mu}_i)^2\right\}^{-1}.$$

The estimated $\widehat{\boldsymbol{W}}$ for fixed ψ is assumed to vary little or not at all as a function of the mean so we use $\boldsymbol{W}$ evaluated at the true $\boldsymbol{\beta}$ directly. This is a typical assumption in the literature on generalized linear models (e.g. Breslow and Clayton, 1993). We assume the same for $\widehat{\boldsymbol{G}}$.

To compare $\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)^T \boldsymbol{W}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)$ with $(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T \boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})$ for $\boldsymbol{z} = \boldsymbol{X}_\psi\boldsymbol{\beta} + \boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu})$, we then note that

$$\text{bias}\left(\hat{\boldsymbol{\beta}}_\psi\right) = \text{E}\left(\hat{\boldsymbol{\beta}}_\psi\right) - \boldsymbol{\beta} = \left\{0, (\boldsymbol{X}_2'\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_{[\psi,\psi_0]}^T\boldsymbol{W}\boldsymbol{X}_{[\psi,\psi_0]}(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)\right\}^T. \qquad (10)$$

To see this, we approximate $\hat{\boldsymbol{\beta}}_\psi$ via Fisher-scoring as $\hat{\boldsymbol{\beta}}_\psi = \left(\boldsymbol{X}_\psi^T\boldsymbol{W}\boldsymbol{X}_\psi\right)^{-1}\boldsymbol{X}_\psi^T\boldsymbol{W}\hat{\boldsymbol{z}}$, then, exploiting that $\hat{\boldsymbol{z}}$ is the working variable obtained in the last (m-th) iteration, calculate

$$\begin{aligned}
\text{E}(\hat{\boldsymbol{z}}) = \text{E}(\boldsymbol{z}_m) &= \text{E}\left\{\boldsymbol{G}_m(\boldsymbol{y} - \boldsymbol{\mu}_m) + \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m\right\} = \boldsymbol{G}_m(\text{E}(\boldsymbol{y}) - \boldsymbol{\mu}_m) + \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m \\
&= \boldsymbol{G}_m\{h(\boldsymbol{\eta}) - h(\boldsymbol{\eta}_m)\} + \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m \approx \boldsymbol{G}_m\left[\frac{\partial h}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}_m)\left\{\boldsymbol{X}_{\psi_0}\boldsymbol{\beta} - \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m\right\}\right] + \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m \\
&= \boldsymbol{G}_m\boldsymbol{G}_m^{-1}\left\{\boldsymbol{X}_{\psi_0}\boldsymbol{\beta} - \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m\right\} + \boldsymbol{X}_\psi(\boldsymbol{\beta}_\psi)_m \\
&= \boldsymbol{X}_{\psi_0}\boldsymbol{\beta},
\end{aligned}$$

and get

$$\begin{aligned}
E\left(\hat{\boldsymbol{\beta}}_\psi\right) &= (\boldsymbol{X}_\psi^T\boldsymbol{W}\boldsymbol{X}_\psi)^{-1}\boldsymbol{X}_\psi^T\boldsymbol{W}\,\text{E}(\hat{\boldsymbol{z}}) = \begin{Bmatrix}(\boldsymbol{X}_1^T\boldsymbol{W}\boldsymbol{X}_1)^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & (\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\end{Bmatrix}\boldsymbol{X}_\psi^T\boldsymbol{W}\,\text{E}(\hat{\boldsymbol{z}}) \\
&= \begin{Bmatrix}(\boldsymbol{X}_1^T\boldsymbol{W}\boldsymbol{X}_1)^{-1}\boldsymbol{X}_1^T\boldsymbol{W} \\ (\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^T\boldsymbol{W}\end{Bmatrix}\left\{(\boldsymbol{X}_1 + \boldsymbol{X}_{[\psi,\psi_0]})\boldsymbol{\beta}_1 + (\boldsymbol{X}_2 - \boldsymbol{X}_{[\psi,\psi_0]})\boldsymbol{\beta}_2\right\} \\
&= \begin{Bmatrix}\boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 + (\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_{[\psi,\psi_0]}(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)\end{Bmatrix}.
\end{aligned}$$

It is helpful to further keep in mind that

$$\begin{aligned}
\text{E}\,\hat{\boldsymbol{\mu}} &= \text{E}\left\{h\left(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)\right\} \approx \text{E}\left\{h(\boldsymbol{X}_\psi\boldsymbol{\beta}) + \boldsymbol{G}^{-1}\left(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi - \boldsymbol{X}_\psi\boldsymbol{\beta}\right)\right\} \\
&= h(\boldsymbol{X}_\psi\boldsymbol{\beta}) + \boldsymbol{G}^{-1}\boldsymbol{X}_\psi\,\text{E}\left(\hat{\boldsymbol{\beta}}_\psi - \boldsymbol{\beta}\right) = h(\boldsymbol{X}_\psi\boldsymbol{\beta}) + \boldsymbol{G}^{-1}\boldsymbol{X}_\psi\,\text{bias}\,\hat{\boldsymbol{\beta}}_\psi
\end{aligned}$$

and

$$\text{var}\,\hat{\boldsymbol{\mu}} \approx \text{var}\left\{h(\boldsymbol{X}_\psi\boldsymbol{\beta}) + \boldsymbol{G}^{-1}\left(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi - \boldsymbol{X}_\psi\boldsymbol{\beta}\right)\right\} = \left(\boldsymbol{G}^{-1}\right)^2\text{var}\left(\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right),$$

consequently,

$$\hat{\boldsymbol{\mu}} = \text{E}\,\hat{\boldsymbol{\mu}} + \mathcal{O}_p\left(\sqrt{\text{var}\,\hat{\boldsymbol{\mu}}}\right) \approx h(\boldsymbol{X}_\psi\boldsymbol{\beta}) + \boldsymbol{G}^{-1}\boldsymbol{X}_\psi\,\text{bias}\,\hat{\boldsymbol{\beta}}_\psi + \boldsymbol{G}^{-1}\mathcal{O}_p\left(\sqrt{\text{var}\,\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right). \quad (11)$$

We now define $\boldsymbol{H} = \boldsymbol{W}^{1/2}\boldsymbol{X}_2(\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2)^{-1}\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_{[\psi,\psi_0]}$ and use (10) and (11) to obtain

$$
\begin{aligned}
-\ell_p(\psi) &\propto \left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right)^T \boldsymbol{W}\left(\hat{\boldsymbol{z}} - \boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi\right) \\
&\approx (\boldsymbol{y}-\hat{\boldsymbol{\mu}})^T\boldsymbol{G}\boldsymbol{W}\boldsymbol{G}(\boldsymbol{y}-\hat{\boldsymbol{\mu}}) \\
&= \{\boldsymbol{y} - h(\boldsymbol{X}_\psi\boldsymbol{\beta})\}^T\boldsymbol{G}\boldsymbol{W}\boldsymbol{G}\{\boldsymbol{y} - h(\boldsymbol{X}_\psi\boldsymbol{\beta})\} \\
&\qquad + 2\{\boldsymbol{y} - h(\boldsymbol{X}_\psi\boldsymbol{\beta})\}^T\boldsymbol{G}\boldsymbol{W}\boldsymbol{G}\{h(\boldsymbol{X}_\psi\boldsymbol{\beta}) - \hat{\boldsymbol{\mu}}\} + \{h(\boldsymbol{X}_\psi\boldsymbol{\beta}) - \hat{\boldsymbol{\mu}}\}^T\boldsymbol{G}\boldsymbol{W}\boldsymbol{G}\{h(\boldsymbol{X}_\psi\boldsymbol{\beta}) - \hat{\boldsymbol{\mu}}\} \\
&\approx (\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta}) \\
&\qquad - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}\left\{\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi + \mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right)\right\} \\
&\qquad + \left\{\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi + \mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right)\right\}^T\boldsymbol{W}\left\{\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi + \mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right)\right\} \\
&= (\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta}) \\
&\qquad - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}\left\{\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi + \mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right)\right\} \\
&\qquad + \left(\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi\right)^T\boldsymbol{W}\left(\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi\right) + 2\left(\boldsymbol{X}_\psi \operatorname{bias}\hat{\boldsymbol{\beta}}_\psi\right)^T\boldsymbol{W}\mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right) \\
&\qquad + \mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right)^T\boldsymbol{W}\mathcal{O}_p\left(\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right) \\
&= (\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta}) \\
&\qquad + \left\{(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)^T\boldsymbol{H}^T - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}^{1/2}\right\}\boldsymbol{H}(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2) \\
&\qquad + \left\{2(\boldsymbol{\beta}_1 - \boldsymbol{\beta}_2)^T\boldsymbol{H}^T - 2(\boldsymbol{z} - \boldsymbol{X}_\psi\boldsymbol{\beta})^T\boldsymbol{W}^{1/2}\right\}^T\mathcal{O}_p\left(\boldsymbol{W}^{1/2}\sqrt{\operatorname{var}\boldsymbol{X}_\psi\hat{\boldsymbol{\beta}}_\psi}\right) \\
&\qquad + \mathcal{O}_p(2p),
\end{aligned}
$$

Derivation of equation (8)

We obtain the approximate posterior (8) as follows. Laplace approximation produces

$$
\begin{aligned}
&\int_{\mathbb{R}^p}\int_{\mathbb{R}^p} p(\boldsymbol{y}|\boldsymbol{\beta}_1,\boldsymbol{\delta},\psi,\phi,\sigma_\delta^2,\boldsymbol{X},\boldsymbol{q})p(\boldsymbol{\delta}|\sigma_\delta^2)d\boldsymbol{\delta}d\boldsymbol{\beta}_1 \\
&\qquad = (2\pi)^{-p/2}|\sigma_\delta^2\boldsymbol{I}_p|^{-1/2}\int_{\mathbb{R}^p}\int_{\mathbb{R}^p}\exp\{-\kappa(\boldsymbol{\delta},\boldsymbol{\beta}_1)\}\,d\boldsymbol{\delta}d\boldsymbol{\beta}_1 \\
&\qquad = (2\pi)^{p/2}|\sigma_\delta^2\boldsymbol{I}_p|^{-1/2}\exp\left\{-\kappa\left(\hat{\boldsymbol{\delta}},\hat{\boldsymbol{\beta}}_1\right)\right\}\left|\frac{\partial^2\kappa}{\partial(\boldsymbol{\delta},\boldsymbol{\beta}_1)\partial(\boldsymbol{\delta},\boldsymbol{\beta}_1)^T}(\hat{\boldsymbol{\delta}},\hat{\boldsymbol{\beta}}_1)\right|^{-1/2} + \mathcal{O}\left(n^{-1}\right)
\end{aligned}
$$

for $\kappa(\boldsymbol{\delta}, \boldsymbol{\beta}_1) = -\sum_{i=1}^{n} \frac{y_i\theta_i - b(\theta_i)}{\phi} - c(y_i, \phi) + \frac{1}{2\sigma_\delta^2}\boldsymbol{\delta}^T\boldsymbol{\delta}$ and $\left(\hat{\boldsymbol{\delta}}, \hat{\boldsymbol{\beta}}_1\right) = \underset{(\boldsymbol{\delta}, \boldsymbol{\beta}_1) \in \mathbb{R}^{2p}}{\operatorname{argmax}} -\kappa(\boldsymbol{\delta}, \boldsymbol{\beta}_1)$.
Given the derivatives

$$\frac{\partial \kappa}{\partial \boldsymbol{\delta}}(\boldsymbol{\delta}) = -\sum_{i=1}^{n} \frac{(y_i - \mu_i)(\boldsymbol{X}_2)_i}{\phi b''(\theta_i) g'(\mu_i)} + \frac{1}{\sigma_\delta^2}\boldsymbol{\delta} = -\boldsymbol{X}_2^T \boldsymbol{W}\boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu}) + \frac{1}{\sigma_\delta^2}\boldsymbol{\delta},$$

$$\frac{\partial \kappa}{\partial \boldsymbol{\beta}_1}(\boldsymbol{\beta}_1) = -\sum_{i=1}^{n} \frac{(y_i - \mu_i)(\boldsymbol{X})_i}{\phi b''(\theta_i) g'(\mu_i)} = -\boldsymbol{X}^T \boldsymbol{W}\boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu}),$$

and

$$\partial^2 \kappa \Big/ \partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)\partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)^T = \begin{pmatrix} \boldsymbol{X}_2^T \boldsymbol{W}\boldsymbol{X}_2 + (1/\sigma_\delta^2)\, \boldsymbol{I}_p & \boldsymbol{X}_2^T \boldsymbol{W}\boldsymbol{X} \\ \boldsymbol{X}^T \boldsymbol{W}\boldsymbol{X}_2 & \boldsymbol{X}^T \boldsymbol{W}\boldsymbol{X} \end{pmatrix} \tag{12}$$

for $\boldsymbol{W}^{-1} = \operatorname{diag}\{\phi b''(\theta_i) g'(\mu_i)^2\}$ and $\boldsymbol{G} = \operatorname{diag}\{g'(\mu_i)\}$, we obtain

$$\left|\partial^2 \kappa \Big/ \partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)\partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)^T\right| = \left|\boldsymbol{X}_2^T \boldsymbol{W}\boldsymbol{X}_2 + \left(1/\sigma_\delta^2\right) \boldsymbol{I}_p\right| \left|\boldsymbol{X}^T \boldsymbol{V}^{-1} \boldsymbol{X}\right|$$

using basic matrix algebra.

To find $\hat{\boldsymbol{\delta}}$ and $\hat{\boldsymbol{\beta}}_1$, we iteratively solve

$$\boldsymbol{X}_2^T \boldsymbol{W}\boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu}) = \frac{1}{\sigma_\delta^2}\boldsymbol{\delta} \text{ and } \boldsymbol{X}^T \boldsymbol{W}\boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu}) = 0$$

via Fisher-scoring: Starting at $\hat{\boldsymbol{\delta}} = \boldsymbol{\delta}_0$ and $\hat{\boldsymbol{\beta}}_1 = (\boldsymbol{\beta}_1)_0$, we solve

$$\mathcal{I}(\boldsymbol{\delta}_m, \boldsymbol{\beta}_m) \begin{pmatrix} \boldsymbol{\delta}_{m+1} \\ (\boldsymbol{\beta}_1)_{m+1} \end{pmatrix} = \mathcal{I}(\boldsymbol{\delta}_m, \boldsymbol{\beta}_m) \begin{pmatrix} \boldsymbol{\delta}_m \\ (\boldsymbol{\beta}_1)_m \end{pmatrix} + s(\boldsymbol{\delta}_m, (\boldsymbol{\beta}_1)_m),$$

$\mathcal{I} = \partial^2 \kappa \Big/ \partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)\partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)^T$ and $s = -\partial \kappa \Big/ \partial(\boldsymbol{\delta}, \boldsymbol{\beta}_1)$, or, more explicitely,

$$\left\{\boldsymbol{X}_2^T \boldsymbol{W}_m \boldsymbol{X}_2 + \frac{1}{\sigma_\delta^2}\boldsymbol{I}_p\right\}\boldsymbol{\delta}_{m+1} + \boldsymbol{X}_2^T \boldsymbol{W}_m \boldsymbol{X}(\boldsymbol{\beta}_1)_{m+1} = \boldsymbol{X}^T \boldsymbol{W}_m \boldsymbol{z}_m$$

and

$$\boldsymbol{X}^T \boldsymbol{W}_m \boldsymbol{X}_2 \boldsymbol{\delta}_{m+1} + \boldsymbol{X}^T \boldsymbol{W}_m \boldsymbol{X}(\boldsymbol{\beta}_1)_{m+1} = \boldsymbol{X}^T \boldsymbol{W}_m \boldsymbol{z}_m,$$

where $\boldsymbol{z}_m = \boldsymbol{X}_2 \boldsymbol{\delta}_m + \boldsymbol{X}(\boldsymbol{\beta}_1)_m + \boldsymbol{G}_m(\boldsymbol{y} - \boldsymbol{\mu}_m)$. This yields

$$\hat{\boldsymbol{\beta}}_1 = \left(\boldsymbol{X}^T \boldsymbol{V}^{-1} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{V}^{-1} \tilde{\boldsymbol{z}} \quad \text{and} \quad \hat{\boldsymbol{\delta}} = \sigma_\delta^2 \boldsymbol{X}_2^T \boldsymbol{V}^{-1}(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1),$$

where $\boldsymbol{V} = \boldsymbol{W}^{-1} + \sigma_\delta^2 \boldsymbol{X}_2 \boldsymbol{X}_2^T$ and $\tilde{\boldsymbol{z}} = \boldsymbol{X}_2^T \hat{\boldsymbol{\delta}} + \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 + \boldsymbol{G}(\boldsymbol{y} - \boldsymbol{\mu})$, with $\boldsymbol{W}$, $\boldsymbol{G}$ and $\boldsymbol{\mu}$ evaluated at $\boldsymbol{\delta} = \hat{\boldsymbol{\delta}}$ and $\boldsymbol{\beta}_1 = \hat{\boldsymbol{\beta}}_1$ (Harville, 1977).

With this, we can now further simplify the posterior. Following Breslow and Clayton (1993) in replacing

$$-2\sum_{i=1}^{n}\{y_i\theta_i - b(\theta_i)\} \quad \text{by the chi-squared statistic} \quad \sum_{i=1}^{n}\frac{(y_i-\mu_i)^2}{b''(\theta_i)}$$

we can exploit the identity

$$\boldsymbol{V}^{-1}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right) = \boldsymbol{W}\left(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 - \boldsymbol{X}_2\hat{\boldsymbol{\delta}}\right),$$

which results in

$$\left(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 - \boldsymbol{X}_2\hat{\boldsymbol{\delta}}\right)^T \boldsymbol{W}\left(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 - \boldsymbol{X}_2\hat{\boldsymbol{\delta}}\right) = \left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right)^T \boldsymbol{V}^{-1}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right) - \frac{1}{\sigma_\delta^2}\hat{\boldsymbol{\delta}}^T\hat{\boldsymbol{\delta}},$$

and, hence,

$$\begin{aligned}
&\exp\left\{\sum_{i=1}^{n}\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i,\phi) - \frac{1}{2\sigma_\delta^2}\hat{\boldsymbol{\delta}}^T\hat{\boldsymbol{\delta}}\right\} \\
&\qquad \approx \exp\left\{-\frac{1}{2}\left(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 - \boldsymbol{X}_2\hat{\boldsymbol{\delta}}\right)^T \boldsymbol{W}\left(\tilde{\boldsymbol{z}} - \boldsymbol{X}\hat{\boldsymbol{\beta}}_1 - \boldsymbol{X}_2\hat{\boldsymbol{\delta}}\right) + \sum_{i=1}^{n} c(y_i,\phi) - \frac{1}{2\sigma_\delta^2}\hat{\boldsymbol{\delta}}^T\hat{\boldsymbol{\delta}}\right\} \\
&\qquad = \exp\left\{-\frac{1}{2}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right)^T \boldsymbol{V}^{-1}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right) + \sum_{i=1}^{n} c(y_i,\phi)\right\}.
\end{aligned}$$

Alltogether, this leaves us with

$$\begin{aligned}
&\int_{\mathbb{R}^p}\int_{\mathbb{R}^p} p(\boldsymbol{y}|\boldsymbol{\beta}_1,\boldsymbol{\delta},\psi,\phi,\sigma_\delta^2,\boldsymbol{X},\boldsymbol{q})p(\boldsymbol{\delta}|\sigma_\delta^2)d\boldsymbol{\delta}d\boldsymbol{\beta}_1 \\
&\qquad = (2\pi)^{p/2}|\sigma_\delta^2\boldsymbol{I}_p|^{-1/2}\exp\left\{\sum_{i=1}^{n}\frac{y_i\theta_i - b(\theta_i)}{\phi} + c(y_i,\phi) - \frac{1}{2\sigma_\delta^2}\hat{\boldsymbol{\delta}}^T\hat{\boldsymbol{\delta}}\right\}\left|\boldsymbol{X}^T\boldsymbol{V}^{-1}\boldsymbol{X}\right|^{-1/2} \\
&\qquad\qquad \cdot \left|\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2 + \left(1/\sigma_\delta^2\right)\boldsymbol{I}_p\right|^{-1/2} + \mathcal{O}\left(n^{-1}\right) \\
&\qquad \approx (2\pi)^{p/2}\exp\left\{-\frac{1}{2}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right)^T\boldsymbol{V}^{-1}\left(\tilde{\boldsymbol{z}} - \hat{\boldsymbol{\beta}}_1\right) + \sum_{i=1}^{n} c(y_i,\phi)\right\}\left|\boldsymbol{X}^T\boldsymbol{V}^{-1}\boldsymbol{X}\right|^{-1/2} \\
&\qquad\qquad \cdot \left|\sigma_\delta^2\boldsymbol{X}_2^T\boldsymbol{W}\boldsymbol{X}_2 + \boldsymbol{I}_p\right|^{-1/2} + \mathcal{O}\left(n^{-1}\right).
\end{aligned}$$

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