Discrete Responses in Bivariate Generalized Additive Models

Francesco Donat* and Giampiero Marra

Department of Statistical Science
University College London

Abstract

A conceptual framework for the analysis of dichotomous and ordinal polychotomous responses within a penalized multivariate Generalized Linear Model is introduced. The proposed structure allows for a rather flexible predictor specification through the inclusion of non-parametric and spatial covariate effects, and the characterisation of the distribution of the stochastic model components with copulae of univariate marginals. Analytic derivations for the particular case of Gaussian marginals within a bivariate system of dichotomous outcomes are also provided, and the framework is subsequently illustrated through the estimation of the HIV prevalence in Zambia using the 2007 DHS dataset.

Key-words: Copulae; Generalized Additive Models; HIV Prevalence; Multivariate Discrete Data; Penalized Regression Splines.

1 Introduction

Generalized Linear Models (GLMs, [Nelder and Wedderburn, 1972]) are a comprehensive class of models that allows us to conduct estimation and inference for a variety of response types within the same coherent unifying framework. However, despite their undoubted relevance in applied research, they rely on a purely parametric specification of the covariate effects on the response, which effectively constrains the linear predictors to be a determined fixed-order polynomial, for instance. This is a strong requirement, as one cannot typically expect to know in advance the actual form of covariate-response relationships. This is especially the case in observational studies where their “experimental” situations are not conducted in a controlled manner. An actual risk for the researcher, therefore, would be to incorrectly specify the functional form of covariate effects, hence to potentially generate a non-negligible source of bias whenever these are not adequately represented.

An existing approach to overcome this limitation is to consider a more flexible class of models that permits the representation and estimation of the additive effects of some continuous covariates of interest in a data-driven way. Methods of this kind are usually termed semi-parametric in the statistical literature (although this denomination is generally not shared by econometricians) because they conjugate both a parametric and a non-parametric characterisation of the functional forms of the regressors. Specifically, whenever the baseline structure is that of a GLM, the so-called Generalized Additive Models emerge ([Hastie and Tibshirani, 1986, 1990]), which complement their parametric counterparts by adopting a regression spline approach, implemented in a computationally stable and efficient manner by [Wood (2006a)]. Nonetheless, as any traditional regression analysis, GAMs are effectively models for the mean of a random variable possessing a certain conditional distribution function. To enhance flexibility, therefore, it is

*Corresponding Author. University College London, Gower Street, London, WC1E 6BT, UK. Tel.: +44 (0)2076791223. E-mail: f.w.donat@gmail.com
also licit to extend the framework to qualify the dependence of any moment of order higher than one on some explanatory variables of interest. In this way, the risks of mis-specifying the models and of conducting invalid inference from them is alleviated. This approach usually comes under the name of distributional regression, whose ideas have been variously incorporated within a GAM setting; for example, Rigby and Stasinopoulos (2005) proposed a Generalized Additive Model for Location, Scale and Shape (GAMLSS), whose framework has been recently extended to the multivariate case by Klein et al. (2015). A review of these and of some other existing methodologies is presented in Kneib (2013). This line of research then seeks to achieve a higher degree of flexibility by increasing the number of distributions allowed by the proposed model representations, and by including in their respective specifications various kinds of covariate effects.

The present work aims at following these auspices in the context of discrete outcomes. Starting from the definition of a GAM for a \( J \)-variate vector of categorical responses as a penalized GLM, we discuss the conceptual representation of dichotomous and ordinal polychotomous dependent variables in terms of a triplet \((r, F_J, Z)\), and of a penalty matrix \(S_\lambda\) that allows us to incorporate in the model various instances, like non-parametric, spatial and random covariate effects. A method for dealing with a mixture of those two types of responses is also outlined. We then show how a generic estimation algorithm can be derived and inference subsequently conducted within the resulting multivariate Generalized Additive Model, and we argue that such algorithm can be, \textit{mutatis mutandis}, applied to any model representable in the \((r, F_J, Z)\) form. Although the pace of the discussion is intentionally kept at a quite generic level, connections between the proposed framework and some existing models are made. These have the dual scope of motivating our representation with well-developed examples from the literature and, at the same time, of offering a way to extend them to the more flexible predictor specifications that form the domain of our work. In particular, attention is given to nested models accounting for unmeasured residual confounding: an instance rather frequent in observational studies and that may lead to detrimental consequences on the parameter estimates whenever it is not adequately controlled for (e.g. Becher, 1992). The proposed representation is then used to define a sample selection model for dichotomous responses to credibly assess the human immunodeficiency virus (HIV) prevalence in Zambia. With this empirical illustration, we give evidence of the flexibility of our generic representation which also permits the inclusion of multivariate distributions defined through copulae of univariate marginals, and the dependence of the corresponding association parameter to be expressed as a functional of the available data. In summary, therefore, this paper contributes to the literature by providing a flexible tool for the representation, estimation and inference in multivariate GLMs for discrete responses admitting non-parametric and spatial-dependent covariate effects, and by accounting for the unification of models for residual confounding under the same conceptual frame.

2 A GAM Representation for Discrete Responses

Let \( Y = (Y_1, \ldots, Y_J)^T \) be a random vector with support the discrete set \( K := K_1 \times \cdots \times K_J \), where \( K_j := \{1, \ldots, K_j\} \) and \( #(K_j) = K_j < \infty \) for every \( j \in J, J := \{1, \ldots, J\} \); namely we consider each variable \( Y_j \) to have finite \( K_j \) levels. The set \( K_j \) is assumed here to collect both qualitative and quantitative elements, as well as variables measured on the nominal or ordinal scale (Stevens, 1946). Specifically, the former differentiates items based only on the categories they belong to, whereas the latter allows also for a rank order by which the realisations of \( Y_j \) can be sorted, but still the relative degree of difference between them lacks of any meaningful interpretation. For notational convenience, we represent each \( k_j \) by a natural number, \( K_j \subset \mathbb{N} \), with the convention that, wherever the support of \( Y_j \) is ordinal, we postulate the existence of an isomorphism that maps bijectively each element of the qualitative ordinal set \( K_j^* \) onto \( K_j \). In this case it holds: \( \bar{k}_j^* \leq k_j^* \) in \( K_j^* \) if and only if \( \bar{k}_j \leq k_j \) in \( K_j \), and we take the set \( (K_j, \leq) \) to
be totally ordered.

In analogy with the approach outlined in Peyhardi et al. (2014) for the univariate case, we consider a regression of the probability \( \pi_k = \Pr[Y = k|X = x] \), with \( k := (k_1, \ldots, k_J)^\top \in \mathcal{K} \), on some covariates \( x := (x_1, \ldots, x_J) \) defined through a Generalized Linear Model form

\[
\pi = g^{-1}(\eta) := (r^{-1} \circ F)(\eta_1, \ldots, \eta_{K-1}),
\]

(1)

where \( r: \mathcal{M} \rightarrow \mathcal{P} \) is a diffeomorphism from \( \mathcal{M} := \{(0, 1)^{K-1}|1^\top \pi < 1\} \) to an open subset \( \mathcal{P} \) of \( (0, 1)^{K-1} \), and with \( \pi := \{\pi_k\}_{k \in \mathcal{K} \setminus \{K\}} \). Model \( (1) \) also comprises the map \( F: \mathcal{S} \rightarrow \mathcal{M} \), where \( \mathcal{S} \subset \mathbb{R}^{K-1} \), and the array \( F(\eta) := (F_j(\eta_1), \ldots, F_j(\eta_{K-1}))^\top \) is taken to collect fully-specified \( J \)-variate distribution functions, each of them evaluated at \( \eta_k := (\eta_{k,1}, \ldots, \eta_{J,k})^\top = Z\beta_k \), a linear predictor. Wherever needed, we assume that the elements of \( \mathcal{K} \) obey a lexicographical order, that is \((k_1, \ldots, k_J) \leq (j_1, \ldots, j_J)\) if and only if \( k_j \leq j_j \) for all \( j \in \mathcal{J} \) or \((\tilde{k}_j = k_j \land \tilde{k}_j \leq k_j) \) for some \( j \in \mathcal{J} \). A more traditional GLM representation for the \( k \)-th category can be recovered from \( (\ref{eq:glm}) \) and reads as

\[
r(\pi_k) = F_j(\eta_k) = F_j(Z\beta_k),
\]

(2)

where \( r \) is now a function specific for the type of the responses \( Y \). For instance, in the univariate framework, dichotomous variables would set \( r_j \) such that \( \pi_{k_j} \mapsto \pi_{k_j} \), the identity map, therefore \( (\ref{eq:glm}) \) reduces to any model for the binary outcome, say a logit or a probit, depending on the definition of \( F_1 \). Models for ordinal polychotomous responses, as the Cumulative Link Model (CLM) of McCullagh (1980), also possess this representation and set the left-hand side of \( (\ref{eq:glm}) \) as \( r_j(\pi_{k_j}) = \pi_1 + \cdots + \pi_{k_j} \). Although more specifications of different univariate response types are illustrated in Peyhardi et al. (2014), in this work we confine ourselves to the sole study of dichotomous and ordinal outcomes, since they are the most frequent instances of the class of models we aim at developing.

As \( (\ref{eq:glm}) \) explicates, any GLM for discrete responses is fully characterised by the triplet \((r, F_j, Z)\), where the design matrix \( Z \) depends on the covariates \( x \), though not necessarily coinciding with them. For example, let the polychotomous response \( Y \) follow the model

\[
r(\pi_k) = \sum_{k_1 \leq k_1} \cdots \sum_{k_j \leq k_j} \pi_{k_1, ..., k_j} = F_j(c_k - X\beta) = F_j(Z\beta_k),
\]

(3)

then \( Z := \text{diag}(z_1^\top, \ldots, z_J^\top) \) and \( \beta_{j,k} := \text{vec}(\beta_{1,k}, \ldots, \beta_{J,k}) \), where \( z_j := (1, -x_{j,1}, \ldots, -x_{j,m_j})^\top \) and \( \beta_{j,k} := (c_{j,k_1}, \beta_{1,j}, \ldots, \beta_{J,m_j})^\top \). In the proceeding analysis, we call the \( c_{j,k_1} \)'s threshold parameters or cut points, and we assume they are the only elements in the corresponding linear predictor \( \eta_{j,k_j} \) to depend on the categories of \( Y \). We also stress that only \( K_j - 1 \) cut points are effectively estimable in this framework, because in order to allow the domain of \( F_j \) to coincide with the extended real hyper-plane \( \mathbb{R}^J \), we need to impose \( c_{j,K_j} = \infty \) for any \( j \) and \( c_{j,0} := c_{j,1-1} = -\infty \). As a consequence, a dichotomous response with support \( \mathcal{K}_j := \{0, 1\} \) would set the only threshold to 0, and the model intercept is now estimable.

**Ordinal Polychotomous Outcomes** This instance is of some interest in terms of the proposed GLM specification and worth to be discussed further. Notice first that the given definition of \( r(\pi_k) \) is posing a constraint to the set \( \mathcal{P} \). Specifically, by assuming \( \tilde{k}_j \leq k_j \), we have

\[
r(\pi_k) = \sum_{k_1 \leq k_1} \cdots \sum_{k_j \leq k_j} \pi_{k_1, ..., k_j} \\
= \sum_{k_1 \leq k_1} \cdots \sum_{k_j \leq k_j} \sum_{k_j \in [k_1, k_j]} \sum_{\tilde{k}_j \leq k_j} \pi_{k_1, ..., \tilde{k}_j} \\
= r(\pi_k) + r'(\pi_k) \geq r(\pi_k)
\]
since $r'(\pi_k)$ is the sum of probability measures. We also deduce $\tilde{k} := (k_1, \ldots, \tilde{k}_j, \ldots, k_{J-1}) \preceq (k_1, \ldots, k_j, \ldots, k_J)$ by the assumed lexicographical order. Hence $r(\pi_k) \leq r(\pi_{\tilde{k}})$ for any $\tilde{k} \preceq k$, and $\mathcal{P} := \{r \in (0,1)^{J-1} | r(\pi_k) \leq r(\pi_{\tilde{k}}), \text{ for all } \tilde{k} \preceq k \text{ and } k, \tilde{k} \in \mathcal{K}\}$. 

If this restriction comes from the very construction of a CLM, a second one emerges to let the model meet a general coherency condition. To establish this result, the inspection of \[3\] reveals that the linear predictors $\{\eta_k\}$ depend on the element $k$ of the discrete ordered set $\mathcal{K}$ that one attempts to model. The sought coherency requires, therefore, the definition of a specific correspondence between the order relations existing in $k \in \mathcal{K}$ with those in $\eta_k \in \mathcal{S}$. This is identified, in particular, in the order embedding of each $X_j$, into a relevant subset of the real line as induced by the thresholds $\{c_{j,k}\}$: in this way, it is possible to construct non-overlapping hyper-rectangles in $\mathbb{R}^J$ isomorphic to $(k_1, \ldots, k_J) \in \mathcal{K}$. In terms of a multivariate CLM, the order embedding is guaranteed by taking the cut points $\{c_{j,k}\}$ to be an increasing sequence in $k$ for every $j \in J$ wherever, as stated above, the threshold parameters are the only quantities in the linear predictors depending on the categories of $Y_j$. Consequently, it follows the isomorphism $\{\eta_k\} \cong \{k\}$, meaning that there exists a bijection $\varphi : \mathcal{K} \rightarrow \mathcal{S}$ such that $\varphi(\tilde{k}) := \eta_k \preceq \eta_{\tilde{k}} := \varphi(k)$ in $\mathcal{S}$ if and only if $\tilde{k} \preceq k$ in $\mathcal{K}$. In this case, the domain of $\mathcal{F}$ is then restricted to be the set $\mathcal{S} := \{\eta \in \mathbb{R}^{K-1} | \eta_k \preceq \eta_{\tilde{k}}, \text{ for all } \tilde{k} \preceq k \text{ and } \tilde{k}, k \in \mathcal{K}\}$. In the bivariate case, $J = 2$, Dale (1986) imposed a strict monotonicity on the cut points to imply a non-degenerate probability measure on $\mathcal{K}$. Although this condition would in turn debar one possible source of the Maximum Likelihood Estimator to be located at the boundary of the parameter space with non-null probability (refer to Haberman, 1980 for the univariate case), we reckon this restriction has to be avoided as it arbitrarily excludes a still admissible estimate, albeit at the boundary. Arguably, two congruent subsequent cut points are not in contrast with the coherency principle. In fact, given any two elements $\tilde{k}$ and $k$ of $\mathcal{K}$ such that either $\tilde{k}_j = k_j$ or $\tilde{k}_j < k_j$, the coherency implies that the occurrence $c_{j,\tilde{k}_j} = c_{j,k_j}$ is verified if and only if $\tilde{k}_j = k_j$, that is whenever $\mathcal{K} := \mathcal{K}_1 \times \cdots \times (\mathcal{K}_j \setminus \{\tilde{k}_j\}) \times \cdots \times \mathcal{K}_{J}$, unless $\tilde{k}_j$ is an element of zero probability mass in $\mathcal{K}$. Either cases correspond to observing zero counts for the $k_j$-th category, but with the coherency would be still in place.

Under this principle, it is possible to motivate ordinal polychotomous responses through a generating continuous latent random vector $Y^* := (Y^*_1, \ldots, Y^*_j)^\top$ in $\mathbb{R}^J$ in such a way that, upon letting $\epsilon$ be the stochastic component in the regression $Y^* = X\beta + \epsilon$, it holds

$$\{Y \preceq k\} \iff \{\epsilon \leq \eta_k\}, \quad (4)$$

where the right-hand side is intended component-wise as $\epsilon_j \leq \eta_{j,k_j}$ for every $j$.

### 2.1 Specification of the Linear Predictors in a Penalized GLM

Linear predictors enter representations \[1\] or \[2\] as domain of the distribution functions collected in $\mathcal{F}$, and are fully characterised by the design matrix $Z$ for any vector of parameters $\beta_k$. In the proceeding, we assume that each predictor $\eta_{j,k_j}$ depends parametrically on some covariates $x_j$, and through an additive form of unknown smooth functions $s_{j,L_j} : \mathbb{R} \rightarrow \mathbb{R}$ for the remaining continuous regressors $v_j := (v_{j,1}, \ldots, v_{j,L_j})^\top$. The resulting functional form is then termed semi-parametric, and defines the class of (Vector) Generalized Additive Models (VGAMs; Yee and Wild, 1996). We prefer, however, to adopt the alternative terminology of penalized GLMs as, in our opinion, it reflects better the features of the class of models we discuss beyond the traditional domain of GAMs.

For dichotomous and ordinal polychotomous responses we define the linear predictor to be

$$\eta_{j,k_j}(x_j, v_j, \theta) = c_{j,k_j} - x_j^{\top} \beta_j - s_{j,1}(v_{j,1}) - \cdots - s_{j,L_j}(v_{j,L_j}) \quad v_{j,L_j} \in \mathbb{R}, \quad (5)$$

where $\theta$ denotes the parameter vector, and the smooth functions are represented by regression splines using the approach popularised in the literature by Eilers and Marx (1994). Assume
first that we have a sample of \( n \) observations indexed by the subscript \( i \). The underlying idea of the method is to approximate each curve by a linear combination of known basis spline functions, \( b_{j,l}(h_i) \), for \( h_j = 1, \ldots, H_j \), and unknown regression parameters to be estimated within the system, \( \delta_{j,l} \). In our notation, \( h_j \) is employed to count the bases, as delimited by some knot points in the interior of \([v_{j,l}(1), v_{j,l}(n)]\) for every \( j \). Upon defining \( b_{j,l}(v_{j,l,i}) := (b_{j,l,1}(v_{j,l,i}), \ldots, b_{j,l,H_j}(v_{j,l,i}))^\top \), and \( \delta_{j,l} \) the corresponding \( H_j \)-dimensional vector of parameters associated with the smooths, it holds

\[
s_{j,l}(v_{j,l,i}) \approx \delta_{j,l}^\top b_{j,l}(v_{j,l,i}).
\]

The evaluation of \( b_{j,l} \) for each \( i \) yields \( H_j \) curves – encompassing different degrees of complexity – that give, once multiplied by some real-valued parameter vector and then summed, an estimated curve for \( s_{j,l} \). Basis functions are usually chosen to have convenient mathematical properties and good numerical stability: possible instances are B-splines, cubic regression and low-rank thin plate regression splines (e.g. [Ruppert et al. 2003 and Wood 2003]). For identifiability purposes, a centering constraint such as \( \sum s_{j,l}(z_{j,l,i}) = 0 \) for every \( i \) has to be imposed, which is automatically incorporated in our model representation using the parsimonious approach of [Wood (2006a)]

We are now in the position to express the functional form of linear predictors through a more compact and comprehensive representation. To this end, let us define \( \beta_{j,l} := \delta_{j,l} \) the sub-vector of \( \beta \) corresponding to the \((j, l)\)-th smooth and, accordingly, \( X_{j,l} \) the covariate matrix whose \( j \)-th row is \( b_{j,l}^\top(v_{j,l,i}) \). It then follows that the \( n \)-dimensional vector of linear predictors for the \( j \)-th response can be written as:

\[
\eta_j := c_j - X_{j,1}\beta_{j,1} - \cdots - X_{j,M_j}\beta_{j,M_j} = Z_j\beta_j,
\]

where \( Z_j := (1_n, -X_{j,1}, \ldots, -X_{j,m_j}, \ldots, -X_{j,M_j}) \) and \( \beta_j := \text{vec}(c_j, \beta_{j,1}, \ldots, \beta_{j,M_j}) \). We further assume \( j = 1, \ldots, J \), with \( J \geq J \) to possibly specify any association parameter implied by the distribution \( F_j \) in terms of some observed independent variables. So re-written, the linear predictors conform notionally with the GLM given in [3], with the caveat that now they can be indifferently used to represent linear and non-linear covariate effects within a generic GLM for multivariate discrete data. To see this, set \( \eta := (\eta_1, \ldots, \eta_J) \) to be the array whose \( i \)-th row is \( \eta_k = (\eta_{1,k,1}, \ldots, \eta_{1,k,i}, \ldots, \eta_{j,k})^\top \) and, accordingly, \( \beta_k := \text{vec}(\beta_{1}, \ldots, \beta_{j}) \). Thus \( Z_i := \text{diag}(z_{i,j,1}, \ldots, z_{i,j,i}) \), with \( z_{i,j,i} \) being the \( i \)-th row of \( Z_j \), and the linear form that defines the right-hand side of [3] is now recovered as \( \eta_k := Z_j\beta_k \).

**Characterisation and Definition of a GAM as a Penalized GLM.** To enforce certain properties of the covariate effects, a ridge-type penalisation is assigned to each component of \( Z_j \), namely \( P_{j,m_j} := \lambda_{j,m_j}\beta_{j,m_j}^\top \mathbf{S}_{j,m_j} \beta_{j,m_j} \), where the dimension of \( \mathbf{S}_{j,m_j} \) is generically denoted by \( q \). The smoothing (or tuning) parameter \( \lambda_{j,m_j} \in [0, \infty) \), in particular, is introduced here to control the trade-off between smoothness and fitting in the non-parametric estimation of \( s_{j,m_j} \). Specifically, as \( \lambda_{j,m_j} \) tends to zero, less penalisation is attached to the regression coefficient \( \beta_{j,m_j} \) and the estimation occurs either at the pre-specified polynomial form for the parametric model components, or at the spline interpolation for the unknown functions. On the other hand, an infinite value of \( \lambda_{j,m_j} \) results in the fitting of a straight line, a situation also known as over-smoothing.

The penalty \( P_{j,m_j} \) can be used to describe several covariate effects in the same unifying manner. In particular, a parametric functional form would set \( \mathbf{S}_{j,m_j} = 0_{q,q} \), and the corresponding \( X_{j,m_j}\beta_{j,m_j} \) reduces to \( x_{j,m_j,}\beta_{j,m_j} \), with \( x_{j,m_j} := (x_{j,m_j,1}, \ldots, x_{j,m_j,n})^\top \) whereas, in the presence of non-parametric effects, one can specify the penalty through the symmetric and positive semi-definite matrix

\[
\mathbf{S}_{j,m_j} := \int_{v_{j,m_j}} b_{j,m_j}'(b_{j,m_j}''')^\top dv_{j,m_j},
\]
a generic measure of the curvature of the estimated \( (j, m_j) \)-th smooth function (see Green and Silverman [1994] for a detailed introduction to this roughness penalty approach to curve estimation).

Furthermore, \( \mathcal{P}_{j,m_j} \) is compatible with the specification of random effects models \( (\mathbf{S}_{j,m_j} = \mathbf{I}_q) \), as well as with the definition of spatial covariate dependence. As recently outlined by Klein et al. (2015) and Marra et al. (2015), this approach can be employed wherever the phenomenon of interest to possesses characteristics that vary according to the geographical location of each individual. Let \( r_i \in \mathcal{R}, \mathcal{R} := \{1, \ldots, R\} \), be the region to which the \( i \)-th observation belongs, and define \( \mathbf{R} \) the corresponding \( n \times R \) design matrix of the spatial effects. This sets \( \mathbf{X}_{j,m_j,i} \beta_{j,m_j,i} \equiv \mathbf{x}_{r_i} \beta_{r_i} \) so that we estimate separate parameters \( \beta_1, \ldots, \beta_R \) for each region, and \( \mathbf{R} \) is an incidence matrix, namely an array such that \( \mathbf{R}_{[i,r]} = 1 \) if observation \( i \) belongs to \( r \in \mathcal{R} \), and 0 otherwise. Then, for discrete spatial effects, a Markov random field (e.g. Rue and Held 2005) induces the estimation).

Once every component in \( \mathbf{Z}_j \) is endowed with a proper penalisation depending on the desired effect one is willing to model, and \( \mathbf{S}_{j,m_j} \) adequately adjusted to meet the splines’ centering constraint, an overall penalty for the whole model can be constructed as \( \mathcal{P}_\mathbf{X} := \mathbf{d}^\top \mathbf{S}_\mathbf{X} \mathbf{d} \), where \( \mathbf{S}_\mathbf{X} \) corresponds to \( \mathbf{S}_\mathbf{\lambda} \) padded with zeros so that \( \mathbf{d}^\top \mathbf{S}_\mathbf{\lambda} \mathbf{d} = \mathbf{\beta}^\top \mathbf{S}_\mathbf{\lambda} \mathbf{\beta} \). \( \mathbf{S}_\mathbf{\lambda} := \text{diag}(\mathbf{S}_{j,m_j})_{m_j,i} \) and \( \lambda := \{\lambda_{j,m_j}\}_{m_j,i} \). A penalized GLM is therefore defined as any model in the form of (2) augmented with a non-zero penalty \( \mathcal{P}_\mathbf{X} \).

In the next section, we qualify the generic framework to describe a class of models widely used in applications, and we show how it can be represented within the \( (\mathbf{r}, \mathbf{F}_j, \mathbf{Z}) \) frame. In this way, these models can be extended beyond the parametric specification of their functional form of covariate effects, and their estimation and inference will then be a direct consequence of those of a generic multivariate penalized GLM for discrete responses.

2.2 Some Bivariate Models in the Class of Penalized GLMs

The analysis of observational data may be difficult as they often depart from the ideal conditions underlying any (also rather simple) regression model. They are commonly characterised by a lack of randomisation that may result either in a non-random selection of individuals in the sample, or even in the non-random allocation of a predictor of interest among the population (hence inducing a distorted association with the outcome). The former is commonly referred to non-random sample selection, and arises whenever individuals select themselves in or out of the relevant sample. It is often the case that some factors that determine the membership to the selected sample are also associated with those that determine the outcome itself. In the empirical illustration accompanying this work, and concerning the estimation of the HIV prevalence in Zambia, the refusal of people to be tested for the virus may be induced by factors associated to their HIV status. For example, they may already know or correctly predict their seropositivity and so fear others will learn about it if tested. The latter instance is regarded instead as a form of endogeneity as it is denominated in the econometric literature, and it may stem from different sources, including, but not limited to, the direct unmeasured confounding problem; Wooldridge [2002] discusses this in detail as well as other generating sources of endogeneity, and we refer to him for a more thoughtful illustration of the topic. This situation arises whenever a common background variable affects simultaneously both the outcome of interest and one of its regressors, and it is not readily observable or quantifiable by the researcher. The affected covariate is then termed endogenous, and its effect on the outcome results confounded. A pedagogical example is the estimation of the effect of education on wages. Both the relevant
variables in this study can be co-determined by factors such as personal ability and motivation that are likely to be explainable to both individual’s level of education and salary, but hardly measurable (see for example [Imbens, 2014] for an interesting survey on the topic).

When not accounted for, non-random sample selection and endogeneity can both lead to inconsistent parameter estimates for the whole model. To deal with these issues, in some early works, [Heckman, 1978, 1979] devised a two-step estimation procedure for a prototypical recursive bivariate system of equations in a dichotomous responses setting, with $Y = (Y_1, Y_2)^\top$ and $Y_2(Y_1)$. His proposals specified a binary rule for the observability of the outcome of interest, $Y_2$, for the non-random sample selection case, and related the conditional mean of the endogenous regressor, $Y_1$, to various other predictors when endogeneity is suspected. In either scenario, identification of the true association between the elements of $Y$ would require to be able to qualify the dependence of $Y_1$ on a relevant variable which is assumed to be independent of both $Y_2|Y_1$ and the unmeasured confounder(s).

**Unmeasured Confounding** We consider the case where both the responses are discrete, and we specify the following triangular generating structure for the $j$-th categorical response in terms of a latent variable formulation, as of Case 3 in [Heckman, 1978],

$$Y_j^* = 1_{j=2}(\psi Y_1^*) + \mathbf{x}_{j,1}^\top \beta_{j,1} + \cdots + \mathbf{x}_{j,M_j}^\top \beta_{j,M_j} + \epsilon_j \quad (\epsilon_1, \epsilon_2)^\top \sim \mathcal{N}_2(0, \Omega; \rho),$$

where $\mathbf{x}_{j,m_j}$ denotes the $(j, m_j)$-th row of $\mathbf{X}_{j,m_j}$. The given distributional assumption is in line with the considerations of [Greene and Hensher, 2010] and with the current practice in multivariate discrete response modelling. In particular, we set $\Omega := \text{Var}[\epsilon]$ to have unit main diagonal elements for identifiability purposes and correlation coefficient $\rho$. Let us next define the following quantities:

$$\Gamma := \begin{bmatrix} 1 & 0 \\ -\psi & 1 \end{bmatrix} \quad \text{and} \quad L := \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1+2\rho+\psi^2} \end{bmatrix},$$

where $L$ is a lower triangular, positive definite matrix since $(1+2\psi+\psi^2) = (1-\rho^2)+(\rho+\psi)^2 > 0$, and with $LY^* = L\Gamma^{-1}(X\theta + \epsilon)$ distributed as Standard Normal random vector with covariance matrix $\Sigma = L\Gamma^{-1}\Omega\Gamma^{-1}L^\top$. This structure constitutes the most general one we discuss in this paper, as it nests the vast majority of the other model specifications for unmeasured confounding and non-random sample selection currently proposed in the literature. Notice that the manifest polychotomous ordinal responses can now be recovered from (4) via the series of equivalences

$$\{Y \preceq k\} \iff \{\Gamma Y^* \leq c_k\} \iff \{L\Gamma^{-1}\epsilon \leq L\Gamma^{-1}Z\beta\},$$

which implies that the predictor $L\Gamma^{-1}\eta_k$ is non-linear in $\theta$, an occurrence that has to be accounted for in the derivation of the estimation algorithm. The corresponding $(r, F_2, Z)$ definition of the triangular form (7) for every $k \in \mathcal{K}$ is then

$$\left(\sum_{k_1 \leq k_1} \sum_{k_2 \leq k_2} \pi_{k_1,k_2} F_2(\eta_{1,k_1}, \eta_{2,k_2}; \Sigma), L\Gamma^{-1}Z_1\right),$$

where $Z$ is defined as in [4] and, in the case of $\mathcal{K} := \{0,1\} \times \{0,1\}$, the first entry of the triplet becomes $r(\pi_k) = \pi_{k_1,k_2}$ while the design matrix has to be modified accordingly in order to accommodate the instance $\epsilon_{j,0} = 0$ for any $j$. This representation of the recursive structure allows explicitly for a latent endogenous predictor to be a determinant of the intentions about $Y_2$. That is, if one interprets the intentions towards a manifest discrete outcome (the actual action) as the result of an underlying choice mechanism as described by $Y_j^*$, then (8) really assumes the existence of unobservables that influence simultaneously the intentions about the
components of Y. For example, there is a vast economic literature pointing out that the choice of investing in both health and education are confounded by individual time preferences, in the sense that people with low (high) rates of time preference are more (less) likely to decide to invest in both schooling and health [Sander (1995), Fuchs (1982), van der Pol (2011)]. In this case, endogeneity is regarded to act at the level of the choice of how much to invest in education and future health status. A researcher could nonetheless be interested in modelling the effects of an observed endogenous variable (where the intentions have been revealed by the actual choices undertaken) on the discrete response Y2: this instance then specifies \( \mathbf{\Gamma} = \mathbf{L} = \mathbf{I}_2 \) and \( \mathbf{Z} \) is assumed to include the levels of the manifest \( Y_1 \). A discussion about the distinctive features of these different modelling strategies can be found in Vossmeier (2014), who also introduced a formal Bayesian model comparison framework to test these two competing models against the observed data.

Models for a mixture of dichotomous and ordinal polytomous responses can also be reconciled within this representation by giving a proper definition of \( r(\pi_2) \). In fact, this is the only element which is directly affected by the types of responses considered, whereas the design matrix mainly attains the functional form assumed for the predictors, and \( F_2 \) specifies the link function. To describe this situation, we may think of \( r \) as the composition function \( r = r_1 \circ r_2 \), where the subscripts correspond to the elements of the 2-dimensional vector \( Y \) they refer to. Therefore, by setting

\[
    r_j(\pi_k) = \pi_{k_j,k_j} \quad \text{and} \quad \pi_j(\pi_k) = \sum_{k_j < k_j} \pi_{k_j,k_j},
\]

we have \( r_j(r_j(\pi_j)) = r_j(\pi_k) \) for any \( k_j,k_2 \in \mathcal{K} \) and \( j := \mathcal{J} \setminus \{j\} \). The result follows because, for dichotomous responses, \( r_j \) is the identity map, meaning that it is also indifferent the order in which the types of the outcomes appear in \( Y \) in terms of the model representation. In other words, irrespectively from whether \( Y_1 \) or \( Y_2 \) is the dichotomous variable, the function composition \( r_j \circ r_j \) is commutative:

\[
    (r_j \circ r_j)(\pi_k) = r_j(\pi_k) = r_j(r_j(\pi_k)) = (r_j \circ r_j)(\pi_k).
\]

**Non-random Sample Selection** In this case, it is assumed that the outcome \( Y_2 \in \mathcal{K}_2 \) is observed if and only if \( \{0, 1\} \ni Y_1 = 1 \), whereas it is labelled as missing otherwise. As a consequence, the vector \( \pi \) results further constrained: every element in the form of \( \pi_{0,k_2} \) is now not a sensible quantity in the model for any \( k_2 \), since it refers to a missing value in the realisation of \( Y_2 \). Hence, one can only describe the corresponding marginal probability \( \pi_0 \), which is translated mathematically into the map \( \mathcal{M} \rightarrow \mathcal{M}^s \) defined by \( \pi_{0_,k_2} \mapsto \sum_{k_2 \in \mathcal{K}_2} \pi_{0,k_2} =: \pi_0 \), and \( \pi_{1,k_2} \mapsto \pi_{1,k_2} \) for any \( k_2 \in \mathcal{K}_2 \setminus \{k_2\} \), where \( \mathcal{M}^s := \{ \pi^s \in (0, 1)^{\mathcal{K}_2} \mid \pi^s < 1 \} \). Notice that, in complete analogy with the general case, if \( \pi^s \) is augmented with \( \pi_{1,k_2} \), the components of the resulting vector will sum up to the unity. Hence, the \( (r, F_2, Z) \) representation of this generic sample selection model would require just to exploit the corresponding function \( r \) as depending on the type of the response \( Y_2 \). In particular, for a dichotomous response \( Y_2 \),

\[
    r(\pi^s) = (\pi_0, \pi_{1,0})^\top = (\Phi_2(-\eta_1, \infty, \Omega), \Phi_2(\eta_1, -\eta_2, \Omega))^\top = \mathcal{F}(\eta), \quad (9)
\]

where \( \Omega \) stems from \( \Sigma \) upon imposing the restrictions \( \mathbf{\Gamma} = \mathbf{L} = \mathbf{I}_2 \), and \( \Phi_2(-\eta_1, \infty) = \Phi_2(-\eta_1, -\eta_2) + (\Phi_2(-\eta_1, \eta_2) - \Phi_2(-\eta_1, -\eta_2)) = \Phi(-\eta_1) \) as from the map characterising the sample selection problem. This bivariate probit model was originally proposed by Heckman (1979) and subsequently extended to encompass penalized regression splines by [Marra and Radice (2013)]. As a natural generalisation, one can also consider the support of \( \mathcal{K}_2 \) to be totally ordered, \#(\mathcal{K}_2) > 2 like in [Miranda and Rabe-Hesketh (2006)], whose corresponding representation within our framework comprises

\[
    r(\pi) = (\pi_0, \pi_{1,1}, \ldots, \pi_{1,1} + \cdots + \pi_{1,K_2-1})^\top,
\]
\[ \mathcal{F}(\eta) = \left( \Phi(-\eta_1), r^{-1}(\Phi_2(\eta_{1,1}, \eta_{2,1}; \Omega)), \ldots, r^{-1}(\Phi_2(\eta_{1,K}, \eta_{2,K}; \Omega)) \right)^\top, \]

where the generic \( r^{-1}(F_2(\eta_{1,k}, \eta_{2,k})) \) can be computed as the non-negative volume of the rectangles \([\eta_{1,k_1-1}, \eta_{1,k_1}] \times [\eta_{2,k_2-1}, \eta_{2,k_2}] \) in \( \mathbb{R}^2 \).

3 Estimation

Let the conditional distribution of \((Y|X = x)\) obey a Categorical distribution \(C(\pi(x))\) with mass function

\[ f_{Y|X}(y|x) = \prod_{k \in \mathcal{K}} \pi_k(x)^{1_y=k}, \quad (10) \]

where \( \mathbb{1}_{y=k} \) is a Boolean function that takes value 1 if \((y_1 = k_1 \land \ldots \land y_J = k_J)\) and 0 otherwise. Then, after having re-defined the response vector \( \bar{y} = (\mathbb{1}_{y=1}, \ldots, \mathbb{1}_{y=K})^\top \), the distribution \((10)\) can be written as

\[ f_{Y|X}(\bar{y}|x) = \exp \left\{ \bar{y}^\top \theta - b(\theta) \right\}, \]

where

\[ \theta_k = \ln \left\{ \frac{\pi_k}{1 - \sum_k \pi_k} \right\}, \quad \theta_K = 0 \quad \text{and} \quad b(\theta) = \ln \left\{ 1 + \sum_k \exp(\theta_k) \right\}, \]

which shows that \(C(\pi(x))\) can be expressed in the exponential form, and hence all the standard properties implied by this family of distributions follow. If we further take \(\{(x_i, y_i)\}_{i=1}^n\) a sample from \(F_Y\) and \(F_X\), where the \(y_i\)'s are assumed conditionally independent given the regressors, then equation \((10)\) can also be used to derive the log-likelihood function of any multivariate model for discrete data admitting a \((r, F_J, Z)\) form. Specifically, by denoting \(\ell_i(\theta)\) the contribution of the \(i\)-th observation to the log-likelihood, the iterative application of the chain rule results in

\[ \nabla_{\theta_i} \ell_i = \frac{\partial \eta_k}{\partial \theta} \left( \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \frac{\partial \theta_k}{\partial \theta_k} \right) = D_i^\top u_i \quad \text{and} \quad \nabla_{\theta \theta_i} \ell_i = D_i^\top W_i D_i + K_i, \quad (11) \]

where

\[ W_i = \frac{\partial^2 F_k}{\partial \eta_k \partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \frac{\partial \theta_k}{\partial \theta_k} \frac{\partial \ell_i}{\partial \theta_k} + \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \left( \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \right)^\top \left\{ \frac{\partial^2 \theta_k}{\partial \theta_k} \frac{\partial \ell_i}{\partial \theta_k} + \left( \frac{\partial \theta_k}{\partial \theta_k} \right)^2 \frac{\partial^2 \ell_i}{\partial \theta_k^2} \right\} \]

and

\[ K_i = \frac{\partial^2 \eta_k}{\partial \theta \partial \theta} \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \frac{\partial \theta_k}{\partial \theta_k} \frac{\partial \ell_i}{\partial \theta_k}. \]

These expressions are analogous to those derived by Green (1984) in the context of iterative re-weighted least squares (IRLS) estimation of likelihood functions. Indeed, the baseline model is rather similar, with the sole relevant difference being the acknowledgment that only in some special cases \(r(\pi) = \pi\). In particular, wherever \(r\) is the identity map, \(u = \text{vec}(u_1, \ldots, u_n)\) reduces to the same simplified expression, \(\partial \ell_i / \partial \eta_k\), that appears in Green (1984). Factor \(K_i\) is somehow unusual, and generally it is not reported in the relevant literature on GLMs. In fact, it is structurally equal to \(0_{p,p}\) wherever each \(\eta_k\) is linear in the parameter vector; however, this may not be true in some instances as shown, for example, in the triangular systems of equations having representation \((8)\). The Information Matrix can also be derived: recalling that, for the exponential family of distributions, \(\partial \ell_i / \partial \theta_k = \bar{y}_k - \pi_k\), \(b'(\theta_k) = \pi_k\) and \(\partial \theta_k / \partial \pi_k = [b''(\theta_k)]^{-1} = \text{Var}[(\bar{y}_k)^{-1} = [\pi_k(1 - \pi_k)]^{-1}\), we have \(\mathbb{E}[K_i] = 0_{p,p}\), while

\[ \mathbb{E}[W_i] = - \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \left( \frac{\partial F_k}{\partial \eta_k} \frac{\partial \pi_k}{\partial r_k} \right)^\top \frac{1}{\pi_k(1 - \pi_k)} = - W_i, \]
Each individual matrix is finally aggregated into appropriate arrays to get a global representation of score and Hessian as follows: \(D := (D_1, \ldots, D_p)^\top\), \(u := \text{vec}(\mathbf{u}_1, \ldots, \mathbf{u}_n, 0_p)\), \(-W := \text{diag}(W_1, \ldots, W_n, K)\), with \(K := \sum_i K_i\), so that \(\nabla_\vartheta \ell(\hat{\vartheta}) = D^\top u\), and \(\nabla_{\vartheta^\top} \ell(\hat{\vartheta}) = -D^\top WD\).

### 3.1 Penalized Likelihood

The quantities derived above have been obtained only by the knowledge of the \((r, F, Z)\) representation of the model that, alongside with the penalty matrix \(S_\lambda\), embodies all the information needed to achieve estimation. Recall that any covariate effect other than a purely parametric specification requires the exploitation of certain features as included in the penalisation term \(P_\lambda\). To account for them, a Penalized Likelihood (PL) is usually set up for estimation, and the corresponding MPLE is then defined as solution of the following optimisation problem

\[
\hat{\vartheta} := \arg\max_{\vartheta \in \Theta} \ell_p(\vartheta, \lambda) = \left\{ \sum_{i=1}^n \ell_i(\eta_i(\vartheta)) - \frac{1}{2} \vartheta^\top S_\lambda \vartheta \right\}, \quad (12)
\]

which is obtained from any fixed value of the smoothing parameter vector \(\lambda\). Because the quadratic form \(P_\lambda\) is positive semi-definite by construction, the joint estimation of \((\vartheta, \lambda)\) would clearly lead to over-fitting since an optimal value for \(\ell_p(\vartheta)\) would be reached at a state where \(\lambda = 0\). Our estimation strategy comprises therefore two alternating steps based on the outer iteration scheme originally proposed by O’Sullivan et al. (1986). Specifically, an estimate \((\hat{\vartheta}|\lambda = \lambda')\) is first obtained from any value \(\lambda'\) via the maximisation of \(\ell_p(\vartheta|\lambda = \lambda')\), which is then used to update a value of the tuning parameter vector. The whole procedure is iterated until convergence.

Although a solution to problem (12) can in principle be obtained through any numerical optimisation algorithm, our subsequent analysis requires some of its iterations to be either of Newton-Raphson or of Fisher scoring-type to match with the derivation of the smoothing parameters vector.

### P-IRLS Scheme for Estimation

Rather than handling the log-likelihood maximisation directly, it is convenient to define a penalized iteratively re-weighted least squares (P-IRLS) scheme based on quantities (11). Let us first derive the Taylor series approximation of the function \(\nabla_\vartheta \ell_{p,i}\) about the vector \(\hat{\vartheta} = \vartheta - \vartheta_0\),

\[
\nabla_{\vartheta_0} \ell_{p,i} \approx \nabla_{\vartheta_0} \ell_{p,i} + \nabla_{\vartheta_0} \nabla_{\vartheta_0}^\top \ell_{p,i}(\hat{\vartheta} - \vartheta_0) = 0_p,
\]

where the last equality holds from \(\hat{\vartheta}\) being the MPLE, and with \(\nabla_{\vartheta} \ell_{p,i}\) standing for \(\nabla_\vartheta \ell_{p,i}|_{\vartheta = \hat{\vartheta}}\). Under the assumptions that \(D\) has full rank \(p\), and \(W\) is positive definite throughout the parameter space \(\Theta\), a Newton-Raphson algorithm comprises the non-singular \(p \times p\) system of equations for \(\vartheta\)

\[
\begin{align*}
(\nabla_{\vartheta^\top} \ell(\vartheta^{[\alpha]}) - S_\lambda)\vartheta^{[\alpha+1]} &= (\nabla_{\vartheta^\top} \ell(\vartheta^{[\alpha]}) - S_\lambda)\vartheta^{[\alpha]} + (S_\lambda \vartheta^{[\alpha]} - \nabla_\vartheta \ell(\vartheta^{[\alpha]})) \\
(D^\top WD + S_\lambda)\vartheta^* &= D^\top Wz,
\end{align*}
\]

where \(z := D\vartheta + W^{-1}u\) defines the pseudo-data vector associated with any \((r, F, Z)\) model. Moreover, equation (13) is expressed in terms of \(\vartheta^* := \vartheta^{[\alpha+1]}\), while the dependence of all the other variables on the \([\alpha]\)-th iteration is neglected to avoid clutter in the notation. Finally, by noticing that the above system can be recovered directly from the normal equations of a Generalized Least Squares (GLS) regression of \(z\) onto the columns of \(D\), using a weight matrix
and a ridge-type penalisation, it follows that Eq. 13 corresponds to the closed-form solution of the problem

$$\vartheta^* = \arg\min_{\vartheta \in \Theta} \| \sqrt{W}(z - Dt) \|^2 + t^T S_\lambda t.$$  

In other words, at every $[\alpha]$-th iteration, the GLS recursion produces a closed-form expression to update the optimisation algorithm, and this is repeated until convergence. Apart from giving an elegant solution to the log-likelihood maximisation problem, the P-IRLS algorithm also establishes a correspondence between MPLE and GLS, and this provides us with an equivalent expression smoothing parameter selection can be based on.

**Remark 1.** The use of matrix $D$ in the computations above reflects the possibility of dealing with models involving non-linear predictors. In other simpler instances, this quantity reduces to the design matrix $Z$, with potential gains in the computational time of the P-IRLS procedure. In fact, $D$ would usually depend on some functions of the parameter vector which need to be updated at every iteration; whereas, in the case of $D = Z$, this quantity can be stored outside the iteration loop.

### 3.2 Smoothing Parameter Selection

The correct specification of the “right” amount of smoothness is important for any practical modelling in non-parametric regression. In what follows, we adapt the Un-biased Risk Estimator (UBRE; e.g. Wood, 2006a) to the present context, so that smoothness selection is achieved from quantities that are directly stemming from the $(r, F, Z)$ representation of the model; a stable and efficient computational method to implement this criterion is discussed in Wood (2004).

In principle, vector $\lambda$ should be estimated in such a way that the fitted curves are as close as possible to the true unknown functions. To this end, let us consider the large sample approximation

$$-\nabla_{\vartheta} \ell(\vartheta) \overset{p}{\rightarrow} I$$

implied by the likelihood model and, under the regularity conditions listed in Section 1.1, it follows $D^TWD \overset{p}{\rightarrow} D^TDW$, where $W = \text{diag}(W_1, \ldots, W_n, 0_{p,p})$. Since $E[K] = 0_{p,p}$, it also holds that $E[K] = 0_{p,p}$ from the linearity of the expectation, hence $K = o_p(1)$ and $W = \tilde{W} + o(1)$ as $n \to \infty$. Further let

$$P = \sqrt{\tilde{W}D^TDW + S_\lambda}^{-1}D^\top \sqrt{\tilde{W}}$$

denote the influence matrix of the associated GLS model, namely the array such that the predicted values of the response $\sqrt{\tilde{W}}z$ can be written as $\hat{\mu} := \sqrt{\tilde{W}D} \vartheta^* = P\sqrt{\tilde{W}}z$, and $z := z(\tilde{W})$ be the pseudo-data vector evaluated at the asymptotic weight matrix. Then, by letting $\mu := E[\sqrt{\tilde{W}}z] = \sqrt{\tilde{W}D} \vartheta$ be the expected value of the GLS response, we define $\hat{\lambda}$ as the minimiser of the expected Mean Squared Error (MSE) of $\hat{\mu}$. Namely

$$\nabla^{-1}\mu - \hat{\mu}]^2 = \nabla^{-1}E[\sqrt{\tilde{W}}z - P\sqrt{\tilde{W}}z - \varepsilon]^2$$

$$= \nabla^{-1}E[\|\sqrt{\tilde{W}}(z - D\vartheta)\|^2 + \|\varepsilon\|^2 - 2\langle \sqrt{\tilde{W}}z - P\sqrt{\tilde{W}}z; \varepsilon \rangle],$$

where the stochastic term above is given by $W^{-1/2}u = \varepsilon \sim (0_n, I_n)$ since $E[u] = 0_p$ and $\text{Var}[u] = \tilde{W}$, while the expectation of the inner product results in

$$-2\nabla^{-1}E\langle \sqrt{\tilde{W}}z - P\sqrt{\tilde{W}}z; \varepsilon \rangle = -2\nabla^{-1}E[\varepsilon^\top (I_n - P)(\sqrt{\tilde{W}D} \vartheta + \varepsilon)]$$

$$= -2 + 2\nabla^{-1}E[\varepsilon^\top P \varepsilon] = -2 + 2\nabla^{-1}\text{tr}(P).$$

Then, the corresponding UBRE criterion for the $[\alpha + 1]$-th iteration step reads as

$$\lambda^{[\alpha+1]} := \arg\min_{\lambda} V_u(\lambda) := \| \sqrt{\tilde{W}}^{[\alpha+1]}(z^{[\alpha+1]} - D^{[\alpha+1]} \vartheta^{[\alpha+1]}) \|^2 / \tilde{n} - 1 + 2\kappa\text{tr}(P^{[\alpha+1]}) / \tilde{n}, \quad (14)$$
attractive in the context of unmeasured confounding as it allows to account for various degrees
parameter explained through an additive linear predictor (Radice et al., 2015). This feature is
doing this, we specialise our structure to describe a bivariate probit regression with association
4 Real Data Illustration: HIV Prevalence in Zambia

detailed in Supplementary Materials S.1 and S.2, respectively.

estimators as well as a method to compute confidence intervals for the included smooths are
of its ability to recover the unknown smooth functions shown in Figure 1 by a simulation study
The structure of the resulting fitting procedure is detailed in Algorithm 1, and an illustration
where

\[ \tilde{n} \]

is a given multiple of the sample size as determined by the dimension of \( \eta_k \), and
accounts for the multivariate nature of the framework. For instance, if we consider a bivariate
model where both the responses are ordinal polychotomous with just one association parameter
\( \gamma \), it follows that, for every individual \( i \), the corresponding array

\[ \eta_k = (\eta_{k_1-k_1-1}, \eta_{k_1-k_2}, \eta_{k_1-k_2-1}, \eta_{k_1}, \eta_{k_2})^T \]

is 5-dimensional and \( \tilde{n} = 5n + p \). An additional inflation parameter \( \kappa \) has been included in the
UBRE criterion and it can be increased from its usual value of 1 in order to obtain smoother
models. In effect, based on experimental results, Kim and Gu (2004) suggested to locate
\( \kappa \in [1.2, 1.4] \) to correct the tendency of prediction error criteria to over-fit the estimated curves.
Notice that the trace of the influence matrix \( P \) represents the effective degrees of freedom of the
model; in a penalised framework, they usually differ from the number of parametric model
components. In effect, based on experimental results, Kim and Gu (2004) suggested to locate
\( \kappa \) in order to obtain smoother estimated curves.

Algorithm 1

Pseudo-code for MPLE Computation under a Outer Iteration Scheme

Require: \( \alpha \in (0, \text{iter.max}) \); \( \kappa \geq 1 \); \( (r, F_j, Z) \); \( S_{\lambda} \)

\[ \theta^0, \lambda^0 \]

while \( \alpha \leq \text{iter.max} \) \lor \( \max |\theta^{(\alpha+1)} - \theta^{(\alpha)}| \geq 10^{-5} \) do

\[ \theta^{(\alpha+1)} \leftarrow \max_\theta \left[ \ell(\theta^{(\alpha)}) - \theta^{(\alpha)}S_{\lambda(\alpha)}\theta^{(\alpha)} \right] \]

\[ D_i^{(\alpha+1)} = \left. \frac{\partial \eta_i^{(\alpha+1)}}{\partial \theta} \right|_{\theta = \theta^{(\alpha+1)}} \quad u_i^{(\alpha+1)} = \left. \frac{\partial F_k \eta_i^{(\alpha+1)}}{\partial \eta_i} \right|_{\theta = \theta^{(\alpha+1)}} \]

\[ W_i^{(\alpha+1)} = \frac{1}{\pi} \left[ t_i^{(\alpha+1)} u_i^{(\alpha+1)} \right]^{\top} \quad K_i^{(\alpha+1)} = \left. \frac{\partial \eta_i^{(\alpha+1)}}{\partial \eta_i} \right|_{\theta = \theta^{(\alpha+1)}} \]

compute \( D^{(\alpha+1)}, u^{(\alpha+1)}, K^{(\alpha+1)}, W^{(\alpha+1)}, z^{(\alpha+1)} \) and \( P^{(\alpha+1)} \)

\[ \lambda^{(\alpha+1)} \leftarrow \min_\lambda \left[ \frac{1}{2} \left( z^{(\alpha+1)} - D^{(\alpha+1)} \theta^{(\alpha+1)} - \tilde{u}^{(\alpha+1)} \right) \right] + 2 \kappa \text{tr}(P^{(\alpha+1)})/\tilde{n} \]

end while

4 Real Data Illustration: HIV Prevalence in Zambia

We illustrate now the proposed framework via the estimation of a sample selection instance. In
doing this, we specialise our structure to describe a bivariate probit regression with association
parameter explained through an additive linear predictor (Radice et al., 2015). This feature is
attractive in the context of unmeasured confounding as it allows to account for various degrees
The resulting model is then applied to data from the 2007 Zambia Demographic Health Survey (DHS) to flexibly estimate the prevalence of HIV in the Zambian male population. Our analysis complements the study of McGovern et al. (2015) through the inclusion of non-parametric covariate effects, and the specification of the aforementioned elements proper of a distributional regression. The following discussion is further extended by Marra et al. (2015), to which we refer the reader for more extensive and thoughtful argumentations. All the relevant computations presented in the study are performed in the R environment (R Development Core Team, 2015) using the package SemiParBIVProbit (Marra and Radice, 2015) which implements the ideas discussed in this article for the binary case, and whose corresponding representation in the $(r, F_2, Z)$ form has been previously given in (9). Notice, however, that because of existing restrictions in the original data-set diffusion, just a one generated from it can be used for reproducibility purposes, and it can be accessed from the above-mentioned package (hiv); details on the employed model specification can be found in McGovern et al. (2015).

4.1 A Dichotomous Regression Defined Through Bivariate Copulae

The models presented in Section 2.2 where originally defined through a bivariate Gaussian distribution. This may be a strong assumption though, especially in applied disciplines where symmetries are unlikely or implausible: a mitigation of these constraints can then be achieved by extending the framework to copulae. As a first definition, let $F_{1,j}$ be the marginal distribution of the $j$-th component of $Y^*$, and consider the map $C_J : [0, 1]^J \rightarrow [0, 1]$, such that

$C_J(F_{1,1}(Y_1^*), \ldots, F_{1,J}(Y_J^*)) =: C_J(U_1, \ldots, U_J)$

is the joint cumulative distribution function of $(U_1, \ldots, U_J)^\top$. Then $U_j$ is uniformly distributed for each $j \in J$, and $C_J$ is called the $J$-variate copula of the vector $(Y_1^*, \ldots, Y_J^*)^\top$ which is a bona fide multivariate distribution function under the Sklar’s Theorem (Sklar, 1959). Notice that, simply by denoting $F_J(\eta_k) \equiv C_J(F_{1,1}(\eta_{1,k_1}), \ldots, F_{1,J}(\eta_{J,k_J}))$, any copula representation in principle belongs already to the class of models we have introduced; for a full account of copulae and their properties we refer to the monograph of Nelsen (2006).
A bivariate copula regression for dichotomous responses sets the probability of any $\pi_k \in \pi$, for $k \in \{0, 0\}, (0, 1), (1, 0), (1, 1) =: K$, as

$$
\pi_k := \mathbb{P}[Y_1 = k_1, Y_2 = k_2]
= (r^{-1} \circ C_2)(F_{1,1}(\eta_{1,k_1}), F_{1,2}(\eta_{2,k_2}); \gamma) = C_2(F_{1,1}(\eta_{1,k_1}), F_{1,2}(\eta_{2,k_2}); \gamma),
$$

where the last equality follows for $r$ being the identity map, and with $\gamma$ being an association parameter measuring the dependence between the two marginals. For optimisation purposes it is sometimes desirable to unbound the support of $\gamma$, hence a specific copula-dependent transformation $\gamma^*$ may be applied, which is taken here to be a function of the covariate vector $x_3$. Since the corresponding $(r, F_2, Z)$ representation of this model for non-random sample selection is given by

$$(\pi_k^*, C_2(\Phi(\eta_{1,k_1}), \Phi(\eta_{2,k_2}); \gamma^*(x_3)), Z),$$

in the proceeding all the IRLS quantities needed to perform estimation and inference can be derived from this, while the binding copula is intentionally left unspecified.

The specialisation of the model for dichotomous responses simplifies the generic framework considerably. In particular, by neglecting any triangular structure ($F = L = I_3$), $D_i$ reduces to the $3 \times p$ design matrix $X_i = (x_{i1}, x_{i2}, x_{i3})^T$, and $K_i = 0_{p,p}$; whereas the GLM representation implies $\partial^i_\ell / \partial \theta_k = 1 = \pi_k$ for any $k \in K$ actually observed, $\partial^2 \theta_k / \partial \pi^2_k = \pi_k^{-1}(1 - \pi_k)^{-2} - \pi_k^{-2}(1 - \pi_k)^{-1}$ and $\partial^2 \ell / \partial \theta_k^2 = -b''(\theta_k) = -\pi_k(1 - \pi_k)$. Let now $\eta_k = (\eta_{1,i}, \eta_{2,i}, \gamma_i^*)$ be the vector of the linear predictors evaluated at the $i$-th individual, where the subscript for $\gamma_i^*$ is introduced to remark its dependence on $x_{3,i}$, then we can further decompose

$$
\frac{\partial F_k}{\partial \eta_i} = \frac{\partial F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} \text{ and } W_i = \frac{1}{\pi_k} \frac{\partial^2 F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} \left( \frac{\partial F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} \right)^T
$$

with

$$
\frac{\partial^2 F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} \left( \frac{\partial F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} \right)^T = \frac{\partial^2 F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i}.
$$

If we further assume Standard Normal marginals for both the components of $Y$, \((15)\) specialises as

$$
\frac{\partial F_k}{\partial \eta_k} = \begin{bmatrix}
\frac{\partial \phi(\eta_{1,i})}{\partial \eta_{1,i}} & 0 & 0 \\
0 & \frac{\partial \phi(\eta_{2,i})}{\partial \eta_{2,i}} & 0 \\
0 & 0 & \frac{\partial \gamma_i}{\partial \gamma_i}
\end{bmatrix}
= \begin{bmatrix}
\frac{\partial \phi(\eta_{1,i})}{\partial \eta_{1,i}} & \frac{\partial \phi(\eta_{2,i})}{\partial \eta_{2,i}} & \frac{\partial \gamma_i}{\partial \gamma_i}
\end{bmatrix}
= \begin{bmatrix}
-\eta_{1,i} & -\eta_{2,i} & h_{3,i} \frac{\partial^2 \gamma_i}{\partial \gamma_i^2}
\end{bmatrix},
$$

where $h_{j,i}$ and $\partial \gamma_i / \partial \gamma_i^*$ are quantities specific to the copula employed. Moreover, $\partial^2 C_k / \partial F_k \partial F_k^T$ is the symmetric matrix with generic element $h_{l,m,i} = \partial h_{l,i} / \partial \Phi(\eta_{m,i})$, $l, m = 1, \ldots, 3$, under the notational abuse $\eta_{3,i} := \gamma_i$, and

$$
\frac{\partial^2 F_k}{\partial \eta_i} \frac{\partial C_k}{\partial \eta_i} \frac{\partial F_k}{\partial \eta_i} = \text{diag}\left(-h_{1,i} \phi(\eta_{1,i}) \eta_{1,i}, -h_{2,i} \phi(\eta_{2,i}) \eta_{2,i}, h_{3,i} \frac{\partial^2 \gamma_i}{\partial \gamma_i^2}\right).
$$

The derivations above make it clear that $W_i$ is a symmetric 3-dimensional matrix whose generic element $w_{l,m,i}$, for $l, m \neq 3$, after some tedious algebra, is given by

$$
w_{l,m,i} = \frac{1}{\pi_k} \left[h_{l,m,i} \phi(\eta_{1,i}) \phi(\eta_{m,i}) - 1_{l=m} h_{l,i} \phi(\eta_{1,i}) \eta_{1,i} \right] - \frac{1}{\pi_k} h_{l,i} h_{m,i} \phi(\eta_{1,i}) \phi(\eta_{m,i}) \quad l, m \neq 3,
$$

and expressions for $l, m = 3$ can be obtained in a similar fashion as based on the quantities derived above. Finally, the $i$-th addendum defining the Hessian matrix is simply $H_i = X_i^T W_i X_i$, and the pseudo-data vector $z_i = X_i \hat{\gamma} - W_i^{-1} u_i$ is $3 \times 1$, with $u_i = \pi_k^{-1}(\partial F_k / \partial \eta_i)$. 


4.2 Background and Results

HIV prevalence in a population is defined as the fraction of people who are infected or, expressed equivalently, as the probability that a randomly drawn individual has the disease. Accurate estimation of the HIV prevalence is essential to policy makers to develop effective control programmes and interventions. Only in recent years, however, in countries where the diffusion of the virus is generalised epidemic, the lack of available administrative data has been overcome by the intensive use of population-based surveys [Boerma et al., 2003]. This is an important new source of data: prior to their introduction, national estimates have prevalently relied on some number of sentinel antenatal clinics [UNAIDS-World Health Organization, 2007], whose data may nonetheless present different sources of bias. First of all, their samples are based only on sexually active women who are pregnant and attend a clinic; secondly the location of the facilities, mostly concentrated in urban areas, may also induce a bias even in the subpopulation of pregnant women. These points have been elucidated and discussed with greater details in Montana et al. (2008) and Arpino et al. (2014), among the others.

On the other hand, participation rates for HIV testing in national surveys are generally low, and ranges from 72% for men to 77% for women in the 2007 Zambia DHS [Hogan et al., 2012], although even lower peaks are recorded in the 2004 Malawi DHS (63% and 70%, respectively). There are potentially many reasons inducing this pattern, including concerns, lack of incentive to participate, survey fatigue or migration of those targeted for interview [Gersovitz, 2011; Sterck, 2013; McGovern et al., 2015]; missing data on respondents’ HIV status represent therefore a not necessarily less severe cause of bias than the ones already mentioned above. This case study focuses on refusal to be tested for HIV, which is commonly regarded as the main reason of missingness in surveys.

Notice, however, that the use of imputation or weighting techniques are likely to produce biased estimates if the selection mechanism does not occur at random, an assumption violated wherever the reasons of the refusal to test are caused by some unobserved factors. This is the case, for example, when individuals refuse to screen because they already know (or correctly predict) their HIV status, and fear others will learn about their seropositivity if they participate in the survey [McGovern et al., 2015]. The framework introduced in this article allows us to estimate a Heckman-type selection model which is able to account for the possibility that data are missing not at random. Specifically, this is achieved by modelling item non-response as a function of unobserved variables that also affect the individual HIV status, and by specifying the selection mechanism together with an assumption on the distribution of the unobservables.

To foster the identification of the causal mechanism in the study an exclusion restriction is imposed: that is we qualify the dependence of the missing data mechanism on a relevant variable independent of both the outcome of interest given the willingness to take the test, and the unobservables. This is usually labelled an instrument in econometrics and epidemiology, and the interviewer identity is regarded here as a valid instrument to be employed. In fact, previous researches, including Bärnighausen et al. (2011), Hogan et al. (2012), Janssens et al. (2014) and McGovern et al. (2015), have successfully included such a variable in their studies, on the grounds that interviewer identity generally predicts consent to be tested, but it is unlikely it also affects the actual HIV status.

A pictorial representation of the effects on the estimates of applying a sample selection model is reported in Figure 2. By comparison with the first map, the second one shows immediately how the simple imputation of the values under a random missingness assumption may severely underestimate the HIV prevalence in the Zambian provinces. The imputation has been conducted by making predictions from the univariate model upon discarding the missing values. The third map depicts instead how the association parameter of the employed copula varies among the different regions of the country, and it has been constructed by exploiting its dependence on the geographical location where the survey took place.

Figure 3 then reports the smooth function estimates for the treatment and outcome equa-
First two panels: HIV prevalence for the male population in nine of the ten Provinces of Zambia (Northern, Muchinga, as well as part of Eastern have been merged because of the data availability) applying an imputation model not accounting for the possible presence of values missing not at random, and the corresponding estimates when a bivariate model is fitted instead, respectively. Third panel: the estimated absolute values of the association parameter, with range \((1, \infty)\), in a Joe copula rotated counterclockwise of \(90^\circ\). The higher its value, the stronger the estimated association between the two equations; that is, the more relevant the impact of neglecting unobservables in the estimation of the HIV prevalence. The spatial effects are obtained here by specifying appropriately the penalty matrix as described in Section 2.1.

As a final remark, we shall stress that the assumption of distinct distributions may in principle lead to different estimates of the HIV prevalence (although it seems not to be an issue in this particular application as reported, for instance, by McGovern et al., 2015), as well as these can be impacted by the specific functional form of the covariates employed. To deal with this critic, some authors advanced instead the identification of a region (rather than of a singleton) of plausible values in which the parameters of interest necessarily lie, given the available data and the maintained assumptions. This switch from point to partial identification is discussed in general terms in Manski (1995, 2003) and Horowitz and Manski (2000), and applied to a similar HIV context by Arpino et al. (2014). Although theoretically valid and appealing, a major drawback of this approach is the realistic possibility of obtaining large width of the estimated bounds: this in turn may let the communication of any result to policymakers harsh even in the case where the identifying region is shrunken by the imposition of a monotone instrumental variable.

Acknowledging this issue, our estimated model extends the traditional Heckman-type by accounting for three degrees of flexibility: the inclusion of non-parametric effects in the representation of the covariate-response functional form, the specification of bivariate copulae to detect more complex dependence structures than classical distributions usually assume, and the direct modelling of the association parameters in terms of some predictors. It is our hope, in this way, to conjugate both the point and partial identification strengths by providing the
researchers with a set of flexible tools aimed at exploring the identifying region widely, and so to make better informed judgments about the robustness of their results wherever a point estimate is sought.

5 Discussion

This paper has devised a generic framework for the representation and estimation of a Generalized Linear Model for a \( J \)-dimensional vector of discrete responses, with a ridge-type penalisation term employed in the fitted algorithm. The resulting class of models allows us to include non-parametric and spatial covariate effects, among the others, as represented through the penalty matrix \( S_\lambda \). In this way, a baseline multivariate Generalized Additive Model has been effectively extended to encompass different kind of modelling instances within the same unifying framework. In fact, by translating the approach of Peyhardi et al. (2014) to the multivariate case, only the \((r,F_j,Z)\) form and the matrix \( S_\lambda \) are formally required to apply the proposed estimation algorithm and related inferential results to different models in the class.

In particular, once the class has been described in some generality, we have introduced a number of bivariate models employed in the literature to account for the possible presence of residual confounding in observational studies. The proposed representation provided us with a flexible machinery able to extend these models in various directions, foremost towards the additive semi-parametric specification of the linear predictors in the spirit of (V)GAMs. This is, \textit{per se}, already a relevant issue in applied research, since it permits to handle a data-driven
representation of the covariate-response relationship and hence to alleviate a possible source of bias stemming from model mis-specification. Moreover, we have described how the framework can be further specified in order to include multivariate distributions as computed by copulae of univariate marginals: some analytical results have been derived for Normal marginals within a bivariate dichotomous regression model.

A further feature illustrated by the article has been the direct modelling of any copula association parameter in terms of known predictors. As shown in the analysis of non-random sample selection for the 2007 DHS Zambia dataset, this characteristic is attractive as it allowed to quantify the strength of the unobservables within the different provinces of the country, and this in turns enabled us to provide new insights about the severity of the non-response issue in the study. In particular, Figure 2 showed that the magnitude of the copula association parameter can vary considerably even between geographically close provinces, like Northern and Luapula in the example. On this point, the relevant literature has already stressed that demographic and environmental factors, like the presence of cities or high density housing, may impact the estimates of the HIV prevalence. Hence, the combination of this knowledge with the possibility of letting the association parameters depend on observed variables seems to us an attractive feature that could be investigated more closely.

As a natural specification of the proposed framework, the practical implementation of models involving ordinal responses are being developed, whereas the estimation of higher dimensional systems of equations is still limited by the necessity of computing multivariate integrals with a good degree of accuracy. Under this respect, the exploitation of a more comprehensive class of models for copula distributions may be beneficial, possibly by allowing the non-parametric estimation of the marginals and/or the corresponding copulae. These are only some of the possible avenues of future research that will be undertaken.

References

Arpino, B., De Cao, E., and Peracchi, F. (2014). Using panel data for partial identification of Human Immunodeficiency Virus prevalence when infection status is missing not at random. Journal of the Royal Statistical Society, Series A, 177(3):587–606.

Barndorff-Nielsen, O. and Cox, D. (1994). Inference and Asymptotics. Chapman & Hall, London, UK.

Bärnighausen, T., Bor, J., Wandira-Kazibwe, S., and Canning, D. (2011). Correcting HIV prevalence estimates for survey nonparticipation using Heckman-type selection models. Epidemiology, 22(1):27–35.

Becher, H. (1992). The concept of residual confounding in regression models and some applications. Statistics in Medicine, 11(13):1747–1758.

Boerma, J., Ghys, P., and Walker, N. (2003). Estimates of HIV-1 prevalence from national population-based surveys as a new gold standard. The Lancet, 362(9399):1929–1931.

Dale, J. (1986). Global cross-ratio models for bivariate, discrete, ordered responses. Biometrics, 42(4):909–917.

Eilers, P. and Marx, B. (1996). Flexible smoothing with B-splines and penalties. Statistical Science, 11(2):89–121.

Fuchs, V. (1982). Economic Aspects of Health, chapter Time Preference and Health: An Exploratory Study. University of Chicago Press, Chicago, IL.
Gersovitz, M. (2011). HIV testing: Principles and practice. The World Bank Research Observer, 26(1):1–41.

Green, P. (1984). Iteratively Reweighted Least Squares for Maximum Likelihood estimation, and some robust and resistant alternatives (with discussion). Journal of the Royal Statistical Society, Series B, 46(2):149–192.

Green, P. and Silverman, B. (1994). Nonparametric Regression and Generalized Linear Models. A Roughness Penalty Approach. Chapman & Hall, London, UK.

Greene, W. and Hensher, D. (2010). Modeling Ordered Choices. A Primer. Cambridge University Press, Cambridge, UK.

Haberman, S. (1980). Discussion of McCullagh (1980). Journal of the Royal Statistical Society, Series B, 42(2):136–137.

Hastie, T. and Tibshirani, R. (1986). Generalized Additive Models (with discussion). Statistical Science, 1(3):297–318.

Hastie, T. and Tibshirani, R. (1990). Generalized Additive Models. Chapman & Hall, London, UK.

Heckman, J. (1978). Dummy endogenous variables in a simultaneous equation system. Econometrica, 46(4):931–959.

Heckman, J. (1979). Sample selection bias as a specification error. Econometrica, 47(1):153–161.

Hogan, D., Salomon, J., Canning, D., Hammitt, J., Zaslavsky, A., and Bärnighausen, T. (2012). National HIV prevalence estimates for Sub-Saharan Africa: Controlling selection bias with Heckman-type selection models. Sexually Transmitted Infections, 88:i17–i23.

Horowitz, J. and Manski, C. (2000). Nonparametric analysis of randomized experiments with missing covariate and outcome data. Journal of the American Statistical Association, 95(449):77–84.

Imbens, G. (2014). Instrumental variables: An econometrician’s perspective. Statistical Science, 29(3):323–358.

Janssens, W., van der Gaag, J., de Wit, T., and Tanović, Z. (2014). Refusal bias in the estimation of HIV prevalence. Demography, 51(3):1131–1157.

Kauermann, G. (2005). Penalized spline smoothing in multivariable survival models with varying coefficients. Computational Statistics & Data Analysis, 49(1):169–186.

Kauermann, G., Krivobokova, T., and Fahrmeir, L. (2009). Some asymptotic results on generalized penalized spline smoothing. Journal of the Royal Statistical Society, Series B, 71(2):487–503.

Kim, Y. and Gu, C. (2004). Smoothing spline Gaussian regression: More scalable computation via efficient approximation. Journal of the Royal Statistical Society, Series B, 66(2):337–356.

Klein, N., Kneib, T., Klasen, S., and Lang, L. (2015). Bayesian structured additive distributional regression for multivariate responses. Journal of the Royal Statistical Society, Series C (in press).

Kneib, T. (2013). Beyond mean regression. Statistical Modelling, 13(4):275–303.
Manski, C. F. (1995). *Identification Problems in the Social Sciences*. Harvard University Press, Cambridge, MA.

Manski, C. F. (2003). *Partial Identification of Probability Distributions*. Springer-Verlag, New York, NY.

Marra, G. and Radice, R. (2013). A Penalized Likelihood estimation approach to semiparametric sample selection binary response modeling. *The Electronic Journal of Statistics*, 7:1432–1455.

Marra, G. and Radice, R. (2015). *SemiParBIVProbit: Semiparametric Bivariate Probit Modelling*. R package version 3.3.

Marra, G., Radice, R., Bärnighausen, T., Wood, S., and McGovern, M. (2015). A unified modeling approach to estimating HIV prevalence in Sub-Saharan African countries. *Research Report No. 324, Department of Statistical Science, University College London*.

Marra, G. and Wood, S. (2012). Coverage properties of confidence intervals for Generalized Additive Model components. *Scandinavian Journal of Statistics*, 39(1):53–74.

McCullagh, P. (1980). Regression models for ordinal data (with discussion). *Journal of the Royal Statistical Society, Series B*, 42(2):109–142.

McGovern, M., Bärnighausen, T., Marra, G., and Radice, R. (2015). On the assumption of bivariate normality in selection models. A copula approach applied to estimating HIV prevalence. *Epidemiology*, 26(2):229–237.

Miranda, A. and Rabe-Hesketh, S. (2006). Maximum Likelihood Estimation of endogenous switching and sample selection models for binary, ordinal, and count variables. *The Stata Journal*, 6(3):285–308.

Montana, L., Mishra, V., and Hong, R. (2008). Measuring the HIV/AIDS epidemic: Approaches and challenges. *Sexually Transmitted Infections*, 84:i78–i84.

Nelder, J. and Wedderburn, R. (1972). Generalized Linear Models. *Journal of the Royal Statistical Society, Series A*, 135(3):370–384.

Nelsen, R. (2006). *An Introduction to Copulas*. Springer, New York, NY.

Nychka, D. (1988). Bayesian confidence intervals for smoothing splines. *Journal of the American Statistical Association*, 83(404):1134–1143.

O’Sullivan, F., Yandell, B., and Raynor, W. (1986). Automatic smoothing of regression functions in Generalized Linear Models. *Journal of the American Statistical Association*, 81(393):96–103.

Peyhardi, J., Trottier, C., and Guédon, Y. (2014). A new specification of Generalized Linear Models for categorical data. [arXiv:1404.7331v2](https://arxiv.org/abs/1404.7331v2).

R Development Core Team (2015). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Radice, R., Marra, G., and Wojtyś, M. (2015). Copula regression spline models for binary outcomes. *Statistics and Computing (in press)*.

Rigby, R. and Stasinopoulos, D. (2005). Generalized Additive Models for Location, Scale and Shape. *Journal of the Royal Statistical Society, Series C*, 54(3):507–554.
Rue, H. and Held, L. (2005). *Gaussian Markov Random Fields*. Chapman & Hall/CRC, Boca Raton, FL.

Ruppert, D., Wand, M., and Carroll, R. (2003). *Semiparametric Regression*. Cambridge University Press, Cambridge, UK.

Sander, W. (1995). Schooling and quitting smoking. *The Review of Economics and Statistics*, 77(1):191–199.

Silverman, B. (1985). Some aspects of the spline smoothing approach to non-parametric regression curve fitting (with discussion). *Journal of the Royal Statistical Society, Series B*, 47(1):1–52.

Sklar, A. (1959). Fonctions de répartition à n dimensions et leurs marges. *Publications de l’Institut de Statistique de l’Université de Paris*, 8:229–231.

Sterck, O. (2013). Why are testing rates so low in Sub-Saharan Africa? Misconceptions and strategic behaviors. *Forum for Health Economics & Policy*, 16(1):219–257.

Stevens, S. (1946). On the theory of scales of measurement. *Science*, 103(2684):677–680.

UNAIDS-World Health Organization (2007). *Guidelines for Conducting HIV Sentinel Serosurveys among Pregnant Women and Other Groups*. UNAIDS, Geneva, CH.

van der Pol, M. (2011). Health, education and time preference. *Health Economics*, 20(8):906–920.

Vossmeyster, A. (2014). Determining the proper specification for endogenous covariates in discrete data settings. *Advances in Econometrics*, 34:223–247.

Wahba, G. (1983). Bayesian “confidence intervals” for the cross-validated smoothing spline. *Journal of the Royal Statistical Society, Series B*, 45(1):133–150.

Wood, S. (2003). Thin plate regression splines. *Journal of the Royal Statistical Society, Series B*, 65(1):481–493.

Wood, S. (2004). Stable and efficient multiple smoothing parameter estimation for Generalized Additive Models. *Journal of the American Statistical Association*, 99(467):673–686.

Wood, S. (2006a). *Generalized Additive Models. An Introduction With R*. Chapman & Hall/CRC, Boca Raton, FL.

Wood, S. (2006b). On confidence intervals for Generalized Additive Models based on penalized regression splines. *Australian & New Zealand Journal of Statistics*, 48(4):445–464.

Wooldridge, J. (2002). *Econometric Analysis of Cross Section and Panel Data*. MIT Press, Cambridge, MA.

Yee, T. and Wild, C. (1996). Vector Generalized Additive Models. *Journal of the Royal Statistical Society, Series B*, 58(3):481–493.
S.1 Asymptotic Behaviour of the Estimator

This section provides some arguments about the asymptotic behaviour of the proposed MPL estimator. Analogous results were also achieved by [Kauermann, 2005] in the context of survival models, and by [Radice et al., 2015] for a bivariate system of dichotomous outcomes. Although our derivations are based on the somehow theoretically stringent assumption that the dimension of the spline bases does not increase with the sample size, this instance is still worth to be considered because, in practice, the bases’ dimensions have to be fixed in order to achieve estimation. Nonetheless, by taking the number of the bases relatively rich such to appropriately describe the unknown curves in the model, it is possible to assume heuristically that the approximation bias is negligible compared to the estimation variability (Kauermann, 2005). To the best of our knowledge, at present the relaxation of this assumption has been confined to the sole analysis of B-splines for their convenient representation and handling as, for instance, did [Kauermann et al., 2009]. Therefore, despite the theoretical relevance of these results, they still do not encompass the whole range of smooths allowed by this work.

Let \( \vartheta_0 \) be the “true” parameter vector, in the sense that it induces the best approximating likelihood corresponding to the structure that has generated the data. Namely, \( \vartheta_0 := \text{arg min}_{\vartheta \in \Theta} \text{KL}(L_t|L_n) = \mathbb{E}[\ell_t - \ell_n(\vartheta)] \), where the expectation above is carried out with respect to the true model distribution. As a consequence, by direct differentiation of the above equation, we are implicitly defining \( \vartheta_0 \) to be the vector such that
\[
0 = \mathbb{E}[\nabla_{\vartheta_0} \ell_n].
\]
For the proceeding analysis we rely on the following regularity conditions:

\[ \begin{align*}
\text{(A.1)} & \quad \nabla_{\vartheta_0} \ell_n = O_p(n^{1/2}) ; \\
\text{(A.2)} & \quad \mathbb{E}[\nabla_{\vartheta_0} \vartheta_0^T \ell_n] = O(n) ; \\
\text{(A.3)} & \quad \nabla_{\vartheta_0} \vartheta_0^T \ell_n - \mathbb{E}[\nabla_{\vartheta_0} \vartheta_0^T \ell_n] = O_p(n^{1/2}) ; \text{ and} \\
\text{(A.4)} & \quad S_\lambda = o(n^{1/2}).
\end{align*} \]

Following [Kauermann, 2005], this assumption can be equivalently restated as \( \lambda_j, m_j = o(n^{1/2}) \) from the very construction of the penalty matrix, and from the fact that its dimensionality is taken fixed as \( n \) increases.

The above (A.1)-(A.3) are the standard conditions for the consistency of the unpenalized ML estimator, whereas (A.4) ensures that, in the large sample limit, \( P_\lambda \) becomes irrelevant for the fitting. For a further investigation, we also need an additional condition aimed at describing the behaviour of the log-likelihood third derivatives, and it guarantees the asymptotic Normal distribution of the score:

\[ \text{(A.5) for every } \vartheta \in \varTheta, (\partial^3/\partial \vartheta^3) \ell_n(\vartheta) \text{ exists and satisfies for every point } x \in \mathbb{R} \text{ and every parameter in the neighbourhood of } \vartheta^*_0; \quad |(\partial^3/\partial \vartheta^3) \ell_n(\vartheta)| \leq M(x), \text{ with } \mathbb{E}[M(x)|\vartheta^*_0] < \infty; \text{ and let } 0 \leq I(\vartheta^*_0) < \infty. \]

Then it follows:

**Proposition 2.** Let \( \vartheta_0 \) be the parameter vector defined as in (S1) and assume that conditions (A.1)-(A.5) hold; then the MPL estimator \( \hat{\vartheta} := \text{arg max}_{\vartheta \in \Theta} \ell(\vartheta) - 1/2 \vartheta^T S_\lambda \vartheta \) satisfies
\[
\hat{\vartheta} - \vartheta_0 = F^{-1}(\lambda)(\nabla_{\vartheta_0} \ell(\vartheta_0) - S_\lambda \vartheta_0)[1 + o_p(1)], \tag{S1}
\]
with \( F^{-1}(\lambda) = (S_\lambda - \mathbb{E}[\nabla \vartheta_0 \vartheta_0^\top \ell(\vartheta_0)])^{-1} \). In particular, the leading stochastic component in \( S_1 \) has asymptotic order \( O_p(n^{-1/2}) \).

**Proof.** We first set the notation. Let us denote by \( \vartheta^j \) the \( j \)-th component of the parameter vector \( \vartheta = (\vartheta^1, \ldots, \vartheta^p)^\top \), and define subsequently \( \ell_{p,j} := \partial \ell_p/\partial \vartheta^j \) the partial derivative of the penalized log-likelihood with respect to \( \vartheta^j \); higher order derivatives are denoted subsequently. Also, the “hat” notation \( \hat{\ell}_p \) stands for \( \ell_p(\hat{\vartheta}) \), while the convention of omitting the listing of parameters is used wherever the relevant quantities are evaluated at the best coefficient \( \vartheta_0 \), that is \( \ell_p := \ell_p(\vartheta_0) \).

Using the Einstein summation convention, we expand \( \hat{\ell}_p \) around \( \ell_{p,r} \) using a second order Taylor approximation:

\[
0 = \hat{\ell}_{p,r} = \ell_{p,r} + \ell_{p,rs}(\hat{\vartheta} - \vartheta_0)^s + \frac{1}{2} \ell_{p,rs}(\hat{\vartheta} - \vartheta_0)^s \ell_{p,rt} + \cdots
\]

with \( (\hat{\vartheta} - \vartheta_0)^s := \vartheta^s - \vartheta_0^s \) and \( (\hat{\vartheta} - \vartheta_0)^st = (\vartheta^s - \vartheta_0^s)(\vartheta^t - \vartheta_0^t) \). Solving the above equation for \( \hat{\vartheta} - \vartheta_0 \), and denoting by superscripts the inverses of the respective quantities, we get (Barndorff-Nielsen and Cox 1994):

\[
(\hat{\vartheta} - \vartheta_0)^s = -\ell_{p,rs}^{-1} + \frac{1}{2} \ell_{p,rs}^{-1} \ell_{p,rt} + \cdots \quad (S2)
\]

where \( \ell_{p,rs} := \ell_{p,rs}(\vartheta) \) and \( \ell_{p,rs} \) is the \( (r,s) \)-th element of the inverse observed (penalized) Fisher Information. Equation \( (S2) \) can be simplified as follows (see, for example, Kauermann 2005): \( \ell_{p,rs} := f_{rs}(\lambda) + r_{rs} \), where \( f_{rs}(\lambda) := f_{rs}(0) - s_{rs}^\lambda \) is the penalized expected Fisher Information contribution: \( f_{rs}(0) := \mathbb{E}[\partial \ell_p/\partial \vartheta^r \partial \vartheta^s] \), and \( r_{rs} := \ell_{rs} - f_{rs}(0) \).

Under assumptions \( (A.2) \) and \( (A.4) \) we find that \( f_{rs}(\lambda) \) is of asymptotic order \( O(n) \), and that \( r_{rs} = O_p(n^{1/2}) \) directly from \( (A.3) \). We can then simplify the first term of \( (S2) \) as

\[
-\ell_{p,rs} = \mathbb{E}[\ell_{p,rs} \ell_{p,rs}]^{-1} \mathbb{E}[\ell_{p,rs} \ell_{p,rs}]^{-1} \mathbb{E}[\ell_{p,rs} \ell_{p,rs}]^{-1} (\mathbb{E}[\ell_{p,rs} \ell_{p,rs}] + \ell_{p,rs})
\]

\[
= -f_{rs}(\lambda) + f_{rs}(\lambda) f_{su}(\lambda)(-f_{rs}(\lambda) + \ell_{p,rs})
\]

that is \( \ell_{p,rs} = f_{rs}(\lambda)[1 + O(n^{-1})O_p(n^{1/2})] = f_{rs}(\lambda)[1 + O_p(n^{-1/2})] \).

We need to characterise next the order of \( \ell_{p,rs} \), which in turns depend on the one of \( \ell_{p,stu} \). First note that \( \ell_{p,stu} = \ell_{stu} \) from the very construction of the penalized likelihood estimator, so that we can safely apply \( (A.5) \) implying that we can bound in probability the third derivative of the log-likelihood. Then, by the strong law of large numbers, we have that, for almost every sequence of \( \{x_1, \ldots, x_n\} \) and every \( \vartheta \in \Theta \),

\[
|n^{-1} \ell_{stu}| \leq n^{-1} \sum_i M(x_i) \xrightarrow{a.s.} \mathbb{E}[M(x)]
\]

as \( n \to \infty \), hence \( n^{-1} \ell_{stu} = O_p(1) \). It is then implied \( \ell_{stu} = O_p(n) \) and, after some tedious computations, \( \ell_{p,stu} = f_{stu}(\lambda) f_{stu}(\lambda)(\omega_{stu}(\lambda)O_p(n) = O_p(n^{2}) \) so that \( \ell_{p,stu} = O_p(n^{1/2} - o(n^{1/2})) \). We also find that \( \ell_{p,stu} \) has order \( O_p(n^{-1/2} + o(n^{-1/2})) \), that is the second addendum in \( (S2) \) becomes asymptotically negligible compared to \( \ell_{p,stu} \). We can then write \( (\hat{\vartheta} - \vartheta_0)^s = -f_{rs}(\lambda) f_{rs}(\lambda)[1 + o_p(1)] \), whose leading terms, in matrix notation, are \( F^{-1}(\lambda)\nabla S_{\lambda} \ell(\vartheta_0) - S_{\lambda} \ell(\vartheta_0) \), from which the assertion follows.

The stochastic order of the above terms then stems from \( f_{rs}(\lambda) f_{rs}(\lambda) = O_p(n^{-1/2}) + o_p(n^{-1/2}) = O_p(n^{-1/2}) \).
The above derivations also allows us to characterise the bias and the variance of the MPL estimator, as well as their corresponding asymptotic orders. In particular, we find that

$$\mathbb{E}[\hat{\vartheta}] - \vartheta_0 = \mathbf{F}^{-1}(\lambda)\mathbf{S}_\lambda \vartheta_0[1 + o(1)]$$

(S3)

and

$$\mathbb{V} \text{ar}[\hat{\vartheta}] = -\mathbf{F}^{-1}(\lambda)\mathbb{E}[\nabla \vartheta_0 \vartheta_0^T \ell(\vartheta_0)]\mathbf{F}^{-1}(\lambda)[1 + o(1)],$$

(S4)

with orders of $o(n^{-1/2})$ and $O(n^{-1})$, respectively. In fact, we immediately obtain the (asymptotic) equivalence

$$\hat{\vartheta} - \vartheta_0 \rightarrow -f^s(\lambda)\ell_p,s[1 + o_p(1)]$$

from which

$$\mathbb{E}[\hat{\vartheta} - \vartheta_0]^r = -\mathbb{E}[f^s(\lambda)(\ell_s - s^*_\lambda \vartheta_0)][1 + o(1)] = f^s \lambda_{s} \vartheta_0[1 + o(1)]$$

and

$$\mathbb{V} \text{ar}[\hat{\vartheta}] = (f^s(\lambda))^2\mathbb{V} \text{ar}[\ell_s][1 + o(1)] = - (f^s(\lambda))^2 f_{r,s}(0)[1 + o(1)].$$

Finally, invoking (A.2) and (A.4) and since $f^s(\lambda)$ is $O(n^{-1})$, we compute $\mathbb{E}[\hat{\vartheta} - \vartheta_0]^r = O(n^{-1})o(n^{1/2}) = o(n^{-1/2})$, while $\mathbb{V} \text{ar}[\hat{\vartheta}]$ is led by terms of order $O(n^{-2})O(n) = O(n^{-1})$.

### S.2 Confidence Intervals Computation

At convergence of the estimation algorithm, the penalised GLS representation of the model induces a covariance matrix of the estimator of the form $\mathbf{V}_{\hat{\vartheta}} = \mathcal{H}_p^{-1} \mathcal{H}_p^{-1}$ which can in principle be used to compute the standard errors of each component of $\hat{\vartheta}$. An appealing alternative approach to conduct inference, however, is to advocate a Bayesian reasoning as based on the posterior distribution of $\vartheta|w$

$$\vartheta|w \sim \mathcal{N}_p([\mathbf{D}^T \mathbf{W}d + \mathbf{S}_\lambda]^{-1} \mathbf{D}^T \mathbf{Wz}, [\mathbf{D}^T \mathbf{W}d + \mathbf{S}_\lambda]^{-1})$$

which is equivalent to choose $\vartheta|w \sim \mathcal{N}_p([\mathbf{D}^T \mathbf{W}d + \mathbf{S}_\lambda]^{-1} \mathbf{D}^T \mathbf{Wz}, [\mathbf{D}^T \mathbf{W}d + \mathbf{S}_\lambda]^{-1})$, with $\mathbf{V}_\vartheta := -\mathcal{H}_p^{-1}$. The Bayesian framework above emerges naturally from the specification of the model through a roughness penalty approach. In effect, as [Wahba 1983] and [Silverman 1985] recognised, the imposition of any kind of penalisation in the estimating procedure corresponds to the explication of some kind of prior beliefs about the likely features of the true model. Specifically, the definition of a normal prior for $\vartheta$, $f_\vartheta \propto \exp\{-1/2 \vartheta^T \mathbf{S}_\lambda \vartheta\}$, implies that smoother models are more likely than wiggly ones, while it gives equal probability density to all models of equal smoothness ([Wood 2006b]). The stated posterior distribution is then a consequence of the asymptotic normality of $w := \mathbf{D}^T \mathbf{Wz}$. Upon re-writing $w = \mathbf{D}^T \mathbf{W}d\vartheta + \mathbf{D}^T \mathbf{u}$, it holds that the last addendum is asymptotically bounded by a random vector with distribution $\mathcal{N}_p(0_p, \mathbf{D}^T \mathbf{W}d)$ because of [A.5] whereas the first one converges in probability to $\mathbf{D}^T \mathbf{W}d\vartheta$ from which the desired distribution follows.

For the construction of confidence intervals of the non-parametric model components, the employment of $\mathbf{V}_\vartheta$ is usually preferred to $\mathbf{V}_{\hat{\vartheta}}$. In fact, as argued by [Marra and Wood 2012] in the context of GAMs, the former can produce intervals with close to nominal “across-the-function” frequentist coverage probabilities, as resulting from the inclusion in $\mathbf{V}_\vartheta$ of both a bias and a variance component, a feature which is not shared instead by $\mathbf{V}_{\hat{\vartheta}}$. A key requirement at the basis of the result is that the magnitude of the bias component is substantially of a small portion compared to the sampling variability, an occurrence that is guaranteed wherever heavily over-smoothing is prevented ([Nychka 1988]). Point-wise confidence intervals for the estimated non-parametric curve $\hat{s}_{j,l,j}$ are then obtained from $\mathcal{N}(s_{j,l,j}(v_{j,l,j},i), b^T_{j,l,j,i} \mathbf{V}_{\vartheta,j,l,j}[b_{j,l,j,i}], \mathbf{V}_{\vartheta,j,l,j}[b_{j,l,j,i}])$,

3
Let us consider first a Taylor expansion of $-2\ell(\hat{\theta}^*)$ about $\hat{\theta}$:

$$-2\ell(\hat{\theta}^*) \approx -2\ell(\hat{\theta}) - 2(\hat{\theta}^* - \hat{\theta})^\top \nabla_{\hat{\theta}}\ell(\hat{\theta}) - (\hat{\theta}^* - \hat{\theta})^\top \nabla_{\theta^*} \ell(\theta^* - \hat{\theta}),$$

and recall that, in the large sample approximation, $-\nabla_{\theta^*} \ell(\theta^*) = D^\top WD \overset{p}{\to} D^\top \overline{W} D$, hence we can write the addenda in the above expression as:

$$(\hat{\theta}^* - \hat{\theta})^\top D^\top \overline{W} D(\hat{\theta}^* - \hat{\theta}) = \|\sqrt{\overline{W}}(\overline{Z} - D\hat{\theta}^*)\|^2 + \|\sqrt{\overline{W}}^{-1} u\|^2 - 2 \langle \overline{Z} - D\hat{\theta}^*; u \rangle$$

where $V_{\theta, [j,l_j]}$ is the sub-matrix of $V_\theta$ corresponding to the parameters associated to the $(j, l_j)$-th smooth.

More generally, confidence intervals for a non-linear function $T(\hat{\theta})$ of the MPLE can be constructed by a convenient simulation scheme from the posterior distribution $\theta|\bf{w}$, as illustrated in the pseudo-code given in Algorithm S1.

To conclude, the asymptotic equivalence between the frequentist and the Bayesian variance estimators can be established as follows:

**Corollary 1** (to Proposition 2). Under assumptions (A.1)-(A.5) the re-scaled frequentist and Bayesian variance estimators $\sqrt{n}V_{\hat{\theta}}$ and $\sqrt{n}V_\theta$, respectively, converge to the same quantity

$$-\sqrt{n}E^{-1}[\nabla_{\hat{\theta}} \ell(\hat{\theta})]$$

as $n \to \infty$.

**Proof.** Using equation (S5) above, we derive

$$\text{Var}[\hat{\theta}^*] = (f^{rs}(\lambda))^2 \text{Var}[\hat{\ell}_a][1 + o(1)] = -(f^{rs}(\lambda))^2 f_{rs}(0)[1 + o(1)],$$

from which

$$\sqrt{n} \text{Var}[\hat{\theta}^*] = -\sqrt{n}(f_{rs}(0) - s_{rs}^*)^{-2} f_{rs}(0)[1 + o(1)]$$

$$\approx -\sqrt{n}^{-1}(\sqrt{n}^{-1} f_{rs}(0) - o(1))^{-2} f_{rs}(0) \approx -\sqrt{n}(f_{rs}(0))^2 f_{rs}(0) = -\sqrt{n}(f_{rs}(0))^{-1};$$

this corresponds immediately to the statement once written in matrix notation. Similarly, we can compute the asymptotic limit of the Bayesian variance estimator: reminding that $V_\theta = -(\nabla_{\theta^*} \ell_p(\theta))^{-1}$, analogous arguments as above lead to:

$$-\sqrt{n}f_{rs}^{rs} = -\sqrt{n}f_{rs}(\lambda)[1 + o(1)] \approx -\sqrt{n}(f_{rs}(0))^{-1}$$

which concludes the proof. 

---

**Algorithm S1 Approximate $(1 - \alpha)\%$ Confidence Interval (CI$_{1-\alpha}$) for $T(\hat{\theta})$**

**Require:** $\hat{\theta}$; D; W; S$_{\lambda}$; N$_{\text{sim}}$

$V_{\hat{\theta}} \leftarrow (D^\top WD + S_{\lambda})^{-1}$

draw $\{\hat{\theta}_r\}^N_{r=1} \sim N_p(\hat{\theta}, V_{\hat{\theta}}(\hat{\theta}))$

$\{T^*_r\} \leftarrow \{T(\hat{\theta}_r)\}_r$

$T^* := \{T^*_1, \ldots, T^*_N\}$ such that $T^*_r \leq T^*_r \leq T^*_r$, \forall $r = 1, \ldots, N_{\text{sim}}$

define $T^*_{1-\alpha}$ as the smallest $[N_{\text{sim}}\alpha]$-th value of $T^*$

$\text{CI}_{1-\alpha} \leftarrow [T^*_{1/2}, T^*_{1-\alpha}/2]$
and 

$$(\vartheta^* - \vartheta)^\top D^\top u = \|\sqrt{W}^{-1} u\|^2 - \langle z - D \vartheta^*; u \rangle.$$ 

Then we have 

$$-2\ell(\vartheta^*) \approx -2\ell(\vartheta) - \|\sqrt{W}^{-1} u\|^2 + \|\sqrt{W}(z - D \vartheta^*)\|^2$$ 

and, by noticing that the smoothing parameter vector affects the latter approximation only through the updated iteration $\vartheta^*$, and that we are interested in optimising a criterion with respect to $\lambda$, it is licit to drop any addendum not depending on it. Hence, one can indifferently consider an equivalent UBRE criterion given by 

$$V_u \propto \|\sqrt{W}(z - D \vartheta^*)\|^2 + 2\text{tr}(P) \equiv 2\text{tr}(P) - 2\ell(\vartheta^*).$$

S.4 Data Generating Process Employed in Figure 1

The simulation results depicted in Figure 1 comprises a bivariate system of equations specified by the following Data Generating Process (DGP):

$$y^*_{1,i} = x_{1,i} + 2x_{2,i} + x_{3,i} + s_{1,1}(v_{1,i}) + s_{1,2}(v_{2,i}) + \epsilon_{1,i}, \quad \epsilon_i \sim \mathcal{N}_2 \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0.9 \\ 0.9 & 1 \end{bmatrix} \right)$$

$$y^*_{2,i} = -0.3y^*_{1,i} + x_{1,i} - 2x_{2,i} + s_{2,1}(v_{1,i}) + \epsilon_{2,i},$$

for a sample size of 10,000 observations, and $N = 100$ replications. The test functions are displayed in red in the figure, and given by $s_{1,1}(v_{1,i}) = 1 - v_{1,i} + 1.6v^2_{1,i} - \sin(5v_{1,i})$, $s_{1,2}(v_{2,i}) = 4v_{2,i}$, and $s_{2,1}(v_{1,i}) = 0.08\{v^4_{1,i}[10(1 - v_{1,i})]^6 + 10(10v_{1,i})^3(1 - v_{1,i})^{10}\}$. Furthermore, the ordered values of $y_{j,i}$ have been computed following the observation rule:

$$y_{j,i} = \sum_{k_j \in K_j} k_j 1_{c_{j,k_j-1} < y^*_{j,i} \leq c_{j,k_j}},$$

for every $j \in \{1, 2\}$, and obtained by setting the threshold parameters at $c_1 := (-2, -1, 0, 2)^\top$ and $c_2 := (-1.4, -0.7, -0.2, 0.7, 3)^\top$. 

5