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Consistent estimation and testing in heteroscedastic polynomial errors-in-variables models

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Abstract The paper concentrates on consistent estimation and testing in functional polynomial measurement errors models with known heterogeneous variances. We rest on the corrected score methodology which allows the derivation of consistent and asymptotically normal estimators for line parameters and also consistent estimators for the asymptotic covariance matrix. Hence, Wald and score type statistics can be proposed for testing the hypothesis of a reduced linear relationship, for example, with asymptotic chi-square distribution which guarantees correct asymptotic significance levels. Results of small scale simulation studies are reported to illustrate the agreement between theoretical and empirical distributions of the test statistics studied. An application to a real data set is also presented.

Keywords Polynomial model · Errors-in-variables · Hypothesis test · Corrected score

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1 Introduction

Measurement errors models with homogeneous variances abound in the literature (see, for example, the books by Fuller, 1987; Carroll et al., 1995; Cheng and Van Ness, 1999). The simple linear regression model relates the response y and the covariate x by means of

$$y_i = \beta_0 + \beta_1 x_i + e_i, \quad (1)$$

with x_i only partially observable through the additive relation

$$w_i = x_i + u_i, \quad (2)$$

with w_i being a surrogate for x_i , $i = 1, \dots, n$.

The functional normal model follows by supposing

$$\begin{pmatrix} e_i \\ u_i \end{pmatrix} \stackrel{\text{indep.}}{\sim} N_2 \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{bmatrix} \sigma_e^2 & 0 \\ 0 & \sigma_u^2 \end{bmatrix} \right), \quad (3)$$

with x_i , $i = 1, \dots, n$, as fixed parameters. Hence, the model encompasses $n + 4$ parameters, the likelihood function is unbounded, and no consistent estimator is available for β . To overcome this problem, additional assumptions are required. One side condition typically adopted is that the variance σ_u^2 is known, leading to the consistent estimator (maximum likelihood estimator under normality)

$$\hat{\beta}_c = \frac{S_{wy}}{S_w^2 - \sigma_u^2}, \quad (4)$$

where $S_{wy} = n^{-1} \sum_{i=1}^n (w_i - \bar{w})(y_i - \bar{y})$ and $S_w^2 = n^{-1} \sum_{i=1}^n (w_i - \bar{w})^2$, with $\bar{w} = n^{-1} \sum_{i=1}^n w_i$ and $\bar{y} = n^{-1} \sum_{i=1}^n y_i$. The asymptotic behavior of this estimator is studied in Cheng and Van Ness (1999). A generalization of model (1) and (2), which did not deserve too much attention in the literature, arises when the measurement errors are heteroscedastic, that is, by assuming that

$$\begin{pmatrix} e_i \\ u_i \end{pmatrix} \stackrel{\text{indep.}}{\sim} N_2 \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{bmatrix} \sigma_{ei}^2 & 0 \\ 0 & \sigma_{ui}^2 \end{bmatrix} \right), \quad (5)$$

$i = 1, \dots, n$, which is discussed in Fuller (1987), Ripley and Thompson (1987), and Galea-Rojas et al. (2003) from a maximum likelihood point of view with the variances $(\sigma_{ei}^2, \sigma_{ui}^2)^\top$ known and greater than 0, $i = 1, \dots, n$. A corrected score estimator (Stefanski, 1989; Nakamura, 1990; Gimenez and Bolfarine, 1997) and its asymptotic behavior are discussed in de Castro et al. (2006). The lack of interest in the heterogeneous model may be due to the fact that both σ_{ei}^2 and σ_{ui}^2 need to be known, $i = 1, \dots, n$. However, this is a common setup in areas such as Analytical Chemistry (Ripley and Thompson, 1987; Riu and Rius, 1996; Galea-Rojas et al., 2003; Nguyet et al., 2004, among others). Walter (1997) develops some examples in Meta-analysis. In many applications, for each observation, variances are estimated by sub-dividing the original sample into subsamples. Cases where an error in the equation of unknown variance is present will be not studied in our paper.

In the present paper we extend the corrected score approach to treat the polynomial heteroscedastic functional measurement errors model, which seems

to the best of our knowledge, not yet discussed in the literature. Indeed, this problem seems not even being mentioned, as can be inferred from important references on the subject, such as Chan and Mak (1985), Fuller (1987), Moon and Gunst (1993), Cheng and Schneeweiss (1998), Schneeweiss and Nittner (2001), Cheng and Schneeweiss (2002), Kuha and Temple (2003), and Kukush et al. (2005). A goodness-of-fit test is presented in Cheng and Kukush (2004). The cases focused are the case σ_u^2 known (most frequent), the knowledge of the ratio of variances (σ_e^2/σ_u^2) (Chan and Mak, 1985), and the situation where the covariance matrix in (3) is fully or partially known, with $\sigma_{eu} = \text{cov}(e_i, u_i)$ not necessarily null. One of the drawbacks in Chan and Mak (1985) is the fact that the determinant of the asymptotic covariance matrix of the curve parameter estimators in the quadratic model vanishes under the hypothesis that the quadratic coefficient is null. Moreover, there is no formal proof in the literature implying that estimating equations yield consistent and asymptotically normal estimators for the functional situation, that is, when incidental parameters are present. Gimenez and Bolfarine (1997) however, provide rigorous proofs for consistency and asymptotic normality for the estimators obtained by solving estimating equations that follows by using the corrected score approach (Stefanski, 1989; Nakamura, 1990) in functional situations. In the structural model, Thamerus (1998) concerns with heteroscedastic measurement errors for all kind of nonlinear models.

The route we take is based on the corrected score methodology (Stefanski, 1989; Nakamura, 1990; Gimenez and Bolfarine, 1997), that when feasible, yields consistent estimators for the regression line parameters and also enables consistent estimation of the asymptotic covariance matrix of the estimators. Results are simple to implement with existing statistical software. The paper is organized as follows. Section 2 deals with the main methodological aspects, covering model formulation, parameter estimation and hypothesis testing. Results of simulation studies and a real data application are reported in Sects. 3 and 4. The Appendix provides an abridged account of the corrected score technique.

2 The corrected score approach for the heteroscedastic polynomial functional model

In this section we postulate that the relationship between the response y and the covariate x , with both variables carrying measurement errors, can be expressed by using

$$y_i = \beta_0 + \beta_1 x_i + \dots + \beta_p x_i^p + e_i, \tag{6}$$

with

$$w_i = x_i + u_i,$$

$i = 1, \dots, n$, $p \geq 1$, and $n > p + 1$. We also assume distribution (5) with σ_{ei} and σ_{ui} known, $i = 1, \dots, n$. Values for σ_{ei} and σ_{ui} can be obtained by using replications. The unknown x_i are taken as fixed so that the model formulated is a functional polynomial model. The assumptions above imply that the (unobserved) log-likelihood function can be written as

$$l(\beta; \mathbf{x}, \mathbf{y}) = \text{constant} - \frac{1}{2} \sum_{i=1}^n \frac{(y_i - \beta_0 - \beta_1 x_i - \dots - \beta_p x_i^p)^2}{\sigma_{ei}^2}, \tag{7}$$

where $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_p)^\top$, $\mathbf{x} = (x_1, \dots, x_n)^\top$, and $\mathbf{y} = (y_1, \dots, y_n)^\top$. Note that the above likelihood is unobserved because it depends on the unknown (unobserved) x_i , $i = 1, \dots, n$. The unobserved score function of $\boldsymbol{\beta}$ follows by differentiating (7) and is given by

$$U_s(\boldsymbol{\beta}; \mathbf{x}, \mathbf{y}) = \frac{\partial l(\boldsymbol{\beta}; \mathbf{x}, \mathbf{y})}{\partial \beta_s} = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left(y_i - \sum_{j=0}^p \beta_j x_i^j \right) x_i^s,$$

$s = 0, 1, \dots, p$.

Substituting w_i for x_i we construct the naive log-likelihood function

$$l(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = \text{constant} - \frac{1}{2} \sum_{i=1}^n \frac{(y_i - \beta_0 - \beta_1 w_i - \dots - \beta_p w_i^p)^2}{\sigma_{ei}^2}, \tag{8}$$

where $\mathbf{w} = (w_1, \dots, w_n)^\top$. Differentiating the likelihood (8) with respect to β_s , the naive score for $\boldsymbol{\beta}$ is given by

$$U_s(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = \frac{\partial l(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y})}{\partial \beta_s} = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left(y_i - \sum_{j=0}^p \beta_j w_i^j \right) w_i^s,$$

$s = 0, 1, \dots, p$. As is well known, the solution of the equations $U_s(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = 0$, $s = 0, 1, \dots, p$ (weighted least squares estimating equations), leads to an inconsistent estimator of $\boldsymbol{\beta}$, since

$$E[U(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y})] \neq \mathbf{0}.$$

To obtain a consistent estimator, we start from a corrected score $\mathbf{U}^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y})$ satisfying

$$E[U_s^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) | \mathbf{x}, \mathbf{y}] = U_s(\boldsymbol{\beta}; \mathbf{x}, \mathbf{y}),$$

so that

$$E[U_s^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y})] = E[E[U_s^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) | \mathbf{x}, \mathbf{y}]] = E[U_s(\boldsymbol{\beta}; \mathbf{x}, \mathbf{y})] = 0,$$

$s = 0, 1, \dots, p$. Hence, by using the corrected score \mathbf{U}^* , solving the equations $\mathbf{U}^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = \mathbf{0}$ yields a consistent estimator for $\boldsymbol{\beta}$. The unbiased corrected score is given by

$$U_s^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left(y_i t_{i,s} - \sum_{j=0}^p \beta_j t_{i,j+s} \right), \tag{9}$$

$s = 0, 1, \dots, p$, where $t_{i,j}$ is defined such that $E[t_{i,j}] = x_i^j$ and can be computed recursively from

$$t_{i,0} = 1, \quad t_{i,1} = w_i, \quad \text{and} \quad t_{i,j+1} = w_i t_{i,j} - j \sigma_{ui}^2 t_{i,j-1},$$

$j = 1, \dots, 2p - 1, i = 1, \dots, n$. Stefanski (1989) derived a recursion formula for the homoscedastic case, but his arguments go through also in the heteroscedastic case. Further, since in this case integration and differentiation operations are exchangeable, it can be shown that the corrected log-likelihood function is given by

$$l^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y}) = \text{constant} - \frac{1}{2} \sum_{i=1}^n \log \sigma_{ui}^2 - \frac{1}{2} \sum_{i=1}^n \log \sigma_{ei}^2 - \frac{1}{2} \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left\{ y_i^2 - 2 y_i \sum_{j=0}^p \beta_j t_{i,j} + \sum_{j=0}^p \sum_{s=0}^p \beta_j \beta_s t_{i,j+s} \right\}. \tag{10}$$

Equating $U_s^*(\boldsymbol{\beta}; \mathbf{w}, \mathbf{y})$ in (9) to 0, $s = 0, 1, \dots, p$, the corrected score estimator of $\boldsymbol{\beta}(\hat{\boldsymbol{\beta}})$ is the solution of the linear system

$$\mathbf{T} \boldsymbol{\beta} = \mathbf{y}_t, \tag{11}$$

where

$$\mathbf{T} = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \begin{bmatrix} 1 & t_{i,1} & t_{i,2} & \cdots & t_{i,p} \\ & t_{i,2} & t_{i,3} & \cdots & t_{i,p+1} \\ & & t_{i,4} & \cdots & t_{i,p+2} \\ & & & \ddots & \vdots \\ & & & & t_{i,2p} \end{bmatrix} \tag{12}$$

and

$$\mathbf{y}_t = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} (y_i, y_i t_{i,1}, y_i t_{i,2}, \dots, y_i t_{i,p})^\top.$$

The system of equations (11) can be seen as a generalization of the adjusted least squares (ALS) estimating equations in Cheng and Schneeweiss (1998). In fact, to construct the estimators, we need the knowledge of $\sigma_{ui}^2, i = 1, \dots, n$. With regard to $\text{var}(e_i)$, we can be more flexible, by taking $\text{var}(e_i) = \kappa \sigma_{ei}^2$, with κ unknown and σ_{ei}^2 known, $i = 1, \dots, n$, as before. This formulation changes (10) and solving $\frac{\partial l^*}{\partial \kappa} = 0$ furnishes

$$\hat{\kappa} = n^{-1} \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left\{ y_i^2 - 2 y_i \sum_{j=0}^p \hat{\beta}_j t_{i,j} + \sum_{j=0}^p \sum_{s=0}^p \hat{\beta}_j \hat{\beta}_s t_{i,j+s} \right\}.$$

Large sample properties of the estimators derived above are considered next.

Theorem 1 *Under the polynomial functional model defined in (6), (2), and (5), the corrected score estimator $\hat{\boldsymbol{\beta}} = \mathbf{T}^{-1} \mathbf{y}_t$ in (11) converges in probability to the true $\boldsymbol{\beta}$ and is asymptotically normally distributed, as $n \rightarrow \infty$, provided the conditions C1–C5 in Gimenez and Bolfarine (1997) are satisfied.*

Proof The result follows directly from Theorems 4.1 and 4.2 in Gimenez and Bolfarine (1997) which are general enough to accommodate situations where the distribution of the outcomes change with the sample units as is the case with the heteroscedastic model considered in this paper. \square

Remark 1 Conditions C1–C5 aforementioned involve the incidental parameters $x_i, i = 1, \dots, n$. In our model, if

$$0 < \liminf_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n (x_i - \bar{x})^{2(2p-1)} \leq \limsup_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n (x_i - \bar{x})^{2(2p-1)} < \infty$$

and if there is a $\gamma > 0$ such that

$$\lim_{n \rightarrow \infty} n^{-(1+\gamma/2)} \sum_{i=1}^n |x_i^p|^{2+\gamma} = 0,$$

then C1–C5 are satisfied. The first condition requires that the true unobservable (x) should be neither too much spread out nor too much concentrated when $n \rightarrow \infty$. The second assumption allows an application of Liapounov’s central limit theorem in order to obtain the asymptotic distribution of $\widehat{\beta}$.

Remark 2 By definition of $t_{i,j}, j = 0, 1, \dots, 2p, i = 1, \dots, n$, we have that

$$\mathbf{E}[\mathbf{T}] = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \begin{pmatrix} 1 \\ x_i \\ \vdots \\ x_i^p \end{pmatrix} \begin{pmatrix} 1 \\ x_i \\ \vdots \\ x_i^p \end{pmatrix}^\top \quad \text{and} \quad \mathbf{E}[\mathbf{y}_t] = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \begin{pmatrix} 1 \\ x_i \\ \vdots \\ x_i^p \end{pmatrix} \begin{pmatrix} 1 \\ x_i \\ \vdots \\ x_i^p \end{pmatrix}^\top \beta. \tag{13}$$

Let $T_{k,l}$ and $y_{t,k}$ be generic elements of \mathbf{T} and \mathbf{y}_t , respectively. Writing

$$\widehat{\beta} = (n^{-1} \mathbf{T})^{-1} (n^{-1} \mathbf{y}_t),$$

if $n^{-1} (T_{k,l} - \mathbf{E}[T_{k,l}]) \xrightarrow{\text{a.s.}} 0$ and $n^{-1} (y_{t,k} - \mathbf{E}[y_{t,k}]) \xrightarrow{\text{a.s.}} 0$, then $\widehat{\beta} \xrightarrow{\text{a.s.}} \beta$. By the Kolmogorov’s strong law of large numbers, this is achieved if

$$\sum_{i=1}^{\infty} \frac{\text{var}(t_{i,j})}{i^2} < \infty, \quad j = 1, \dots, 2p, \quad \text{and} \quad \sum_{i=1}^{\infty} \frac{\text{var}(y_i t_{i,j})}{i^2} < \infty, \quad j = 1, \dots, p.$$

Computation of these variances can be performed using the results in Moon and Gunst (1993). We conclude that

$$\sum_{i=1}^{\infty} \frac{x_i^{2(2p-1)}}{i^2} < \infty$$

is a sufficient condition for strong consistency of $\widehat{\beta}$.

Remark 3 Adopting as working assumption the boundedness of the sequence $\{x_i, i = 1, \dots, n\}$, conditions C1–C5 in Gimenez and Bolfarine (1997) and strong consistency of $\widehat{\beta}$ are directly stated. This condition, albeit stringent, is tenable in many situations.

The estimator in (11) is numerically unstable for small samples. Following Cheng et al. (2000), we propose an estimator with better behavior for small and moderate samples. Let $\mathbf{t}_i = (t_{i,0}, t_{i,1}, \dots, t_{i,p})^\top$, $\mathbf{M}_t = \sum_{i=1}^n \mathbf{t}_i \mathbf{t}_i^\top / \sigma_{ei}^2$, and $\mathbf{V} = \mathbf{M}_t - \mathbf{T}$. Let ρ be the smallest positive root of

$$\det \begin{bmatrix} \sum_{i=1}^n y_i^2 / \sigma_{ei}^2 & \mathbf{y}_t^\top \\ \mathbf{M}_t - \rho \mathbf{V} \end{bmatrix} = 0.$$

The modified estimator ($\widehat{\beta}_M$) is obtained by solving

$$(\mathbf{M}_t - a\mathbf{V}) \beta = \mathbf{y}_t, \tag{14}$$

where

$$a = \begin{cases} (n - \alpha)/n, & \text{if } \rho > 1 + 1/n, \\ \rho (n - \alpha)/(n + 1), & \text{if } \rho \leq 1 + 1/n, \end{cases}$$

with $\alpha = p + 2$, as suggested in Cheng et al. (2000). In Sects. 3 and 4 we adopt the modified estimator.

Theorem 2 *Let*

$$\begin{bmatrix} \sum_{i=1}^n y_i^2 / \sigma_{ei}^2 & \mathbf{y}_t^\top \\ \mathbf{M}_t \end{bmatrix} \text{ and } \lim_{n \rightarrow \infty} n^{-1} E[\mathbf{T}]$$

be positive definite matrices, with $E[\mathbf{T}]$ as in (13). Under the polynomial functional model defined in (6), (2), and (5), the corrected score estimator $\widehat{\beta} = \mathbf{T}^{-1} \mathbf{y}_t$ and the modified estimator ($\widehat{\beta}_M$) in (14) are asymptotically equivalent, that is, $n^{-1/2}(\widehat{\beta}_M - \widehat{\beta})$ converges in probability to $\mathbf{0}$, as $n \rightarrow \infty$.

Proof The proof parallels the proofs of the Theorems 1 and 2 in Cheng et al. (2000).

In the simplest instance ($p = 1$), the heterogeneous model reduces to (1), (2), and (5). From (11), the corrected score estimators come as solutions to the equations

$$\begin{bmatrix} \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} & \sum_{i=1}^n \frac{t_{i,1}}{\sigma_{ei}^2} \\ \sum_{i=1}^n \frac{t_{i,2}}{\sigma_{ei}^2} \end{bmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n \frac{y_i}{\sigma_{ei}^2} \\ \sum_{i=1}^n \frac{y_i t_{i,1}}{\sigma_{ei}^2} \end{pmatrix}.$$

Solving the above equations lead to the corrected score estimators

$$\widehat{\beta}_0 = \frac{\sum_{i=1}^n (y_i - \widehat{\beta}_1 w_i) / \sigma_{ei}^2}{\sum_{i=1}^n 1 / \sigma_{ei}^2}$$

and

$$\widehat{\beta}_1 = \frac{\sum_{i=1}^n \frac{w_i y_i}{\sigma_{ei}^2} - \sum_{i=1}^n \frac{y_i}{\sigma_{ei}^2} \sum_{i=1}^n \frac{w_i}{\sigma_{ei}^2} \left(\sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \right)^{-1}}{\sum_{i=1}^n \frac{w_i^2}{\sigma_{ei}^2} - \left(\sum_{i=1}^n \frac{w_i}{\sigma_{ei}^2} \right)^2 \left(\sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \right)^{-1} - \sum_{i=1}^n \frac{\sigma_{ui}^2}{\sigma_{ei}^2}}.$$

Thus, the corrected score approach affords closed form expressions for the estimators of β_0 and β_1 and to the best of our knowledge are not in the literature. On the contrary, maximum likelihood estimators for the linear situation have been considered in Fuller (1987) and Galea-Rojas et al. (2003) and require iterative procedures for its derivation. In the latter paper, simplified expressions are obtained for the asymptotic covariance matrix of the maximum likelihood estimators. Fuller (1987, Sect. 3.1.1) also presents consistent estimators of β_0 and β_1 . These estimators are motivated by the maximum likelihood estimators in the homoscedastic functional model and require the solution of an eigenvalue problem. We emphasize that the likelihood approach seems not feasibly extendable for the functional polynomial situation considered in this paper. Notice that if $\sigma_{ui}^2 \equiv \sigma_u^2$ and $\sigma_{ei}^2 \equiv \sigma_e^2$, $i = 1, \dots, n$, then $\widehat{\beta}_1$ reduces to $\widehat{\beta}_c$ in (4), which can be seen as a corrected least squares estimator (Fuller, 1987).

For the quadratic model (that is, $p = 2$), we have the system

$$\begin{bmatrix} \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} & \sum_{i=1}^n \frac{t_{i,1}}{\sigma_{ei}^2} & \sum_{i=1}^n \frac{t_{i,2}}{\sigma_{ei}^2} \\ & \sum_{i=1}^n \frac{t_{i,2}}{\sigma_{ei}^2} & \sum_{i=1}^n \frac{t_{i,3}}{\sigma_{ei}^2} \\ & & \sum_{i=1}^n \frac{t_{i,4}}{\sigma_{ei}^2} \end{bmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n \frac{y_i}{\sigma_{ei}^2} \\ \sum_{i=1}^n \frac{y_i t_{i,1}}{\sigma_{ei}^2} \\ \sum_{i=1}^n \frac{y_i t_{i,2}}{\sigma_{ei}^2} \end{pmatrix}.$$

If $\sigma_{ui}^2 \equiv \sigma_u^2$ and $\sigma_{ei}^2 \equiv \sigma_e^2$, $i = 1, \dots, n$, this system reduces to the estimating equations found in Kuha and Temple (2003, Sect. 4.2). □

2.1 Asymptotic covariance matrix

By using the sandwich method presented in the Appendix (see also Gimenez and Bolfarine, 1997), a consistent estimator of the asymptotic covariance matrix of the corrected score estimators ($\widehat{\mathbf{V}}$) is available. According to (22), $\widehat{\mathbf{V}} = n^{-1} \widehat{\mathbf{\Omega}}$, where

$$\widehat{\mathbf{\Omega}} = \bar{\mathbf{I}}^{*-1} \bar{\mathbf{S}}^* \bar{\mathbf{I}}^{*-1},$$

with

$$\bar{\mathbf{I}}^* = -n^{-1} \sum_{i=1}^n \frac{\partial}{\partial \boldsymbol{\beta}} \mathbf{U}_i^*(\boldsymbol{\beta}; w_i, y_i) \Big|_{\boldsymbol{\beta}=\boldsymbol{\beta}}$$

and

$$\bar{\mathbf{S}}^* = n^{-1} \sum_{i=1}^n \mathbf{U}_i^*(\widehat{\boldsymbol{\beta}}; w_i, y_i) \mathbf{U}_i^*(\widehat{\boldsymbol{\beta}}; w_i, y_i)^\top.$$

From (9) we arrive at

$$\mathbf{U}_i^*(\boldsymbol{\beta}; w_i, y_i) = \frac{1}{\sigma_{ei}^2} \begin{pmatrix} y_i t_{i,0} - \sum_{j=0}^p \beta_j t_{i,j} \\ y_i t_{i,1} - \sum_{j=0}^p \beta_j t_{i,j+1} \\ \vdots \\ y_i t_{i,p} - \sum_{j=0}^p \beta_j t_{i,j+p} \end{pmatrix},$$

$i = 1, \dots, n$. In this way, we have that $\bar{\mathbf{I}}^* = n^{-1} \mathbf{T}$, which does not depend on $\boldsymbol{\beta}$, so that

$$\widehat{\boldsymbol{\Omega}} = n^2 \mathbf{T}^{-1} \bar{\mathbf{S}}^* \mathbf{T}^{-1}. \tag{15}$$

Hence we have that

Theorem 3 *Under the conditions C1–C5 stated in Gimenez and Bolfarine (1997), as $n \rightarrow \infty$, the estimator $\widehat{\mathbf{V}} = n^{-1} \widehat{\boldsymbol{\Omega}}$ converges in probability to the true asymptotic covariance matrix of the corrected score estimator in Theorem 1.*

Proof The proof follows directly by using results in Theorem 4.2 in Gimenez and Bolfarine (1997). □

2.2 Hypothesis testing

We tackle now the problem of testing

$$H_0 : \boldsymbol{\beta} = \boldsymbol{\beta}_0, \tag{16}$$

where $\boldsymbol{\beta}_0$ is a vector of known constants. Gimenez et al. (2000) propose score and Wald type test statistics based on the corrected score methodology. In order to test (16), two statistics are available, namely,

$$\begin{aligned} W &= n (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)^\top \widehat{\boldsymbol{\Omega}}^{-1} (\boldsymbol{\beta}_0) (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \\ &= n^{-1} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)^\top \mathbf{T} \bar{\mathbf{S}}^* (\boldsymbol{\beta}_0)^{-1} \mathbf{T} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0), \end{aligned}$$

in view of (15), and the score statistic

$$Q = n^{-1} \mathbf{U}^*(\boldsymbol{\beta}_0; \mathbf{w}, \mathbf{y})^\top \bar{\mathbf{S}}^*(\boldsymbol{\beta}_0)^{-1} \mathbf{U}^*(\boldsymbol{\beta}_0; \mathbf{w}, \mathbf{y}). \tag{17}$$

Taking (9) and (11) into account, it follows that

$$\mathbf{T} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) = \mathbf{y}_t - \mathbf{T} \boldsymbol{\beta}_0 = \mathbf{U}^*(\boldsymbol{\beta}_0; \mathbf{w}, \mathbf{y});$$

so, $W = Q$. Hence, we have the following main result of the section.

Theorem 4 *Consider the functional polynomial model defined in (6), (2), and (5). Under H_0 in (16), $W = Q$ is asymptotically distributed according to a chi-square distribution with $p + 1$ degrees of freedom. Moreover, W is asymptotically equivalent to the Wald statistic*

$$W_2 = n^{-1} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)^\top \mathbf{T} \bar{\mathbf{S}}^* (\widehat{\boldsymbol{\beta}})^{-1} \mathbf{T} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0). \tag{18}$$

Proof The proof follows directly from Theorem 3.1 in Gimenez et al. (2000).

As also shown in Gimenez et al. (2000), a likelihood ratio type statistic based on the corrected log-likelihood (10) is distributed as a mixture of chi-square distributions, so that its use is more complicated than the statistic considered in Theorem 4.

Let β be partitioned as $(\beta_\psi^\top, \beta_\lambda^\top)^\top$, where ψ and λ are proper disjoint subsets of $\{0, 1, \dots, p\}$ with q and $p + 1 - q$ elements, respectively. The corrected score estimator $\hat{\beta}$ is partitioned accordingly. We examine in the sequel the hypothesis concerning the subset β_ψ , formulated as

$$H_0 : \beta_\psi = \beta_{\psi 0}. \tag{19}$$

Specifically, we could be interested in testing

$$H_0 : (\beta_1, \beta_2, \dots, \beta_p)^\top = (0, 0, \dots, 0)^\top.$$

Adopting a usual notation for partitioned vectors and matrices, we write

$$U^*(\beta; \mathbf{w}, \mathbf{y}) = \begin{pmatrix} U_\psi^*(\beta; \mathbf{w}, \mathbf{y}) \\ U_\lambda^*(\beta; \mathbf{w}, \mathbf{y}) \end{pmatrix}, \mathbf{T} = \begin{bmatrix} \mathbf{T}_{\psi\psi} & \mathbf{T}_{\psi\lambda} \\ \mathbf{T}_{\lambda\psi} & \mathbf{T}_{\lambda\lambda} \end{bmatrix}, \text{ and } \hat{\Omega} = \begin{bmatrix} \hat{\Omega}_{\psi\psi} & \hat{\Omega}_{\psi\lambda} \\ \hat{\Omega}_{\lambda\psi} & \hat{\Omega}_{\lambda\lambda} \end{bmatrix}.$$

Like in Theorem 4, the statistics proposed by Gimenez et al. (2000) serve to our purposes. First, let $\hat{\beta}_0 = (\beta_{\psi 0}^\top, \hat{\beta}_{\lambda 0}^\top)^\top$, where $\hat{\beta}_{\lambda 0}$ is the corrected score estimator of β_λ restricted to (19). From (9), the corrected score of β_s under H_0 , $s \in \lambda$, can be written as

$$U_s^*(\beta; \mathbf{w}, \mathbf{y}) = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left\{ \left(y_i t_{i,s} - \sum_{j \in \psi} \beta_{j0} t_{i,j+s} \right) - \sum_{j \in \lambda} \beta_j t_{i,j+s} \right\}.$$

The system of linear equations $U_s^*(\beta; \mathbf{w}, \mathbf{y}) = 0$, $s \in \lambda$, takes the form

$$\sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \sum_{j \in \lambda} \beta_j t_{i,j+s} = \sum_{i=1}^n \frac{1}{\sigma_{ei}^2} \left(y_i t_{i,s} - \sum_{j \in \psi} \beta_{j0} t_{i,j+s} \right). \tag{20}$$

Remembering (9) and (11), we conclude that $\hat{\beta}_{\lambda 0}$ is the solution of

$$\mathbf{T}_{\lambda\lambda} \beta_\lambda = \mathbf{y}_{\lambda},$$

where \mathbf{y}_{λ} is the vector with the elements on the right-hand side of (20). In other words, corrected score estimation in a restricted model is straightforward. Finally, the test of the hypothesis (19) is possible with the aid of the next theorem. \square

Theorem 5 Consider the functional polynomial model formulated in (6), (2), and (5). Define $\mathbf{T}_{\psi\psi,\lambda} = \mathbf{T}_{\psi\psi} - \mathbf{T}_{\psi\lambda} \mathbf{T}_{\lambda\lambda}^{-1} \mathbf{T}_{\lambda\psi}$. Under H_0 in (19), the statistics

$$W_\psi = n (\hat{\beta}_\psi - \beta_{\psi 0})^\top \hat{\Omega}_{\psi\psi} (\hat{\beta}_0)^{-1} (\hat{\beta}_\psi - \beta_{\psi 0})$$

and

$$Q_\psi = n U_\psi^*(\hat{\beta}_0; \mathbf{w}, \mathbf{y})^\top \mathbf{T}_{\psi\psi,\lambda}^{-1} \hat{\Omega}_{\psi\psi} (\hat{\beta}_0)^{-1} \mathbf{T}_{\psi\psi,\lambda}^{-1} U_\psi^*(\hat{\beta}_0; \mathbf{w}, \mathbf{y})$$

are asymptotically distributed according to a chi-square distribution with q degrees of freedom, when $n \rightarrow \infty$.

Proof This assertion is a consequence of Theorem 3.1 in Gimenez et al. (2000).

Individual hypothesis regarding one parameter at time, expressed by

$$H_0 : \beta_s = \beta_{s0}, \quad s \in \{0, 1, \dots, p\},$$

can be tested similarly. For these hypothesis we can use

$$Z_s = \frac{\widehat{\beta}_s - \beta_{s0}}{\widehat{v}_{ss}^{1/2}},$$

which for large samples is distributed according to the standard normal distribution, where \widehat{v}_{ss} denotes the s -th entry in the main diagonal of $\widehat{\mathbf{V}}$. \square

3 Simulations

In order to state inferential results in Sect. 2 we resort to asymptotic theory. In view of this, we planned Monte Carlo simulations to evaluate the empirical level and the power of the proposed test statistics at a nominal level of 5%. We chose the quadratic model and the null hypothesis to be tested in (16) is $H_0 : \boldsymbol{\beta} = (0, 1, 0)^\top$. In the simulations we take $\beta_0 = 0$ and $(\beta_1, \beta_2)^\top$ vary as in Table 1, creating different scenarios around H_0 . Sample sizes are $n = 30, 50, 100,$ and 500 . Standard deviations in (5) increase with the true measurements according to

$$\sigma_{ei} = 0.075 E[y_i]^{0.505} \quad \text{and} \quad \sigma_{ui} = 0.16 x_i^{0.503},$$

where $E[y_i] = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 = \beta_1 x_i + \beta_2 x_i^2, i = 1, \dots, n$. For each sample size, true unobservable x_i in (6) are sampled from a gamma distribution (shape and scale parameters taken as 0.45 and 0.65, respectively) and σ_{ui} is computed, $i = 1, \dots, n$. Next, for each pair $\beta_1, \beta_2, E[y_i]$ and σ_{ei} are computed, $i = 1, \dots, n$. Then, keeping these values fixed, rejection rates of the hypothesis in (16) from score (17) and Wald statistics (18) are obtained from 10, 000 replications obeying (2) and (6), contaminated with measurement errors having distribution (5), $i = 1, \dots, n$. Simulated samples resemble data from Example 4 in Galea-Rojas et al. (2003). Computations were performed by using homemade programs written in Ox language (Doornik, 2002). Graphics were drawn in the R system (R Development Core Team, 2004).

Table 1 summarizes the results. The rejections rates from Wald statistics are high, whichever the sample size and the (β_1, β_2) values. For samples generated under H_0 , notwithstanding the increasing sample sizes, rejection rates from Wald statistic are far from the nominal level, rather distinct from the behavior of the score statistic, whose empirical levels, albeit not so close to 5% when $n = 30$ and 50 , seems to suggest a good agreement between empirical and theoretical distributions. A sample size of 500 is compatible with the real data set in the example of Sect. 4.

Figure 1 displays samples generated under the conditions of Table 1 and the line corresponding to the null hypothesis tested. Figure 1a and d represent the clearest departures from H_0 , so that, as expected, for each sample size the largest rejection rates typically are at upper left and lower right corners in Table 1.

Moreover, simulations also indicate that the weighted least squares (WLS) estimators are markedly biased. For sake of space, results from these simulations are omitted.

Table 1 Rejection rates of the null hypothesis $H_0: \beta_1 = 1.00$ and $\beta_2 = 0.00$: (a) Wald statistic and (b) score statistic

β_2	β_1 (a)					β_1 (b)				
	0.90	0.95	1.00	1.05	1.10	0.90	0.95	1.00	1.05	1.10
$n = 30$										
-0.15	0.999	0.995	0.975	0.931	0.860	0.268	0.108	0.034	0.017	0.046
-0.05	0.954	0.874	0.786	0.721	0.719	0.107	0.031	0.018	0.049	0.134
0.00	0.872	0.773	0.711	0.722	0.787	0.054	0.021	0.025	0.085	0.208
0.05	0.785	0.730	0.743	0.800	0.870	0.037	0.023	0.047	0.132	0.302
0.15	0.834	0.859	0.899	0.941	0.968	0.025	0.046	0.126	0.267	0.464
$n = 50$										
-0.15	1.000	1.000	1.000	1.000	1.000	0.300	0.144	0.046	0.014	0.033
-0.05	0.992	0.950	0.837	0.679	0.550	0.170	0.051	0.025	0.056	0.176
0.00	0.784	0.562	0.439	0.503	0.695	0.093	0.030	0.035	0.010	0.268
0.05	0.648	0.677	0.794	0.885	0.954	0.049	0.024	0.062	0.180	0.373
0.15	0.977	0.980	0.985	0.990	0.995	0.023	0.053	0.141	0.310	0.525
$n = 100$										
-0.15	1.000	1.000	1.000	0.994	0.977	0.993	0.857	0.392	0.056	0.076
-0.05	0.998	0.973	0.883	0.824	0.857	0.815	0.312	0.040	0.067	0.378
0.00	0.972	0.869	0.800	0.839	0.939	0.521	0.095	0.033	0.221	0.672
0.05	0.905	0.836	0.859	0.935	0.988	0.242	0.045	0.118	0.494	0.881
0.15	0.945	0.957	0.985	0.998	1.000	0.070	0.117	0.487	0.874	0.989
$n = 500$										
-0.15	1.000	1.000	1.000	1.000	1.0000	1.0000	1.0000	1.000	1.000	0.974
-0.05	1.000	1.000	0.999	0.867	0.941	1.000	1.000	0.928	0.436	0.925
0.00	1.000	0.897	0.229	0.846	1.000	1.000	0.762	0.043	0.832	1.000
0.05	0.961	0.749	0.983	1.000	1.000	0.923	0.620	0.976	1.000	1.000
0.15	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

4 Application

We illustrate with data from Example 4 in Galea-Rojas et al. (2003), where a detailed description can be found. Gold contents (in grams/ton) in 501 samples was analyzed using two methods: a classical method and a screen fire assay. The chief aim is to test the bias of one method relative to the other one. Synek (2001) points out that wide concentration ranges are prone to curvature at higher levels. Figure 2 brings to light this issue and induces us to adopt a quadratic model as a first step beyond the simplest model. Corrected score estimates (and standard errors) are $\hat{\beta}_0 = 0.00746$ (0.00868), $\hat{\beta}_1 = 0.976$ (0.0952), and $\hat{\beta}_2 = -0.125$ (0.0330). Hypothesis $H_0: \beta_0 = 0, \beta_1 = 1$ e $\beta_2 = 0$, which means bias absence between the methods, is rejected at a 5% level ($Q = 9.01$ with three degrees of freedom, p -value = 0.0291). Individual tests show the significance of linear and quadratic coefficients (p -values = 0.390, < 0.0001, and 0.000159, respectively).

5 Conclusions

The paper presents inferential methods for functional polynomial measurement error models with known heterogeneous variances. Contrary to many articles in

the literature, special attention was dedicated to hypothesis testing, either on the whole parameter vector or on a subset of it. As pointed out by a referee, with data like those presented on Fig. 2, goodness-of-fit should be checked. In future work we will address this point, elaborating a test similar to one constructed by Cheng and Kukush (2004). The power of the tests in Sect. 2.2 under local alternatives could also be investigated.

Throughout the paper only the functional model was mentioned. The corrected score estimator is also applicable to the structural counterpart, although distributional information about the covariate could be incorporated in the analysis, resulting in better inferential procedures. We concentrate on the functional model, for our work was fostered by datasets having asymmetric measurements.

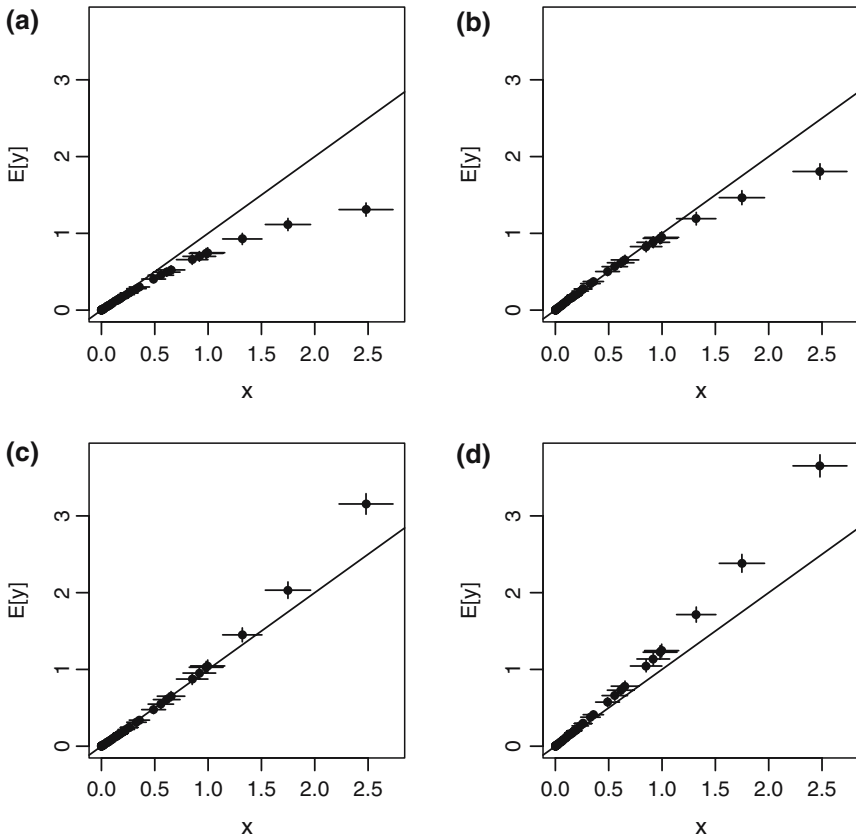


Fig. 1 True 50 unknown x and $E[y]$ values with the standard deviations of the measurement errors: **a** $\beta_1 = 0.90$, $\beta_2 = -0.15$, **b** $\beta_1 = 1.10$, $\beta_2 = -0.15$, **c** $\beta_1 = 0.90$, $\beta_2 = 0.15$, and **d** $\beta_1 = 1.10$, $\beta_2 = 0.15$. Solid line represents the null hypothesis to be tested ($\beta_1 = 1.00$, $\beta_2 = 0.00$)

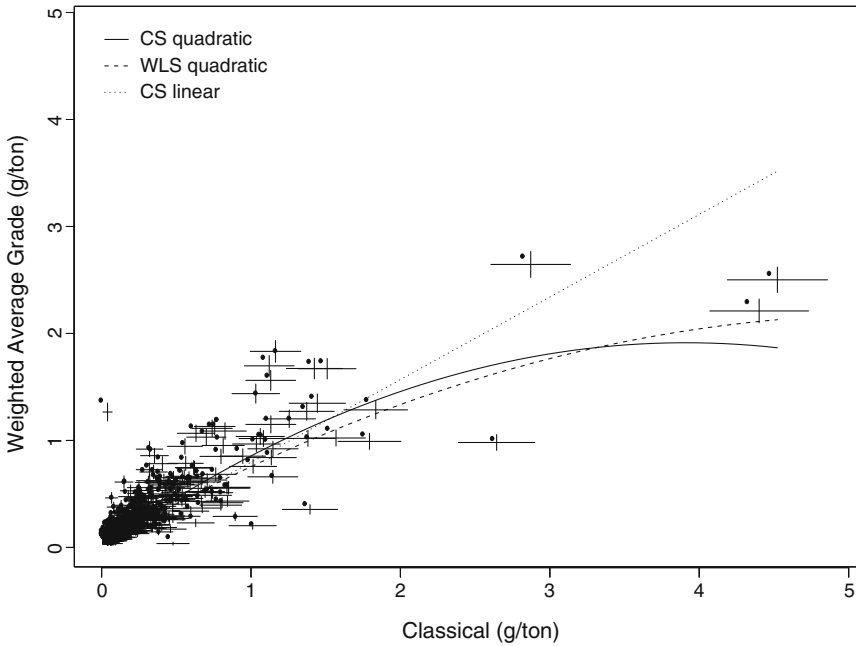


Fig. 2 Gold concentrations, standard deviations of the measurement errors, and adjusted models (“CS” stands for corrected score)

Appendix: the corrected score methodology

Consider a response vector \mathbf{y} of dimension r , \mathbf{x} a covariate vector of dimension k and $\boldsymbol{\theta}$ a parameter vector of dimension p . Denoting by \mathbf{x}_i and \mathbf{y}_i the covariate and response vectors for unit i in a sample of n independent observations, let

$$l(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}) = \sum_{i=1}^n l_i(\boldsymbol{\theta}; \mathbf{x}_i, \mathbf{y}_i),$$

the log-likelihood function of $\boldsymbol{\theta}$ given $\mathbf{X} = (\mathbf{x}_1^\top, \dots, \mathbf{x}_n^\top)$ and $\mathbf{Y} = (\mathbf{y}_1^\top, \dots, \mathbf{y}_n^\top)$, the observed data. Therefore, the score function and the observed information matrix are given by

$$\mathbf{U}(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}) = \frac{\partial}{\partial \boldsymbol{\theta}} l(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}) \tag{21}$$

and

$$\mathbf{I}(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}) = -\frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{U}(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}),$$

supposing that the required derivatives are well defined. Under appropriate regularity conditions (Lehmann, 1998) the maximum likelihood estimator $\hat{\boldsymbol{\theta}}_X$ of $\boldsymbol{\theta}$ comes from solving the estimating equations $\mathbf{U}(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y}) = \mathbf{0}$. It is well known that under suitable regularity conditions, $\hat{\boldsymbol{\theta}}_X$ is consistent and asymptotically normal, with asymptotic covariance matrix given by $\{E[\mathbf{I}(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y})]\}^{-1}$. Now, given that \mathbf{X}

cannot be observed, as happens when it is measured with error, the above scheme is not useful. In the additive model with $r = k = 1$, where $w_i = x_i + u_i$ and $E[u_i] = 0$, for example, we can substitute w_i for x_i (which is not observed) in (21), that is, we can construct the naive score function $\mathbf{U}(\boldsymbol{\theta}; \mathbf{W}, \mathbf{Y})$, where $\mathbf{W} = (w_1, \dots, w_n)^\top$, leading to the naive estimating equations $\mathbf{U}(\boldsymbol{\theta}; \mathbf{W}, \mathbf{Y}) = \mathbf{0}$, which do not yield in general a consistent estimator of $\boldsymbol{\theta}$ (Carroll et al., 1995).

To overcome these difficulties, Stefanski (1989) and Nakamura (1990) proposed to work with a corrected likelihood function, that is, to find a likelihood function $l^*(\boldsymbol{\theta}; \mathbf{W}, \mathbf{Y})$ such that $E[l^*(\boldsymbol{\theta}; \mathbf{W}, \mathbf{Y}) \mid \mathbf{X}, \mathbf{Y}] = l(\boldsymbol{\theta}; \mathbf{X}, \mathbf{Y})$, which, under suitable regularity conditions, will lead to consistent estimators achieved by using the corrected score function

$$\mathbf{U}_i^*(\boldsymbol{\theta}; w_i, y_i) = \frac{\partial}{\partial \boldsymbol{\theta}} l_i^*(\boldsymbol{\theta}; w_i, y_i),$$

$i = 1, \dots, n$. Thus, the corrected score estimator of $\boldsymbol{\theta}$ follows by solving the system $\sum_{i=1}^n \mathbf{U}_i^*(\boldsymbol{\theta}; w_i, y_i) = \mathbf{0}$.

The corrected observed information matrix is given by

$$\bar{\mathbf{I}}^*(\boldsymbol{\theta}; \mathbf{W}, \mathbf{Y}) = -n^{-1} \sum_{i=1}^n \frac{\partial}{\partial \boldsymbol{\theta}} \mathbf{U}_i^*(\boldsymbol{\theta}; w_i, y_i).$$

As shown in Gimenez and Bolfarine (1997), $\hat{\boldsymbol{\theta}}$ is asymptotically normally distributed with mean vector $\boldsymbol{\theta}$ and

$$n^{-1} \bar{\mathbf{I}}^{*-1}(\hat{\boldsymbol{\theta}}; \mathbf{W}, \mathbf{Y}) \bar{\mathbf{S}}^*(\hat{\boldsymbol{\theta}}; \mathbf{W}, \mathbf{Y}) \{\bar{\mathbf{I}}^{*-1}(\hat{\boldsymbol{\theta}}; \mathbf{W}, \mathbf{Y})\}^\top \tag{22}$$

is a consistent estimator of the asymptotic covariance matrix, where

$$\bar{\mathbf{S}}^*(\hat{\boldsymbol{\theta}}; \mathbf{W}, \mathbf{Y}) = n^{-1} \sum_{i=1}^n \mathbf{U}_i^*(\hat{\boldsymbol{\theta}}; w_i, y_i) \mathbf{U}_i^*(\hat{\boldsymbol{\theta}}; w_i, y_i)^\top.$$

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