Understanding nonparametric estimation for clustered data

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SUMMARY

In this note we give an alternative formulation of the nonparametric estimators of Wang (2003) with the identity link. This results in a closed form of the estimator that has computational advantages and gives insight into the rationale behind the estimator.

Some key words: Clustered data; Nonparametric estimation.

1. INTRODUCTION

The development of nonparametric estimators for clustered data has had a relatively long history with limited success until the recent estimator of Wang (2003). The generalised estimating equation approach was examined by Lin & Carroll (2000), who developed optimal estimating equations within a class of estimating equations, and showed that within the class considered the working independence estimator that ignores the correlation within the clusters is the most asymptotically efficient. Ruckstuhl et al. (2000) have examined several approaches and left as an open problem the possibility of obtaining an estimator with uniformly lower mean squared error than that of the working independence estimator. Wang (2003) developed estimating equations for the joint response in contrast to the conditional approach of Huggins (2004) and developed a full theory of her estimator. She showed in simulations and analytically that this estimator was superior to the working independence estimator, but it is not immediately apparent why it should be a good estimator. Here we determine a closed form of the estimator of Wang (2003) when the identity link is used.

2. ESTIMATING EQUATIONS

Let X^T denote the transpose of the matrix X and let $X^{-T} = (X^T)^{-1}$. To develop the estimating equations, consider a single cluster $Y = (Y_1, \dots, Y_m)^T$. Suppose Y has covariance matrix Ω and mean vector $\mu = (\mu(z_1), \dots, \mu(z_m))^T$, which is a function of covariates $(z_1, \dots, z_m)^T$. Let μ_j and Ω_j respectively denote the mean vector and the positive definite covariance matrix of $Y(j) = (Y_1, \dots, Y_j)^T$. We are interested in estimating $\mu(z_0)$ for known Ω . Wang et al. (2005) and Linton et al. (2004) comment on the effects of estimation of Ω . To develop the nonparametric estimators, let $g_p(u) = (1, u, u^2, \dots, u^p)$ so that, for z near z_0 , $\mu(z) \simeq \sum_{k=0}^p b_k(z - z_0)^k = g_p(z - z_0)^T b$, where $b = (b_0, b_1, \dots, b_p)$. If u is a vector $u = (u_1, \dots, u_n)$, let the matrix $G_p(u)$ have j th row $(1, u_j, \dots, u_j^p)$ so that, under regularity conditions, $\mu(z) \simeq G_p(z - z_0)b$.

Let $\bar{\mu}(z)$ denote the estimated value of $\mu(z)$ arising from the working independence estimator, let $\bar{\mu} = (\bar{\mu}(z_1), \dots, \bar{\mu}(z_m))^T$ and let $\bar{\mu}(j)$ have j th value $g_p(z_j - z_0)b$ and, for $k \neq j$, have value $\bar{\mu}(z_k)$. Let d_j be a vector of length m with 1 in the j th position and 0 elsewhere. In the Wang (2003) estimator

with identity link, the contribution of Y to the estimating equations is

$$\sum_{j=1}^m K(z_j - z_0) g_p(z_j - z_0)^T d_j^T \Omega^{-1} \{Y - \bar{\mu}(j)\}. \quad (1)$$

Now let A denote the lower triangular Cholesky decomposition of Ω , so that $\Omega = AA^T$, and similarly define A_j so that $\Omega_j = A_j A_j^T$. Define standardised residuals by $Z_j = (Z_1, \dots, Z_j)^T = A_j^{-1} \{Y(j) - \mu_j\}$.

Write

$$\Omega_{j+1} = \begin{bmatrix} \Omega_j & a_{j+1} \\ a_{j+1}^T & b_{j+1} \end{bmatrix}$$

and let $\ell_{j+1}^T = a_{j+1}^T A_j^{-T}$, $\delta_{j+1} = (b_{j+1} - \ell_{j+1}^T \ell_{j+1}^T)^{1/2}$ and $r_{j+1}^T = -\delta_{j+1}^{-1} a_{j+1}^T \Omega_j^{-1}$. Then, following Stewart (1973, p. 141) we have

$$A_{j+1} = \begin{bmatrix} A_j & 0 \\ \ell_{j+1}^T & \delta_{j+1} \end{bmatrix}, \quad A_{j+1}^{-1} = \begin{bmatrix} A_j^{-1} & 0 \\ r_{j+1}^T & \delta_{j+1}^{-1} \end{bmatrix}.$$

Hence

$$Z_{j+1} = r_{j+1}^T \{Y(j) - \mu_j\} + \delta_{j+1}^{-1} (Y_{j+1} - \mu(z_{j+1})) = \delta_{j+1}^{-1} [Y_{j+1} - \mu(z_{j+1}) - a_{j+1}^T \Omega_j^{-1} \{Y(j) - \mu_j\}].$$

Let $\tilde{Y}_{j+1} = Y_{j+1} - a_{j+1}^T \Omega_j^{-1} \{Y(j) - \mu_j\}$, so that, as $Z_{j+1} = \delta_{j+1}^{-1} (\tilde{Y}_{j+1} - \mu(z_{j+1}))$, the pseudo-observations $\tilde{Y}_j$ have means $\mu(z_j)$ and are uncorrelated.

Define $\bar{Z}(j) = A^{-1} \{Y - \bar{\mu}(j)\}$ and $\bar{Y}_k = Y_k - a_k^T \Omega_{k-1}^{-1} \{Y(k-1) - \bar{\mu}_{k-1}\}$, where

$$\bar{\mu}_{k-1} = (\bar{\mu}(z_1), \dots, \bar{\mu}(z_{k-1}))^T.$$

Note that $d_j^T A^{-T}$ has first nonzero element δ_j^{-1} and that the remaining terms are the j th elements of r_k ($k > j$). We denote these elements by r_{kj} and let $\mathcal{R}$ be the matrix with rows $\mathcal{R}_j = (0, \dots, 0, r_{j+1,j}, \dots, r_{m,j})$. Then (1) is

$$\begin{aligned} \sum_{j=1}^m K(z_j - z_0) g_p(z_j - z_0)^T d_j^T A^{-T} A^{-1} \{Y - \bar{\mu}(j)\} &= \sum_{j=1}^m g_p(z_j - z_0)^T K(z_j - z_0) \delta_j^{-1} \bar{Z}_j(j) \\ &\quad + \sum_{j=1}^{m-1} g_p(z_j - z_0)^T K(z_j - z_0) \sum_{k=j+1}^m r_{kj} \bar{Z}_k(j) \\ &= G_p(z - z_0)^T W \{\bar{Y} - G_p(z - z_0)b\} + G_p(z - z_0)^T K \bar{D} \\ &= G_p(z - z_0)^T W \{\bar{Y} - G_p(z - z_0)b + \Delta^2 \bar{D}\}, \end{aligned} \quad (2)$$

where $W = K(z)^{1/2} R^{-1} K(z)^{1/2}$ for a diagonal weight matrix $K(z)$ and $R = \text{diag}(\delta_j^2)$, $\bar{D}$ has j th element $\mathcal{R}_j \bar{Z}(j)$ and Δ is a diagonal matrix with j th diagonal δ_j .

The first term of (2) is related to estimating equations of Huggins (2004) and is easily interpreted. Simulations, not reported in detail, showed that estimation based on $G_p^T(z - z_0) W \{\bar{Y} - G_p(z - z_0)b\}$ is far less efficient than that based on (2); in a small simulation study along the lines of that in Wang (2003), the ratios of the averages of the mean squared errors for the working independence estimator and the proposed estimators were 1.17 for the conditional estimator and 1.58 for Wang's estimators. Consider the second term in (2). Note that b enters $\bar{Z}_k(j)$ for $k > j$ through $\bar{\mu}(j)$, where it is only involved in the j th element. Let $\bar{\mu}_k(j)$ be the first k elements of $\bar{\mu}(j)$ and let $\bar{Z} = A^{-1} (Y - \bar{\mu})$. Then, for $k > j$,

$$\begin{aligned} \bar{Z}_k(j) &= \delta_k^{-1} [Y_k - \bar{\mu}_k - a_k^T \Omega_{k-1}^{-1} \{Y(k-1) - \bar{\mu}_{k-1}(j)\}] \\ &= \delta_k^{-1} (Y_k - \bar{\mu}_k) + r_k \{Y(k-1) - \bar{\mu}_{k-1}(j)\} \\ &= \delta_k^{-1} (Y_k - \bar{\mu}_k) + \sum_{\ell=1, \ell \neq j}^{k-1} r_{k\ell} (Y_\ell - \bar{\mu}_\ell) + r_{kj} Y_j - r_{kj} g_p(z_j - z_0)b \\ &= \bar{Z}_k + r_{kj} \{\bar{\mu}_j - g(z_j - z_0)b\} \end{aligned}$$

so that $\bar{Z}(j) = \bar{Z} + v_j\{\bar{\mu} - G_p(z - z_0)b\}$, where v_j has k th row consisting of zeros for $k \leq j$ and $v_{jk} = (0, \dots, r_{kj}, \dots, 0)$ for $k > j$. The contribution of a single cluster to the estimating equations from a single cluster may be expressed as

$$G_p^T(z - z_0)W\{\bar{Y} - G(z - z_0)b + \Delta^2 \mathcal{R}\bar{Z} + \Delta^2 S\bar{\mu} - \Delta^2 Tb\}, \quad (3)$$

where S has j th row $\mathcal{R}_j v_j$ and T has j th row $\mathcal{R}_j v_j G_p(z - z_0)$.

In practice we observe n independent clusters and (3) yields the closed-form estimator,

$$\hat{b} = \mathcal{A}_1^{-1} \sum_{i=1}^n G_p^T(z_i - z_0)W_i(\bar{Y}_i + \Delta^2 \mathcal{R}\bar{Z}_i + \Delta^2 S\bar{\mu}_i),$$

where $\mathcal{A}_1 = \sum_{i=1}^n G_p^T(z_i - z_0)W_i\{G_p(z_i - z_0) + \Delta^2 T_i\}$ and W_i and so on have the obvious definitions for the i th cluster. As (3) is a reformulation of the estimator of Wang (2003) its properties are as given in Wang (2003).

3. DISCUSSION

Lin et al. (2004) also give a closed form of the Wang (2003) estimator, but using pseudo-observations that are constructed differently from our $\bar{Y}_j$, and Linton et al. (2004) also consider an approach based on pseudo-observations that are different again. The common idea is to construct these pseudo-observations so that they have the same mean as Y_j , but a diagonal covariance matrix for each cluster.

At present little theory is available to aid the construction of optimal nonparametric estimators for dependent data. One can construct estimators and derive their properties, but there is no general theory comparable to that of maximum likelihood to provide guidance. Weighted martingale estimators have a role for first-order Markov processes, as in Huggins & Yip (1999) for example. Here the underlying process is not Markovian and efficiency is increased by incorporating this in the estimating equations. The formation of the Wang (2003) estimator derived here makes this explicit. Expression (3) is based on conditional residuals, which contribute in two ways to the estimating equations. The first is directly through the mean of $\bar{Y}$. The second is from noting that the 'conditional offset' $a_k^T \Omega_{k-1}^{-1}(Y_{k-1} - \bar{\mu}_{k-1})$ applied to Y_k is also a function of b for $k > j$. The complicated form of the estimating equations comes from resolving these two roles and (3) is the sum of the residuals in these roles.

Apart from the insights into the estimator that are gained from our derivation, the closed form of the estimator obviates the need for iterative numerical procedures to calculate the estimates. Typically the estimation of $\mu(z)$ requires one to compute several hundred estimates. If it is also necessary to estimate parameters in a model for Ω and use crossvalidation the computations quickly become unmanageable. The form of the estimator suggests several possible improvements. However, in simulations these improvements were not large. The standardised residuals employed here have previously been used in Huggins (1996) to develop robust estimators for clustered data.

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