Model-Based Covariance Estimation for Regression M- and GM-Estimators

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1 Introduction

The population regression model is given by

$$\xi: \quad Y_i = \boldsymbol{x}_i^T \boldsymbol{\theta} + \sigma\sqrt{v_i} E_i, \qquad \boldsymbol{\theta} \in \mathbb{R}^p, \quad \sigma > 0, \quad i \in U,$$

where the population U is of size N; the parameters $\boldsymbol{\theta}$ and σ are unknown; the $\boldsymbol{x}_i$'s are known values (possibly containing outliers), $\boldsymbol{x}_i \in \mathbb{R}^p$, $1 \leq p < N$; the v_i's are known positive (heteroscedasticity) constants; the errors E_i are independent and identically distributed (i.i.d.) random variables with zero expectation and unit variance; it is assumed that $\sum_{i \in U} \boldsymbol{x}_i \boldsymbol{x}_i^T / v_i$ is a non-singular $(p \times p)$ matrix.

It is assumed that a sample s is drawn from U with sampling design $p(s)$ such that the independence structure of model ξ is maintained. The sample regression GM-estimator of $\boldsymbol{\theta}$ is defined as the root to the estimating equation $\widehat{\boldsymbol{\Psi}}_n(\boldsymbol{\theta}, \sigma) = \boldsymbol{0}$ (for all $\sigma > 0$), where

$$\widehat{\boldsymbol{\Psi}}_n(\boldsymbol{\theta}, \sigma) = \sum_{i \in s} w_i \boldsymbol{\Psi}_i(\boldsymbol{\theta}, \sigma) \qquad \text{with} \qquad \boldsymbol{\Psi}_i(\boldsymbol{\theta}, \sigma) = \eta\left(\frac{y_i - \boldsymbol{x}_i^T\boldsymbol{\theta}}{\sigma\sqrt{v_i}}, \ \boldsymbol{x}_i\right) \frac{\boldsymbol{x}_i}{\sigma\sqrt{v_i}},$$

where the function $\eta : \mathbb{R} \times \mathbb{R}^p \to \mathbb{R}$ parametrizes the following estimators

$$\begin{aligned}
&\eta(r, \boldsymbol{x}) = \psi(r) && M\text{-estimator},\\
&\eta(r, \boldsymbol{x}) = \psi(r) \cdot h(\boldsymbol{x}) && \text{Mallows } GM\text{-estimator},\\
&\eta(r, \boldsymbol{x}) = \psi\left(\frac{r}{h(\boldsymbol{x})}\right) \cdot h(\boldsymbol{x}) && \text{Schweppe } GM\text{-estimator},
\end{aligned}$$

where $\psi : \mathbb{R} \to \mathbb{R}$ is a continuous, bounded, and odd (possibly redescending) function, and $h : \mathbb{R}^p \to \mathbb{R}_+$ is a weight function.

2 Covariance estimation

The model-based covariance matrix of $\boldsymbol{\theta}$ is (Hampel, Ronchetti, Rousseeuw, and Stahel, 1986, Chapter 6.3)

$$\mathrm{cov}_{\xi}(\boldsymbol{\theta}, \sigma) = \boldsymbol{M}^{-1}(\boldsymbol{\theta}, \sigma) \cdot \boldsymbol{Q}(\boldsymbol{\theta}, \sigma) \cdot \boldsymbol{M}^{-T}(\boldsymbol{\theta}, \sigma) \qquad \text{for known } \sigma > 0, \tag{1}$$

where

$$\boldsymbol{M}(\boldsymbol{\theta}, \sigma) = \sum_{i=1}^{N} \mathrm{E}_{\xi}\big\{\boldsymbol{\Psi}_i'(\boldsymbol{\theta}, \sigma)\big\}, \quad \text{where} \quad \boldsymbol{\Psi}_i'(\boldsymbol{\theta}, \sigma) = -\frac{\partial}{\partial \boldsymbol{\theta}^*}\boldsymbol{\Psi}_i(Y_i, \boldsymbol{x}_i; \boldsymbol{\theta}^*, \sigma)\Big|_{\boldsymbol{\theta}^* = \boldsymbol{\theta}},$$

and

$$\boldsymbol{Q}(\boldsymbol{\theta}, \sigma) = \frac{1}{N}\sum_{i=1}^{N} \mathrm{E}_{\xi}\big\{\boldsymbol{\Psi}_i(Y_i, \boldsymbol{x}_i; \boldsymbol{\theta}, \sigma)\boldsymbol{\Psi}_i(Y_i, \boldsymbol{x}_i; \boldsymbol{\theta}, \sigma)^T\big\},$$

and E_{ξ} denotes expectation with respect to model ξ. For the sample regression GM-estimator $\widehat{\boldsymbol{\theta}}_n$, the matrices $\boldsymbol{M}$ and $\boldsymbol{Q}$ must be estimated. Expressions of the generic matrices $\boldsymbol{M}$ and $\boldsymbol{Q}$ in (1) are given as foolows.

$$\begin{aligned}
\widehat{\boldsymbol{M}}_M &= -\overline{\psi'} \cdot \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X} & \widehat{\boldsymbol{Q}}_M &= \overline{\psi^2} \cdot \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X} & &M\text{-est.}\\
\widehat{\boldsymbol{M}}_{Mal} &= -\overline{\psi'} \cdot \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{H}\boldsymbol{X} & \widehat{\boldsymbol{Q}}_{Mal} &= \overline{\psi^2} \cdot \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{H}^2\boldsymbol{X} & &GM\text{-est. (Mallows)}\\
\widehat{\boldsymbol{M}}_{Sch} &= -\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{S}_1\boldsymbol{X} & \widehat{\boldsymbol{Q}}_{Sch} &= \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{S}_2\boldsymbol{X} & &GM\text{-est. (Schweppe)}
\end{aligned}$$

where

$$\begin{aligned}
\boldsymbol{W} &= \mathrm{diag}_{i=1,\ldots,n}\{w_i\}, & \boldsymbol{H} &= \mathrm{diag}_{i=1,\ldots,n}\{h(\boldsymbol{x}_i)\},\\
\overline{\psi'} &= \frac{1}{\widehat{N}}\sum_{i \in s} w_i \psi'\left(\frac{r_i}{\widehat{\sigma}\sqrt{v_i}}\right), & \overline{\psi^2} &= \frac{1}{\widehat{N}}\sum_{i \in s} w_i \psi^2\left(\frac{r_i}{\widehat{\sigma}\sqrt{v_i}}\right),\\
\boldsymbol{S}_1 &= \mathrm{diag}_{i=1,\ldots,n}\{s_1^i\}, & s_1^i &= \frac{1}{\widehat{N}}\sum_{j \in s} w_j \psi'\left(\frac{r_j}{h(\boldsymbol{x}_i)\widehat{\sigma}\sqrt{v_j}}\right),
\end{aligned}$$

and

$$\boldsymbol{S}_2 = \mathrm{diag}_{i=1,\ldots,n}\{s_2^i\}, \qquad s_2^i = \frac{1}{\widehat{N}}\sum_{j \in s} w_j \psi^2\left(\frac{r_j}{h(\boldsymbol{x}_i)\widehat{\sigma}\sqrt{v_j}}\right).$$

Remarks.

- The i-th diagonal element of $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ depends on $h(\boldsymbol{x}_i)$, but the summation is over $j \in s$; see also (Marazzi, 1987, Chapter 6).
- When $\boldsymbol{W}$ is equal to the identity matrix $\boldsymbol{I}$, the asymptotic covariance of $\widehat{\boldsymbol{\theta}}_M$ is equal to the expression in Huber (1981, Eq. 6.5), which is implemented in the R packages `MASS` (Venables and Ripley, 2002) and `robeth` (Marazzi, 2020).

- For the Mallows and Schweppe type GM-estimators and given that $\boldsymbol{W} = \boldsymbol{I}$, the asymptotic covariance coincides with the one implemented in package/ library `robeth` for the option "averaged"; see Marazzi (1993, Chapter 4) and Marazzi (1987, Chapter 2.6) on the earlier `ROBETH-85` implementation.

3 Implementation

The main function – which is only a wrapper function – is `cov_reg_model`. The following display shows pseudo code of the main function.

```
cov_reg_model()
{
    get_psi_function()          // get psi function (fun ptr)
    get_psi_prime_function()    // get psi-prime function (fun ptr)
    switch(type) {
        case 0: cov_m_est()             // M-estimator
        case 1: cov_mallows_gm_est()    // Mallows GM-estimator
        case 2: cov_schweppe_gm_est()   // Schweppe GM-estimator
    }
    robsurvey_error()           // signal error in case of failure
}
```

The functions `cov_m_est()`, `cov_mallows_gm_est()`, and `cov_schweppe_gm_est()` implement the covariance estimators; see below. All functions are based on the subroutines in `BLAS` (Blackford et al., 2002) and `LAPACK` (Anderson et al., 1999).

To fix notation, denote the Hadamard product of the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ by $\boldsymbol{A} \circ \boldsymbol{B}$ and suppose that $\sqrt{\cdot}$ is applied element by element.

3.1 M-estimator

The covariance matrix is (up to $\widehat{\sigma}$) equal to (see `cov_m_est`)

$$(\boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X})^{-1} \tag{2}$$

and is computed as follows:

- Compute the factorization $\sqrt{\boldsymbol{w}} \circ \boldsymbol{X} := \boldsymbol{QR}$ (LAPACK: `dgeqrf`).
- Invert the upper triangular matrix $\boldsymbol{R}$ by backward substitution to get $\boldsymbol{R}^{-1}$ (LAPACK: `dtrtri`).
- Compute $\boldsymbol{R}^{-1}\boldsymbol{R}^{-T}$, which is equal to (2); taking advantage of the triangular shape of $\boldsymbol{R}^{-1}$ and $\boldsymbol{R}^{-T}$ (LAPACK: `dtrmm`).

3.2 Mallows GM-estimator

The covariance matrix is (up to $\widehat{\sigma}$) equal to (see `cov_mallows_gm_est`)

$$\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{H}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{H}^2\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{H}\boldsymbol{X}\right)^{-1} \tag{3}$$

and is computed as follows:

- Compute the QR factorization: $\sqrt{\boldsymbol{w}\cdot\boldsymbol{h}}\circ\boldsymbol{X} := \boldsymbol{Q}\boldsymbol{R}$ (LAPACK: `dgeqrf`).
- Invert the upper triangular matrix $\boldsymbol{R}$ by backward substitution to get $\boldsymbol{R}^{-1}$ (LAPACK: `dtrtri`).
- Define a new matrix: $\boldsymbol{A} \leftarrow \sqrt{\boldsymbol{h}}\circ\boldsymbol{Q}$ (extraction of $\boldsymbol{Q}$ matrix with LAPACK: `dorgqr`).
- Update the matrix: $\boldsymbol{A} \leftarrow \boldsymbol{A}\boldsymbol{R}^{-T}$ (taking advantage of the triangular shape of $\boldsymbol{R}^{-1}$; LAPACK: `dtrmm`).
- Compute $\boldsymbol{A}\boldsymbol{A}^T$, which corresponds to the expression in (3); (LAPACK: `dgemm`).

3.3 Schweppe GM-estimator

The covariance matrix is (up to $\widehat{\sigma}$) equal to (see `cov_schweppe_gm_est`)

$$\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{S}_1\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{S}_2\boldsymbol{X}\left(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{S}_1\boldsymbol{X}\right)^{-1}. \tag{4}$$

Put $\boldsymbol{s}_1 = \mathrm{diag}(\boldsymbol{S}_1)$, $\boldsymbol{s}_2 = \mathrm{diag}(\boldsymbol{S}_2)$, and let $\cdot/\cdot$ denote elemental division (i.e., the inverse of the Hadamard product). The covariance matrix in (4) is computed as follows

- Compute the factorization $\sqrt{\boldsymbol{w}\circ\boldsymbol{s}_1}\circ\boldsymbol{X} := \boldsymbol{Q}\boldsymbol{R}$ (LAPACK: `dgeqrf`).
- Invert the upper triangular matrix $\boldsymbol{R}$ by backward substitution to get $\boldsymbol{R}^{-1}$ (LAPACK: `dtrtri`).
- Define a new matrix: $\boldsymbol{A} \leftarrow \sqrt{\boldsymbol{s}_2/\boldsymbol{s}_1}\circ\boldsymbol{Q}$ (extraction of $\boldsymbol{Q}$ matrix with LAPACK: `dorgqr`).
- Update the matrix: $\boldsymbol{A} \leftarrow \boldsymbol{A}\boldsymbol{R}^{-T}$ (taking advantage of the triangular shape of $\boldsymbol{R}^{-1}$; LAPACK: `dtrmm`).
- Compute $\boldsymbol{A}\boldsymbol{A}^T$, which corresponds to the expression in (4); (LAPACK: `dgemm`).

Remark. Marazzi (1987) uses the Cholesky factorization (see his subroutines `RTASKV` and `RTASKW`) which is computationally a bit cheaper than our QR factorization.

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