1 LMVAR: a linear model with heteroscedasticity

This vignette describes in more detail the mathematical aspects of the model with which the \texttt{lmvar} package is concerned. A short description can be found in the vignette 'Intro' of this package. The model has been discussed by various authors [1, 2, 3].

Assume that a stochastic vector $Y \in \mathbb{R}^n$ has a multivariate normal distribution as
\[
Y \sim N_n(\mu^*, \Sigma^*)
\] (1)
in which $\mu^* \in \mathbb{R}^n$ is the expected value and $\Sigma^* \in \mathbb{R}^{n,n}$ a diagonal covariance matrix
\[
\Sigma^*_{ij} = \begin{cases} 0 & i \neq j \\ (\sigma_i^*)^2 & i = j. \end{cases}
\] (2)

Assume that the vector of expectation values $\mu^*$ is linearly dependent on the values of the covariates in a model matrix $X_\mu$:
\[
\mu^* = X_\mu \beta_{\mu}^*
\] (3)
with $X_\mu \in \mathbb{R}^{n,k_\mu}$ and $\beta_{\mu}^* \in \mathbb{R}^{k_\mu}$.

Similarly, assume that the vector $\sigma^* = (\sigma_1^*, \ldots, \sigma_n^*)$ depends on the covariates in a model matrix $X_\sigma$ as
\[
\log \sigma^* = X_\sigma \beta_{\sigma}^*
\] (4)
where $\log \sigma^* = (\log \sigma_1^*, \ldots, \log \sigma_n^*)$, $X_\sigma \in \mathbb{R}^{n,k_\sigma}$ and $\beta_{\sigma}^* \in \mathbb{R}^{k_\sigma}$. The logarithm is taken to be the 'natural logarithm', i.e., with base $e$.

We assume $n \geq k_\mu + k_\sigma$ to avoid having an overdetermined system when we calculate estimators for $\beta_{\mu}^*$ and $\beta_{\sigma}^*$, as explained in the next section.

If we take $X_\sigma$ a $n \times 1$ matrix in which each element is equal to 1, we have the standard linear model.

The parameter vector $\beta_{\mu}^*$ is defined uniquely only if $X_\mu$ is full-rank. If not, the space $\mathbb{R}^{k_\mu}$ can be split into subspaces such that there is a uniquely defined $\beta_{\mu}^*$ in each subspace. The way \texttt{lmvar} treats this is as follows. If the user-supplied $X_\mu$ is not full-rank, \texttt{lmvar} removes just enough columns from the matrix to make it full-rank. This amounts to selecting $\beta_{\mu}^*$ from the subspace in which all vector elements corresponding to the removed columns, are set to zero.

In the same way, if the user-supplied $X_\sigma$ is not full-rank, just enough columns are removed to make it so. This defines a subspace in which $\beta_{\sigma}^*$ is defined uniquely.

In what follows we assume that $X_\mu$ and $X_\sigma$ are the matrices after the columns have been removed, i.e., they are full-rank matrices. The vector elements that are set to zero, drop out of $\beta_{\mu}^*$ and $\beta_{\sigma}^*$ and the dimensions $k_\mu$ and $k_\sigma$ are reduced accordingly. These reduced dimensions are returned by the function \texttt{dfree} in the \texttt{lmvar} package.
2 Maximum-likelihood equations

A vector element $Y_i$ is distributed as

$$Y_i \sim \frac{1}{\sqrt{2\pi} \sigma_i^*} \exp \left( -\frac{1}{2} \left( \frac{Y_i - \mu_i^*}{\sigma_i^*} \right)^2 \right).$$

(5)

The logarithm of the likelihood $L$ is defined as

$$\log L(\beta_{\mu}, \beta_{\sigma}) = -\frac{n}{2} \log(2\pi) - \sum_{k=1}^{n} \left( \log \sigma_k + \frac{(y_k - \mu_k^2)}{2\sigma_k^2} \right).$$

(6)

for all vectors $\beta_{\mu} \in \mathbb{R}^{k_{\mu}}$ and $\beta_{\sigma} \in \mathbb{R}^{k_{\sigma}}$ and $\mu$ and $\sigma$ defined as

$$\mu = X_{\mu} \beta_{\mu}$$

$$\log \sigma = X_{\sigma} \beta_{\sigma}.$$  

(7)

We are looking for $\hat{\beta}_{\mu} \in \mathbb{R}^{k_{\mu}}$ and $\hat{\beta}_{\sigma} \in \mathbb{R}^{k_{\sigma}}$ that maximize the log-likelihood:

$$\left( \hat{\beta}_{\mu}, \hat{\beta}_{\sigma} \right) = \arg \max_{(\beta_{\mu}, \beta_{\sigma}) \in \mathbb{R}^{k_{\mu}} \times \mathbb{R}^{k_{\sigma}}} \log L(\beta_{\mu}, \beta_{\sigma}).$$

(8)

These maximum likelihood estimators are taken to be the estimators of $\beta_{\mu}^*$ and $\beta_{\sigma}^*$. We assume that $\hat{\beta}_{\mu}$ and $\hat{\beta}_{\sigma}$ thus defined, exist and are unique. See section 4 however for a situation in which the maximum log-likelihood is undefined.

Given $\hat{\beta}_{\sigma}$, this is true for $\hat{\beta}_{\mu}$. Namely, given any $\beta_{\sigma}$, $\log L$ is maximized by the $\beta_{\mu}$ which is the solution of

$$\nabla_{\beta_{\mu}} \log L = 0$$

(9)

where $\nabla_{\beta_{\mu}}$ stands for the gradient $(\frac{\partial}{\partial \beta_{\mu,1}}, \ldots, \frac{\partial}{\partial \beta_{\mu,n}})$.

This solution is

$$\beta_{\mu} = (X_{\mu}^T \Sigma^{-1} X_{\mu})^{-1} X_{\mu}^T \Sigma^{-1} y.$$  

(10)

with $\Sigma \in \mathbb{R}^{n,n}$ defined as in (2) but with $\beta_{\sigma}$ arbitrary:

$$\Sigma_{ij} = \begin{cases} 0 & i \neq j \\ \sigma_i^2 & i = j. \end{cases}$$

(11)

Because of our assumption that $X_{\mu}$ is full rank, the inverse of the matrix $X_{\mu}^T \Sigma^{-1} X_{\mu}$ can be taken.

It is easy to see that the solution (10) represents a maximum in the log-likelihood. The matrix $H_{\mu\mu}$ of second-order derivatives

$$(H_{\mu\mu})_{ij} = \frac{\partial^2 \log L}{\partial \beta_{\mu i} \partial \beta_{\mu j}}.$$  

(12)
is given by
\[ H_{\mu\mu} = -X_\mu^T \Sigma^{-1} X_\mu, \] (13)
which is negative-definite for any \( \beta_\sigma \).

Our maximization search can now be carried out in a smaller space:
\[ \hat{\beta}_\sigma = \arg\max_{\beta_\sigma \in \mathbb{R}^{k_\sigma}} \log L_P(\beta_\sigma) \] (14)
where \( L_P \) is the so-called profile-likelihood
\[ L_P(\beta_\sigma) = L(\beta_\mu(\beta_\sigma), \beta_\sigma). \] (15)
with \( \beta_\mu \) depending on \( \beta_\sigma \) as in (10).

To find \( \hat{\beta}_\sigma \) from (14), we must solve
\[ (\nabla_{\beta_\mu} \log L) (\nabla_{\beta_\sigma} \beta_\mu) + \nabla_{\beta_\sigma} \log L = 0 \] (16)
evaluated at \( \beta_\mu = \beta_\mu(\beta_\sigma) \), and \( (\nabla_{\beta_\sigma} \beta_\mu) \) the matrix
\[ (\nabla_{\beta_\sigma} \beta_\mu)_{ij} = \frac{\partial \beta_{\mu i}}{\partial \beta_{\sigma j}}. \] (17)
However, because of (9), the first term in (16) vanishes and we are left to solve
\[ \nabla_{\beta_\sigma} \log L = 0. \] (18)
The derivatives that are the elements of this gradient are given by
\[
\frac{\partial \log L}{\partial \beta_{\sigma i}} = \sum_{k=1}^{n} \left( -\frac{(X_\sigma)_{ki}}{\sigma_k^2} \cdot \left( y_k - \mu_k \right)^2 \right) - \left( \frac{(X_\sigma)_{ki}}{\sigma_k^2} \right) \cdot \left( \frac{(X_\sigma)_{ki}}{\sigma_k^2} \right) \cdot \left( Y_k^2 - 1 \right) \cdot (X_\sigma)_{ki}.
\] (19)
The entire gradient can be written as a matrix-product as
\[ \nabla_{\beta_\sigma} \log L = X_\sigma^T \lambda_\sigma \] (20)
with \( \lambda_\sigma \) a vector of length \( n \) whose elements \( \lambda_{\sigma i} \) are
\[ \lambda_{\sigma i} = \left( \frac{y_i - \mu_i}{\sigma_i} \right)^2 - 1. \] (21)
The maximum-likelihood equations (18) take the form
\[ X_\sigma^T \lambda_\sigma = 0. \] (22)
The estimate \( \mu \) of the expectation value that appears in \( \lambda_\sigma \) depends on \( \beta_\sigma \) as
\[
\mu = X_\mu \beta_\mu = X_\mu \left( X_\mu^T \Sigma^{-1} X_\mu \right)^{-1} X_\mu^T \Sigma^{-1} y.
\] (23)
2.1 Profile-likelihood Hessian

Numerical procedures to solve the maximum-likelihood equations $X^T \lambda_\sigma = 0$ involve the calculation of the Hessian $H_P$ of the profile log-likelihood. $H_P$ is the matrix of second-order derivatives of log $L_P$:

$$(H_P)_{ij} = \frac{\partial^2 \log L_P}{\partial \beta_\sigma j \partial \beta_\sigma i}$$

(24)

Differentiation of (19) gives for the second-order derivatives

$$(H_P)_{ij} = -2 \sum_{k=1}^{n} (X_{ik})_k \frac{y_k - \mu_k}{\sigma_k^2} \left\{ \frac{\partial \mu_k}{\partial \beta_\sigma j} + (y_k - \mu_k)(X_\sigma)_{kj} \right\}$$

(25)

with $\frac{\partial \mu_k}{\partial \beta_\sigma j}$ the element at row $k$ and column $j$ of the matrix $\nabla_\beta \mu$. Given that $\mu = X_\mu \beta_\mu$ and $\beta_\mu$ is given by (10), the $j$-th column vector of the matrix is

$$\frac{\partial \mu}{\partial \beta_\sigma j} = X_\mu \left\{ \frac{\partial (X_\mu^T \Sigma^{-1} X_\mu)}{\partial \beta_\sigma j} X_\mu^T \Sigma^{-1} + (X_\mu^T \Sigma^{-1} X_\mu)^{-1} X_\mu^T \frac{\partial \Sigma^{-1}}{\partial \beta_\sigma j} \right\} y$$

(26)

The matrix $\frac{\partial \Sigma^{-1}}{\partial \beta_\sigma j}$ takes the form

$$\frac{\partial \Sigma^{-1}}{\partial \beta_\sigma j} = \sum_{i=1}^{n} \frac{\partial \Sigma^{-1}}{\partial \sigma_i} \frac{\partial \sigma_i}{\partial \beta_\sigma j}$$

(27)

$$= -2 \begin{pmatrix} (X_\sigma)_{1j} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & (X_\sigma)_{nj} \end{pmatrix} \Sigma^{-1}$$

The $j$-th column vector of the matrix is

$$\frac{\partial \mu}{\partial \beta_\sigma j} = -2 X_\mu (X_\mu^T \Sigma^{-1} X_\mu)^{-1} X_\mu^T \left( \begin{array}{c} \frac{y_1 - \mu_1}{\sigma_1^2} (X_\sigma)_{1j} \\ \vdots \\ \frac{y_n - \mu_n}{\sigma_n^2} (X_\sigma)_{nj} \end{array} \right)$$

(28)

and the element $(\nabla_\beta \mu)_{kj}$ of the matrix $\nabla_\beta \mu$ is given by

$$\frac{\partial \mu_k}{\partial \beta_\sigma j} = -2 \sum_{l=1}^{n} (X_\mu (X_\mu^T \Sigma^{-1} X_\mu)^{-1} X_\mu^T)_{kl} \frac{y_l - \mu_l}{\sigma_l^2} (X_\sigma)_{lj}.$$
If we substitute this result in (25), we obtain for the element at row $i$ and column $j$ of the Hessian:

$$(H_P)_{ij} = 4 \sum_{k,l=1}^{n} (X^T_{\sigma})_{ik} \frac{y_k - \mu_k}{\sigma_k^2} (X_{\mu} (X^T_{\mu} \Sigma^{-1} X_{\mu})^{-1} X^T_{\mu})_{kl} \frac{y_l - \mu_l}{\sigma_l^2} (X_{\sigma})_{lj} +$$

$$-2 \sum_{k=1}^{n} (X^T_{\sigma})_{ik} \left( \frac{y_k - \mu_k}{\sigma_k} \right)^2 (X_{\sigma})_{kj}.$$  \hspace{1cm} (30)

We can write the Hessian as a matrix-product as

$$H_P = X^T_{\sigma} A_1 X_{\mu} (X^T_{\mu} \Sigma^{-1} X_{\mu})^{-1} X^T_{\mu} A_1 X_{\sigma} + X^T_{\sigma} A_2 X_{\sigma} \quad \text{(31)}$$

with two $n \times n$ diagonal matrices

$$(A_1)_{ij} = \begin{cases} 0 & i \neq j \\ 2 \frac{y_i - \mu_i}{\sigma_i^2} & i = j \end{cases} \quad (A_2)_{ij} = \begin{cases} 0 & i \neq j \\ -2 \left( \frac{y_i - \mu_i}{\sigma_i} \right)^2 & i = j. \end{cases} \quad \text{(32)}$$

### 3 Distributions for estimators

Asymptotic theory of maximum-likelihood estimators tells that the vector of the combined estimators $(\hat{\beta}_{\mu}, \hat{\beta}_{\sigma})$ as defined in (8), is distributed approximately as

$$(\hat{\beta}_{\mu}, \hat{\beta}_{\sigma}) \sim \mathcal{N}_{k_{\mu} + k_{\sigma}} ((\beta^*_{\mu}, \beta^*_{\sigma}), \Sigma_{\beta \beta}) \quad \text{for } n \text{ large.} \quad \text{(33)}$$

This distribution is valid in the limit of a large number of observations $n$.

The covariance matrix $\Sigma_{\beta \beta}$ is given in terms of the inverse Fisher information matrix $I_n$:

$$\Sigma_{\beta \beta} = \frac{1}{n} I_n^{-1}. \quad \text{(34)}$$

The Fisher information matrix is given in terms of the expected value of the Hessian at $\beta_{\mu} = \beta^*_\mu$ and $\beta_{\sigma} = \beta^*_\sigma$:

$$I_n = -\frac{1}{n} E[H^*]. \quad \text{(35)}$$

The Hessian $H$ is the Hessian of the full log-likelihood, in contrast to the profile-log-likelihood Hessian:

$$H^* = \begin{pmatrix} H^*_{\mu\mu} & H^*_{\mu\sigma} \\ H^*_{\mu\sigma} & H^*_{\sigma\sigma} \end{pmatrix} \quad \text{(36)}$$

with the three block-matrices defined as

$$\begin{align*}
(H^*_{\mu\mu})_{ij} &= \frac{\partial^2 \log L}{\partial \beta_{\mu i} \partial \beta_{\mu j}}, \\
(H^*_{\mu\sigma})_{ij} &= \frac{\partial^2 \log L}{\partial \beta_{\mu i} \partial \beta_{\sigma j}}, \\
(H^*_{\sigma\sigma})_{ij} &= \frac{\partial^2 \log L}{\partial \beta_{\sigma i} \partial \beta_{\sigma j}}.
\end{align*} \quad \text{(37)}$$
evaluated at $\beta_\mu = \beta_\mu^*$ and $\beta_\sigma = \beta_\sigma^*$.

We have already calculated $H_{\mu\mu}$ in (13). The other block matrices are given by

$$(H_{\mu\sigma}^*)_{ij} = -2 \sum_{k=1}^n \frac{y_k - \mu_k^*}{\sigma_k^*} (X_\mu)_{ki} (X_\sigma)_{kj}$$

$$(H_{\sigma\sigma}^*)_{ij} = -2 \sum_{k=1}^n \left( \frac{y_k - \mu_k^*}{\sigma_k^*} \right)^2 (X_\sigma)_{ki} (X_\sigma)_{kj}.$$ 

In matrix notation:

$$H_{\mu\mu}^* = -X_\mu^T \Sigma_\star^{-1} X_\mu, \quad H_{\mu\sigma}^* = -X_\mu^T \Lambda_1^* X_\sigma, \quad H_{\sigma\sigma}^* = X_\sigma^T \Lambda_2^* X_\sigma. \quad (38)$$

with $\Lambda_1^*$ equal to $\Lambda_1$ with $\mu = \mu^*$ and $\sigma = \sigma^*$, and likewise for $\Lambda_2^*$.

When we take expected values and keep in mind that $E[Y - \mu^*] = 0$

$$E[(Y_i - \mu_i^*)(Y_j - \mu_j^*)] = \begin{cases} 0 & i \neq j \\ \sigma_i^* & i = j \end{cases},$$

we arrive at

$$E[H_{\mu\mu}^*] = -X_\mu^T \Sigma_\star^{-1} X_\mu, \quad E[H_{\mu\sigma}^*] = 0, \quad E[H_{\sigma\sigma}^*] = -2X_\sigma^T X_\sigma \quad (39)$$

This brings the expected value of the Hessian in the form

$$E[H^*] = -\begin{pmatrix} X_\mu^T \Sigma_\star^{-1} X_\mu & 0 \\ 0 & 2X_\sigma^T X_\sigma \end{pmatrix}. \quad (40)$$

The function fisher in the lmvar package calculates the Fisher information matrix. It estimates $E[H^*]$ by replacing the true but unknown $\sigma^*$ by its maximum-likelihood estimator $\hat{\sigma}$ in $\Sigma_\star$.

The expectation value (40) brings the covariance matrix $\Sigma_{\beta\beta}$ in the form

$$\Sigma_{\beta\beta} = \begin{pmatrix} (X_\mu^T \Sigma_\star^{-1} X_\mu)^{-1} & 0 \\ 0 & \frac{1}{2} (X_\sigma^T X_\sigma)^{-1} \end{pmatrix}. \quad (41)$$

This implies that $\hat{\beta}_\mu$ and $\hat{\beta}_\sigma$ are independent stochastic variables distributed as

$$\hat{\beta}_\mu \sim N_{k_\mu} (\beta_\mu^*, (X_\mu^T \Sigma_\star^{-1} X_\mu)^{-1}) \quad \text{for } n \text{ large.} \quad (42)$$

$$\hat{\beta}_\sigma \sim N_{k_\sigma} (\beta_\sigma^*, \frac{1}{2} (X_\sigma^T X_\sigma)^{-1})$$

We obtain for the asymptotic distribution of the maximum-likelihood estimators of $\mu^*$ and $\sigma^*$

$$\hat{\mu} \sim N_n (\mu^*, X_\mu (X_\mu^T \Sigma_\star^{-1} X_\mu)^{-1} X_\mu^T) \quad \text{for } n \text{ large.} \quad (43)$$

$$\log \hat{\sigma} \sim N_n (\log \sigma^*, \frac{1}{2} X_\sigma (X_\sigma^T X_\sigma)^{-1} X_\sigma^T)$$
The expectation value and the variance for an element $\hat{\sigma}_i$ of $\hat{\sigma}$ are

$$
E[\hat{\sigma}_i] = \sigma_i^* \exp \left( \frac{(X_{\sigma} (X_{\sigma}^T X_{\sigma})^{-1} X_{\sigma}^T)_{ii}}{4} \right) \quad \text{for } n \text{ large.}
$$

$$
\text{var}(\hat{\sigma}_i) = (E[\hat{\sigma}_i])^2 \left( \exp \left( \frac{(X_{\sigma} (X_{\sigma}^T X_{\sigma})^{-1} X_{\sigma}^T)_{ii}}{2} \right) - 1 \right)
$$

The function fitted.lmvar (with the option log = FALSE) returns $\hat{\mu}$ and $\hat{\sigma}$.

4 A case in which the maximum log-likelihood is not defined

It happens in practice that the maximum log-likelihood cannot be determined. The routine which calculates it runs into numerical instabilities and exits with warning messages.

If that happens, the following might be the case. Suppose the full set of $n$ observations can be split in two subsets $S_1$, with $n_1$ observations, and $S_2$, with $n_2$ observations, such that $n = n_1 + n_2$. For simplicity and without loss of generality, we assume that the first $n_1$ observations form the set $S_1$ and the remaining observations the set $S_2$. Correspondingly, we split the response vector $y$ in a vector $y_1 \in \mathbb{R}^{n_1}$ and a vector $y_2 \in \mathbb{R}^{n_2}$, the model matrix $X_{\mu}$ in $X_{\mu 1} \in \mathbb{R}^{n_1 k_{\mu}}$ and $X_{\mu 2} \in \mathbb{R}^{n_2 k_{\mu}}$, and likewise for the model matrix $X_{\sigma}$:

$$
y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad X_{\mu} = \begin{pmatrix} X_{\mu 1} \\ X_{\mu 2} \end{pmatrix}, \quad X_{\sigma} = \begin{pmatrix} X_{\sigma 1} \\ X_{\sigma 2} \end{pmatrix}.
$$

The split is made such that:

- $y_1$ is an element of the range of $X_{\mu 1}$, i.e., there exists a vector $\beta_1$ such that $X_{\mu 1} \beta_1 = y_1$, and

- $\ker(X_{\sigma 2}) \neq \emptyset$.

Because $X_{\sigma}$ is full rank there exists a $\beta_2 \in \ker(X_{\sigma 2})$ such that $X_{\sigma} \beta_2 \neq 0$. Moreover, if $v = X_{\sigma 1} \beta_2$ we can choose $\beta_2$ such that $\sum_{k=1}^{n_1} v_k > 0$.

Now consider the log-likelihood $\log \mathcal{L}(\beta_1, \beta_2)$ with $\beta_1 = \beta_1$ and $\beta_2 = -L \beta_2$ with $L > 0$:

$$
\log \mathcal{L}(\beta_1, -L \beta_2) = -\frac{n}{2} \log(2\pi) + L \sum_{k=1}^{n_1} v_k - \frac{1}{2} \sum_{k=n_1+1}^{n} (y_k - \mu_k)^2
$$

which shows

$$
\log \mathcal{L}(\beta_1, -L \beta_2) \to \infty \quad \text{as } L \to \infty.
$$

The option remove.df.sigma = TRUE of the function lmvar tries to recognize this situation. It identifies the set of observations $S_1$ as the observations for which the standard deviation becomes very small. It then removes columns from $X_{\sigma}$ to make $X_{\sigma 2}$ full-rank.
References

