

Generalized Least Squares

- So far, we have focused on modeling the *expected value of the dependent variable* and calculated its standard error. Now we concentrate on the estimating covariance matrix of the *distribution of the random component* and use it to adjust the least squares estimator
- **General Least Squares** (GLS) allows addressing violations of the assumption that the regression disturbances ε are independently identical distributed $\varepsilon \sim N(\mathbf{0}, \sigma^2 \cdot \mathbf{I})$.
- If we assume that the disturbances are normally distributed with $\varepsilon \sim N(\mathbf{0}, \sigma^2 \cdot \mathbf{\Omega})$ then regression models under the violation of i.i.d. can be estimated by identifying $\mathbf{\Omega}$ with the maximum likelihood method.
no longer diagonal matrix
- Let us assume that the disturbances ε have a covariance matrix $E(\varepsilon \cdot \varepsilon^T) = \sigma^2 \cdot \mathbf{\Omega}$.
- The generalized least squares estimator accounting for the covariance structure $\mathbf{\Omega}$ in the disturbance ε becomes:

$$\hat{\beta}_{GLS} = (\mathbf{X}^T \cdot \mathbf{\Omega}^{-1} \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{\Omega}^{-1} \cdot \mathbf{y} .$$

- Alternatively, but equivalently (see Hamilton pp 188-189), after transforming the dependent variable and independent variables by $\mathbf{y}^* = \mathbf{\Omega}^{-\frac{1}{2}} \cdot \mathbf{y}$ and $\mathbf{X}^* = \mathbf{\Omega}^{-\frac{1}{2}} \cdot \mathbf{X}$ we get the standard OLS equation:
after this transformation, all observation becomes independent

$$\hat{\beta}_{GLS} = (\mathbf{X}^{*T} \cdot \mathbf{X}^*)^{-1} \cdot \mathbf{X}^{*T} \cdot \mathbf{y}^* .$$

- For simple covariance structures $\mathbf{\Omega}$, like diagonal matrices $\mathbf{\Omega} = \begin{pmatrix} \omega_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \omega_n \end{pmatrix}$, the inverse

$$\mathbf{\Omega}^{-1} = \begin{pmatrix} \frac{1}{\omega_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\omega_n} \end{pmatrix} \text{ or its inverse square root } \mathbf{\Omega}^{-\frac{1}{2}} \text{ are easily calculated.}$$

For general covariance structures $\mathbf{\Omega}$ more advanced methods such as the **eigen-decomposition** or **Cholesky decomposition** must be applied.

- The covariance matrix of the estimated generalized least squares regression coefficients $\hat{\boldsymbol{\beta}}_{GLS}$ becomes:

$$\text{Var}(\hat{\boldsymbol{\beta}}_{GLS}) = \sigma^2 \cdot (\mathbf{X}^T \cdot \mathbf{\Omega}^{-1} \cdot \mathbf{X})^{-1}.$$

- Why does generalized least squares work?
 - The transformed regression model becomes: $\mathbf{\Omega}^{-\frac{1}{2}} \cdot \mathbf{y} = \mathbf{\Omega}^{-\frac{1}{2}} \cdot \mathbf{X} \cdot \boldsymbol{\beta} + \mathbf{\Omega}^{-\frac{1}{2}} \cdot \boldsymbol{\varepsilon}$.
 - Therefore the **transformed disturbances $\mathbf{\Omega}^{-\frac{1}{2}} \cdot \boldsymbol{\varepsilon}$ will follow an i.i.d normal distribution:**

$$E\left(\mathbf{\Omega}^{-\frac{1}{2}} \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}^T \cdot \mathbf{\Omega}^{-\frac{1}{2}T}\right) = \mathbf{\Omega}^{-\frac{1}{2}} \cdot E(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}^T) \cdot \mathbf{\Omega}^{-\frac{1}{2}T}$$

$$\begin{aligned} &= \mathbf{\Omega}^{-\frac{1}{2}} \cdot \sigma^2 \cdot \mathbf{\Omega} \cdot \mathbf{\Omega}^{-\frac{1}{2}T} \\ &= \sigma^2 \cdot \mathbf{I} \end{aligned}$$

it is a fixed matrix

- The **main problem** is that the covariance structure $\sigma^2 \cdot \Omega$ of the disturbances is usually **unknown**. However, it may be specified by function that just depends on a set of unknown parameters. **These parameters must be estimated from the data.**
- If GLS is used with a ML estimated covariance matrices $\hat{\Omega}$ then it is called **feasible** GLS.

Heteroscedasticity no constant variance

- Remember, we are now explicitly modeling not only the expected value of the dependent variable $E(\mathbf{y}) = \boldsymbol{\mu} = \mathbf{X} \cdot \boldsymbol{\beta}$ but we also focus on the covariance structure among the disturbances $\sigma^2 \cdot \Omega$.

Furthermore, we need the explicit assumption that the dependent variable is normally distributed **$\mathbf{y} \sim N(\boldsymbol{\mu}, \sigma^2 \cdot \Omega)$** in order to perform maximum likelihood estimation.

- If heteroscedasticity is present, that is, $\text{Var}(\varepsilon_i) = \sigma_i^2 = \sigma^2 \cdot \omega_i$, with ω_i being the **individual variation** of the disturbances around the **global variance** σ^2 , the covariance structure takes the special diagonal form of


$$\Omega = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \omega_n \end{bmatrix}$$

with its inverse and square root of its inverse:

$$\mathbf{\Omega}^{-1} = \begin{bmatrix} \frac{1}{\omega_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{\omega_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\omega_n} \end{bmatrix} \quad \text{and} \quad \mathbf{\Omega}^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{\sqrt{\omega_1}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{\omega_2}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{\omega_n}} \end{bmatrix}$$

- The challenge becomes estimating the n unknown variances $\text{VAR}(\varepsilon_i) = \sigma_i^2 = \sigma^2 \cdot \omega_i$.
It is impossible to estimate this many unknown variances since we have only n observations.
Therefore, one needs to build a **functional model** for the individual variances, which depends only on a few unknown parameters $\gamma_0, \dots, \gamma_P$.
- A linear model for the unknown variances could be specified using P **known** external variables $\mathbf{z}_0, \dots, \mathbf{z}_P$.
- All \mathbf{z}_p must be positive **positive** so that the estimated variance remains positive.
- The underlying **multiplicative** model structure becomes, which can be transformed into a linear model structure:

$$\begin{aligned} \sigma_i^2 &= \sigma^2 \cdot z_{i1}^{\gamma_1} \cdot \dots \cdot z_{iP}^{\gamma_P} \quad \text{and with } \sigma^2 = \exp(\gamma_0) \\ &= \exp(\gamma_0 \cdot 1 + \ln(z_{i1}^{\gamma_1}) + \dots + \ln(z_{iP}^{\gamma_P})) \\ &= \exp(\gamma_0 \cdot 1 + \gamma_1 \cdot \ln(z_{i1}) + \dots + \gamma_P \cdot \ln(z_{iP})) \end{aligned}$$

- Therefore, $\sigma^2 = \exp(\gamma_0)$ provides an estimate for the global variance.
- It is important that all variable \mathbf{z}_p **must be** entered in their **logarithmic** form into the model specification for the heteroscedastic error variances (see the help of the function **lmHetero()** in the  package **TexMix**).
- For the simple model with just one weights variable \mathbf{z}_1 , that is,

$$\sigma_i^2 = \exp(\gamma_0 \cdot 1 + \gamma_1 \cdot \ln(z_{i1})),$$

we get the relationships

$\gamma_1 > 0$ σ_i^2 is increasing with increasing z_{i1}

$\gamma_1 \cong 0$ σ_i^2 is not affected by $z_{i1} \Rightarrow$ homoscedasticity

$\gamma_1 < 0$ σ_i^2 is decreasing with increasing z_{i1} spatial condition

- If the estimate coefficient γ_1 does not differ significantly for zero then the model is homoscedastic with regards to the weights variable \mathbf{z}_1 .

Consequently, an adjustment for heteroscedasticity is **not** requires.

- Assuming the model is estimated using the maximum likelihood approach, a likelihood ratio test can be performed with

$$-2 \cdot (\mathcal{LL}(\text{OLS model}) - \mathcal{LL}(\text{weighted model})) \sim \chi_{df=P-1}^2$$

- The R-script **MultiWeightedMaxLike.r** demonstrates the maximum likelihood estimation of the unknown parameters γ and the estimation of the weights vector $\mathbf{w} = \left[\frac{1}{\omega_1}, \dots, \frac{1}{\omega_n} \right]^T$.

Modelling an Autoregressive Spatial Process with FGLS

- Let \mathbf{V} be the a $n \times n$ coded spatial link matrix among the n spatial objects. For a precise definition of the coded link matrix \mathbf{V} see the lecture notes on *Spatial Autocorrelation*.
- The error structure of disturbances for a Gaussian autoregressive spatial process is

$$\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2 \cdot \boldsymbol{\Omega}(\rho))$$

with $\boldsymbol{\Omega}(\rho) = (\mathbf{I} - \rho \cdot \mathbf{V})^{-1} \cdot (\mathbf{I} - \rho \cdot \mathbf{V}^T)^{-1}$. measures the autocorrelation level

- Therefore, $\boldsymbol{\Omega}(\rho)^{-\frac{1}{2}} = [\mathbf{I} - \rho \cdot \mathbf{V}]$ and i.i.d. disturbances can be obtained with the transformation $\boldsymbol{\eta} = \boldsymbol{\Omega}(\rho)^{-\frac{1}{2}} \cdot \boldsymbol{\varepsilon}$ where $\boldsymbol{\eta} = N(\mathbf{0}, \sigma^2 \cdot \mathbf{I})$.
- The generalized least squares model becomes

$$\boldsymbol{\Omega}(\rho)^{-\frac{1}{2}} \cdot \mathbf{y} = \boldsymbol{\Omega}(\rho)^{-\frac{1}{2}} \cdot \mathbf{X} \cdot \boldsymbol{\beta} + \boldsymbol{\eta}$$

which those unknown parameters $\hat{\sigma}^2$, $\hat{\rho}$ and $\hat{\boldsymbol{\beta}}$ with a maximum likelihood estimator using the feasible general least squares approach.

- The R-script **SpatialACItaly.rmd** demonstrates the estimation of a spatial autoregressive process.

Modelling Serial Autocorrelation with GLS (skipped, not test relevant)

- Assuming an autoregressive a stochastic process in the random component ε_t becomes

$$\varepsilon_t = \underbrace{\varphi \cdot \varepsilon_{t-1}}_{\text{AR-process}} + \mu_t \text{ with iid } \mu_t \sim N(0, \sigma^2)$$

- Underlying covariance structure Ω depends on the AR parameter φ .
- For instance, a process with $|\varphi| < 1$ becomes a first order AR process.

Its underlying covariance structure for a process of an equally spaced temporal sequence of observation of length T is

$$\Omega_{(\varphi)} = \frac{1}{1 - \varphi^2} \cdot \begin{bmatrix} 1 & \varphi & \varphi^2 & \dots & \varphi^{T-2} & \varphi^{T-1} \\ \varphi & 1 & \varphi & \dots & \varphi^{T-3} & \varphi^{T-2} \\ \varphi^2 & \varphi & 1 & \dots & \varphi^{T-4} & \varphi^{T-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \varphi^{T-2} & \varphi^{T-3} & \varphi^{T-4} & \dots & 1 & \varphi \\ \varphi^{T-1} & \varphi^{T-2} & \varphi^{T-3} & \dots & \varphi & 1 \end{bmatrix}$$

- Notice, the more time periods Δt two observations are apart the less their stochastic dependence becomes, because for $|\varphi| < 1$ the autocorrelation effect $|\varphi^{\Delta t}| < |\varphi|$ for $\Delta t > 1$.
- Insert $\Omega_{(\varphi)}^{-1/2}$ here.

- Assuming this covariance structure $\mathbf{\Omega}_{(\varphi)}$, the unknown parameters $\{\boldsymbol{\beta}, \sigma^2, \varphi\}$ can be estimated by maximum likelihood assume a distribution of the endogenous variable is $\mathbf{y} \sim N(\mathbf{X} \cdot \boldsymbol{\beta}, \sigma^2 \cdot \mathbf{\Omega}_{(\varphi)})$.
- The R-script **GLSArmaConcord.rmd** demonstrates the estimation of temporally autocorrelated stochastic processes.