Weighted Least Squares (WLS)

Intro

- The **Weighted Least Squares (WLS)** method is an extension of the ordinary least squares (OLS) technique. The model is formulated the same way as in OLS:

$$\hat{y}(\boldsymbol{x}) = \boldsymbol{x}^\mathsf{T}\hat{\boldsymbol{\beta}} + \varepsilon(\boldsymbol{x})$$

  where $\boldsymbol{x}$ is the vector of features, $\boldsymbol{\beta}$ is the vector of parameters, $y(\boldsymbol{x})$ is the target variable, and $\varepsilon(\boldsymbol{x})$ is the error term.

- Each observation $\boldsymbol{x}$ has associated weights $w(\boldsymbol{x})$ that reflect the importance of that particular observation.
- This method minimizes the weighted sum of squared residuals:

$$\mathrm{RSS} = \sum_{\boldsymbol{x}\in X^\ell} w(\boldsymbol{x}) \cdot (y(\boldsymbol{x}) - \hat{y}(\boldsymbol{x}))^2 \to \min_{\boldsymbol{\beta}}.$$

- The solution to this minimization problem is given by:

$$\boldsymbol{\beta}^* = \underbrace{(X^\mathsf{T} W X)^{-1} X^\mathsf{T} W}_{X_W^+}\boldsymbol{y},$$

  where W is the diagonal matrix of weights, and X_W^+ is the weighted pseudo-inverse.

Heteroscedasticity can be eliminated by applying weighted LS.

For a model with non-constant variance of the error term:

$$\boldsymbol{y} = X\beta + \varepsilon, \quad \mathrm{Var}[\varepsilon(\boldsymbol{x})] = y(\boldsymbol{x})^2 \cdot \sigma^2$$

To apply WLS, the weights must have a negative square unit:

$$w(\boldsymbol{x}) = \frac{1}{y(\boldsymbol{x})^2}$$

This leads to the transformations:

$$\boldsymbol{y}' = \frac{\boldsymbol{y}}{\sqrt{w}}, \quad \boldsymbol{x}' = \frac{\boldsymbol{x}}{\sqrt{w}}, \quad \boldsymbol{\varepsilon}' = \frac{\boldsymbol{\varepsilon}}{\sqrt{w}}$$

The weight matrix is:

$$W = \begin{pmatrix} \frac{1}{y(\boldsymbol{x}_1)^2} & & \\ & \ddots & \\ & & \frac{1}{y(\boldsymbol{x}_\ell)^2} \end{pmatrix}$$

and

$$\boldsymbol{y}' = \sqrt{W}\boldsymbol{y}, \quad \boldsymbol{x}' = \sqrt{W}\boldsymbol{x}, \quad \boldsymbol{\varepsilon}' = \sqrt{W}\boldsymbol{\varepsilon}$$

Now, the model can be formulated as a homoscedastic least squares problem:

$$\boldsymbol{y}' = X'\beta + \varepsilon', \quad \mathrm{Var}[\varepsilon'(\boldsymbol{x})] = \sigma^2$$

Formalism

Weight matrix

For a weighted

$$\mathrm{RSS} = \sum_{\boldsymbol{x}\in X^\ell} w(\boldsymbol{x}) \cdot (y(\boldsymbol{x}) - \hat{y}(\boldsymbol{x}))^2$$

let's introduce the weight matrix:

$$\begin{aligned} W &:= \mathrm{diag}(w(\boldsymbol{x}_1), ..., w(\boldsymbol{x}_\ell)) \\ &= \begin{pmatrix} w(\boldsymbol{x}_1) & & \\ & \ddots & \\ & & w(\boldsymbol{x}_\ell) \end{pmatrix} \end{aligned}$$

Matrix form

Thus, we can rewrite the RSS in matrix form as a quadratic form:

$$\mathrm{RSS} = (\boldsymbol{y} - X\beta)^\mathsf{T} W (\boldsymbol{y} - X\beta).$$

Quadratic form is a function of the form:

$$Q(x_1, ..., x_n) = \sum_{i=1}^n \sum_{j=1}^n a_{i,j} x_i x_j.$$

Coefficients $a_{i,j}$ can be arranged in a symmetric matrix A, and the quadratic form can be written in matrix form as:

$$Q(\boldsymbol{x}) = \boldsymbol{x}^T A \boldsymbol{x}.$$

Transformation to standard LS problem

The weighted LS problem can be easily reformulated as a standard LS problem by replacing the original variables with transformed ones:

$$\boldsymbol{y}' := W^{\frac{1}{2}}\boldsymbol{y}, \quad X' := W^{\frac{1}{2}}X, \quad \boldsymbol{\varepsilon}' := W^{\frac{1}{2}}\boldsymbol{\varepsilon}$$

Substituting these transformations into the original model, we get:

$$\boldsymbol{y}' = X'\beta + \varepsilon'$$

Analytical solution

Now, let's solve for $\boldsymbol{\beta}$ in the transformed model. Since W and $W^{\{\frac{1}{2}\}}$ are diagonal matrices, transposing them results in the same matrix:

$$\boldsymbol{\beta}^* = X'^{+}\boldsymbol{y}' = \left(X'^{\top}X'\right)^{-1}X'^{\top}\boldsymbol{y}'$$

Expanding the expressions:

$$\begin{aligned}
\boldsymbol{\beta}^* &= \left(\left(W^{\frac{1}{2}}X\right)^{T}W^{\frac{1}{2}}X\right)^{-1}\left(W^{\frac{1}{2}}X\right)^{\top}W^{\frac{1}{2}}\boldsymbol{y} \\
&= \left(X^{\top}WX\right)^{-1}X^{\top}W\boldsymbol{y}
\end{aligned}$$

Therefore, the solution is:

$$\boldsymbol{\beta}^* = \underbrace{\left(X^{\top}WX\right)^{-1}X^{\top}W}_{X_W^{+}}\boldsymbol{y}$$