

Generalized Least Squares

FW8051 Statistics for Ecologists

Department of Fisheries, Wildlife and Conservation Biology



Learn how to use generalized least squares (GLS) to model data where $Y_i|X_i$ is normally distributed, but the variance of the residuals is not constant and may depend on one or more predictor variables.

Generalized Least Squares

Can be used to model data where $Y_i|X_i$ is normally distributed, but we have:

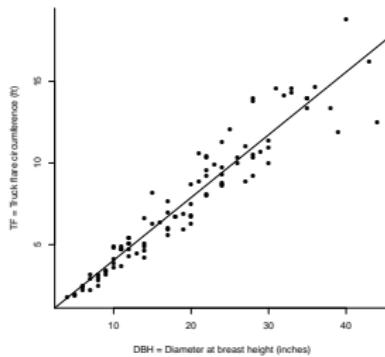
- Non-constant variance (Chapter 5)
- Data that are correlated
 - Multiple measurements on the same sample unit (Chapter 18)
 - Temporal dependence (Chapter 6 of Zuur et al)
 - Spatial dependence (Chapter 7 of Zuur et al)

For this class, we will focus on non-constant variance and multiple measurements on the same sample unit [later in the course]

Trunk Flare Diameter



Linear Model



$$Y_i = \beta_0 + X_i\beta_1 + \epsilon_i$$

Assume ϵ_i are independent, normally distributed, with constant variance.

$$\epsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$$

iid = independent and identically distributed

Generalized Least Squares: Non-Constant Variance

$$Y_i = \beta_0 + X_i\beta_1 + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma_i^2)$$

$$\sigma_i^2 \sim f(X_i; \tau)$$

Model the mean and variance:

- $E[Y_i|X_i] = \beta_0 + X_i\beta_1$
- $\text{Var}[Y_i|X_i] = f(X_i; \tau)$, where τ are additional variance parameters.

Generalized Least Squares: Non-Constant Variance

$$Y_i = \beta_0 + X_i\beta_1 + \epsilon_i$$

$$\epsilon_i \sim N(0, \sigma_i^2)$$

$$\sigma_i^2 \sim f(X_i; \tau)$$

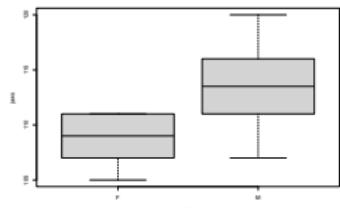
Some options:

- $\sigma_i^2 = \sigma_g^2$ (different σ for each group, g , modeled using a set of multiplicative factors and a reference group)
- $\sigma_i^2 = \sigma^2 X_i$, or $= \sigma^2 |X_i|^{2\delta}$, or $= \sigma^2 e^{2\delta X_i}$ for continuous covariate, X
- $\sigma_i^2 = \sigma^2 E[Y_i|X_i]^{2\theta} = \sigma^2 (\beta_0 + X_i\beta_1)^{2\theta}$. This one is not in Zuur et al. (2009) and can be fit using:
`varPower(form=~fitted(.))`
- Some combination of the above + other options (see Ch. 4 of Zuur et al.)

T-test with unequal variances: Jaw data

```
males<-c(120, 107, 110, 116, 114, 111, 113, 117, 114, 112)
females<-c(110, 111, 107, 108, 110, 105, 107, 106, 111, 111)
jawdat <- data.frame(jaws = c(males, females),
                      sex = c(rep("M", 10), rep("F", 10)))
```

```
boxplot(jaws~sex, data=jawdat)
```



```
summary(gls_ttest)
```

```
## Generalized least squares fit by REML
##  Model: jaws ~ sex
##  Data: jawdat
##      AIC      BIC   logLik 
## 102.0841 105.6456 -47.04206
## 
## Variance function:
##  Structure: Different standard deviations per stratum
##  Formula: ~1 | sex
## Parameter estimates:
##   M       F
## 1.0000000 0.6107279
## 
## Coefficients:
##             Value Std.Error t-value p-value
## (Intercept) 108.6 0.7180211 151.24903 0.0000
## sexM         4.8 1.3775993  3.48432  0.0026
## 
## Correlation:
##   (Intr)
## sexM -0.521
## 
## Standardized residuals:
##            Min          Q1          Med          Q3          Max
## -1.72143457 -0.70466510  0.02689742  0.76657633  1.77522940
## 
## Residual standard error: 3.717829
## Degrees of freedom: 20 total; 18 residual
```

T-test with unequal variances: Jaw data

Y_i = jaw length for jackal i

$$Y_i \sim N(\mu_i, \sigma_i^2) \quad (1)$$

$$\mu_i = \beta_0 + \beta_1 I(\text{sex}=\text{male})_i \quad (2)$$

$$\sigma_i^2 = \sigma_{\text{sex}}^2 \quad (3)$$

```
gls_ttest <- gls(jaws ~ sex,
                  weights = varIdent(form = ~ 1 | sex),
                  data = jawdat)
```

Estimates of regression parameters are obtained by minimizing:

$$\sum_{i=1}^n \frac{(Y_i - \mu_i)^2}{2\sigma_i^2}$$

Summary output

Apparent parameterization:

$\sigma_{\text{sex}}^2 = \sigma^2 \delta_{\text{sex}}^2$, which is the same as $\sigma_{\text{sex}} = \sigma \delta_{\text{sex}}$

with:

- $\delta_{\text{males}} = 1$
- $\delta_{\text{females}} = 0.61$
- $\hat{\sigma} = 3.72$ (residual standard error)

Actual Parameterization

Fraser River Sockeye

Variance model parameterization actually looks like a linear model on the log scale:

$$\log(\sigma_i) = \gamma_0 + \gamma_1 I(\text{sex} = \text{female})_i$$

Ensures that σ_i is positive when we back-transform using $\exp()$.

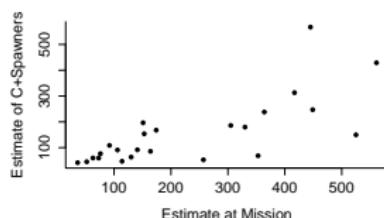
Actual parameterization used by R:

$$\log(\sigma_i) = \log(\sigma) + \log(\delta)I(\text{sex} = \text{female})_i$$

Which is the same as:

$$\sigma_i^2 = \sigma^2 \delta^{2I(\text{sex} = \text{female})}$$

(see book and in-class file for details)



Use historical correlation between the *count at Mission* and $S_t + C_t$ to manage the fishery

Variance increasing with X_j or μ_i

1. Fixed variance model: $\sigma_i^2 = \sigma^2 \text{MisEsc}_i$
2. Power variance model: $\sigma_i^2 = \sigma^2 |\text{MisEsc}_i|^{2\delta}$
3. Exponential variance model: $\sigma_i^2 = \sigma^2 e^{2\delta \text{MisEsc}_i}$
4. Constant + power variance model: $\sigma_i^2 = \sigma^2 (\delta_1 + |\text{MisEsc}_i|^{\delta_2})^2$

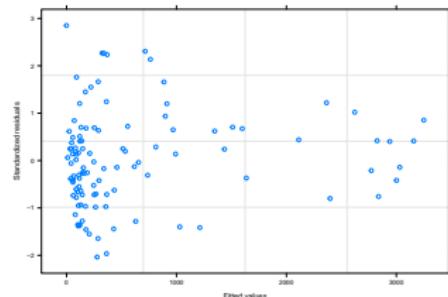
```
varconstp <- gls(SpnEsc ~ MisEsc,  
                    weights = varConstPower(form = ~ MisEsc),  
                    data = sockeye)
```

See textbook via this link.

Standardized residuals

Standardized residuals = $(Y_i - \hat{Y}_i)/\hat{\sigma}_i$, should have approximately constant variance:

```
plot(varconstp)
```



Zuur et al.'s Strategy (Section 4.2.3)

- Start with a "full model" (containing as many predictors as possible) fit using `lm`
- Inspect residuals, consider alternative variance structures if necessary
 - Inspect normalized residuals = $\frac{Y_i - \hat{Y}_i}{\hat{\sigma}_i}$ (these should have constant variance if the variance model is adequate)
 - Compare models using AIC (after refitting the constant variance model using `gls`)
 - Settle on optimal variance model
- Choose best set of predictor variables for the mean of Y_i (using the variance model, chosen above)
- Check diagnostics again and pick best model

... Try to make sense of your results.

Variance depending on μ_i

$$Y_i \sim N(\mu_i, \sigma_i^2)$$
$$\mu_i = \beta_0 + \beta_1 X_i$$
$$\sigma_i^2 = \mu_i^{2\delta}$$

Fit using `varPower(form = ~ fitted(.))`. See textbook via this link.

Approximate Confidence and Prediction Intervals

For a confidence interval, we need to consider:

$$\text{var}(\widehat{E[Y|X]}) = \text{var}(\hat{\beta}_0 + X\hat{\beta}_1)$$

For a prediction interval, we need to consider:

$$\text{var}(\widehat{Y}_i|X_i) = \text{var}(\hat{\beta}_0 + X\hat{\beta}_1 + \epsilon_i)$$

- Confidence interval = captures uncertainty regarding the average value of Y (given by the line)
- Prediction interval = captures uncertainty regarding a particular value of Y (need to also consider spread about the line)

Statistical Theory

- means, sums, regression coefficients will be normally distributed if our sample size, n , is "large" (thanks Central Limit Theorem!)

Consider $(X, Y) \sim MVN(\mu, \Sigma)$.

- $\mu = (E(X), E(Y))$
- $\Sigma = \begin{bmatrix} \sigma_X^2 & \sigma_{X,Y}^2 \\ \sigma_{X,Y}^2 & \sigma_Y^2 \end{bmatrix}$

Then for constants a and b :

- $aX + bY$ will be $MVN(\tilde{\mu}, \tilde{\sigma})$
- $\tilde{\mu} = E(aX + bY) = aE(X) + bE(Y)$
- $\tilde{\sigma} = \text{var}(aX + bY) = a^2\text{var}(X) + b^2\text{var}(Y) + 2ab\text{cov}(X, Y)$

Matrix Multiplication

Matrix multiplication offers a convenient way to calculate variances of linear combinations of random variables (i.e., $aX + bY$)

Let $\Sigma = \begin{bmatrix} \sigma_X^2 & \sigma_{X,Y}^2 \\ \sigma_{X,Y}^2 & \sigma_Y^2 \end{bmatrix}$ give the variance covariance matrix of (X, Y)

- σ_X^2, σ_Y^2 = variance of X, Y
- $\sigma_{X,Y}^2$ = covariance of X and Y

$$\begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = aX + bY$$

$$\begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} \sigma_X^2 & \sigma_{X,Y}^2 \\ \sigma_{X,Y}^2 & \sigma_Y^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = a^2\sigma_X^2 + b^2\sigma_Y^2 + 2ab\sigma_{X,Y}^2$$

Confidence Intervals

$$\text{var}(\widehat{E[Y|X]}) = \text{Var}(\hat{\beta}_0 + X\hat{\beta}_1)$$

$$\begin{bmatrix} a & b \end{bmatrix} = \begin{bmatrix} 1 & X \end{bmatrix} \text{ and } \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}$$

Define:

$$\hat{\Sigma} = \begin{bmatrix} \sigma_{\hat{\beta}_0}^2 & \sigma_{\hat{\beta}_0, \hat{\beta}_1}^2 \\ \sigma_{\hat{\beta}_0, \hat{\beta}_1}^2 & \sigma_{\hat{\beta}_1}^2 \end{bmatrix}$$

$$\widehat{\text{var}}(\widehat{E[Y|X]}) = \text{Var}(\hat{\beta}_0 + X\hat{\beta}_1) = \begin{bmatrix} 1 & X \end{bmatrix} \hat{\Sigma} \begin{bmatrix} 1 \\ X \end{bmatrix}$$

Calculations in R

We can use matrix multiplication to efficiently calculate intervals for multiple observations.

In R, we do this by using %*%

$$\text{Let } X = \text{design matrix} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$$

$\widehat{E[Y|X]} = X \%*% \text{coef(modelname)}$ gives us predicted values for all rows of the X matrix.

$$\widehat{E[Y|X]} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 + X_1\hat{\beta}_1 \\ \hat{\beta}_0 + X_2\hat{\beta}_1 \\ \vdots \\ \hat{\beta}_0 + X_n\hat{\beta}_1 \end{bmatrix}$$

Calculations in R

$$\widehat{\text{var}}(E[Y|X]) = X \% \text{vcov}(\text{modelname}) \% t(X)$$

- `vcov(model) = $\hat{\Sigma}$` = estimated variance-covariance matrix of $\hat{\beta}$ (works for `lm`, `gls`, maybe others)
- We use `t` to get a transpose of a matrix

We end up with a matrix that looks something like:

$$\begin{bmatrix} \text{var}(\hat{Y}_1) & \text{cov}(\hat{Y}_1, \hat{Y}_2) & \cdots & \text{cov}(\hat{Y}_1, \hat{Y}_n) \\ \text{cov}(\hat{Y}_2, \hat{Y}_1) & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \text{cov}(\hat{Y}_{n-1}, \hat{Y}_n) \\ \text{cov}(\hat{Y}_n, \hat{Y}_1) & \cdots & \text{cov}(\hat{Y}_n, \hat{Y}_{n-1}) & \text{var}(\hat{Y}_n) \end{bmatrix}$$

Pull off the diagonal elements (the variances) - see the textbook for code.

Additional Notes

Note, these estimates are approximate in that:

- They rely on asymptotic normality (central limit theorem)
[think difference between t and z]
- They ignore uncertainty in the variance parameters

Prediction Intervals

$$\text{var}(\hat{Y}_i|X_i) = \text{var}(\hat{\beta}_0 + X\hat{\beta}_1 + \epsilon_i)$$

- $\text{var}(\epsilon_i) = \text{var}(Y_i|X_i) = \sigma_i^2$ and estimated by $\hat{\sigma}_i^2$.
- In many cases, $\hat{\sigma}_i^2$ is independent of $[\hat{\beta}_0 \quad \hat{\beta}_1]$
- This implies $\text{cov}(\hat{\sigma}_i^2, \hat{\beta}_0) = \text{cov}(\hat{\sigma}_i^2, \hat{\beta}_1) = 0$

So, to construct a prediction interval, we approximate $\text{var}(\hat{Y}_i|X_i)$ with:

$$\text{var}(\hat{Y}_i|X_i) \approx \widehat{\text{var}}(\hat{\beta}_0 + X\hat{\beta}_1) + \hat{\sigma}_i^2 = X\hat{\Sigma}X' + \hat{\sigma}_i^2.$$

Temporal or Spatial Correlation

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
$$\epsilon_i \sim N(0, \Omega)$$

- Time series: $\text{cor}(\epsilon_i, \epsilon_j) = \rho^{|i-j|}$
- Spatial data: $\text{cor}(\epsilon_i, \epsilon_j)$ depends on distance between points.

If these interest you, I highly recommend taking Brian Aukema's class.