Generalized Least Squares

FW8051 Statistics for Ecologists

Department of Fisheries, Wildlife and Conservation Biology

Learning Objectives

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

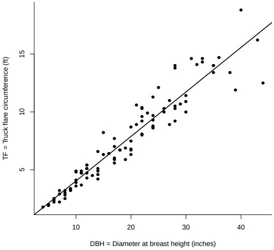
Can be used to model data where $Y_i|X_i$ is normally distributed, but we have:

- 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]

Trunck Flare Diameter

Linear Model



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

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

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

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:

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

Generalized Least Squares: Non-Constant Variance

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

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

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

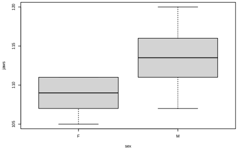
Some options:

- $\sigma_i^2 = \sigma_g^2$ (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

```r
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)))
```

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




```r
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

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

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

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

```r
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:

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

with:

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

Actual Parameterization

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

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

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

Actual parameterization used by R:

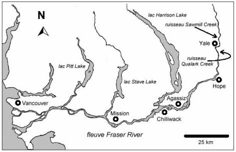
$log(\sigma_i) = log(\sigma) + log(\delta)\text{I(sex = female)}_i$

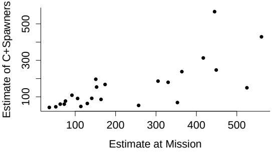
Which is the same as:

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

(see book and in-class file for details)

Fraser River Sockeye





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

Variance increasing with X_i 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: $\sigma_i^2 = \sigma^2 (\delta_1 + |\text{MisEsc}_i|^{\delta_2})^2$

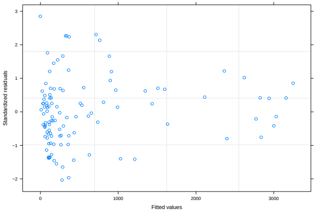
```
varconstp <- gls(SpnEsc ~ MisEsc,
                 weights = varConstPower(form = ~ MisEsc),
                 data = sockeye)
```

See textbook via this link.

Standardized residuals

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

```
plot(varconstp)
```



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.

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 = $\frac{Y_i - \hat{Y}_i}{\widehat{\sigma_i}}$ (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.

Approximate Confidence and Prediction Intervals

For a confidence interval, we need to consider:

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

For a prediction interval, we need to consider:

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

- 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)

Matrix Multiplication: Expected Value

$$\widehat{E[Y|X_i]} = \beta_0 + \hat{\beta}_1 X_i$$

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

Matrix multiplication: Variances

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

Define:

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

Let $\mathbf{X} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$ and $\mathbf{X}'$ be its transpose

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

Calculations in R

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

In R, we do this by using %*%

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

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

Calculations in R

$\widehat{var}(\widehat{E[Y|X]})$ = X%*%`vcov(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:

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

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

Prediction Intervals

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

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

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

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

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

Temporal or Spatial Correlation

$$
\begin{aligned}
y_i &= \beta_0 + \beta_1 x_i + \epsilon_i \\
\epsilon_i &\sim N(0, \Omega)
\end{aligned}
$$

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

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