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)

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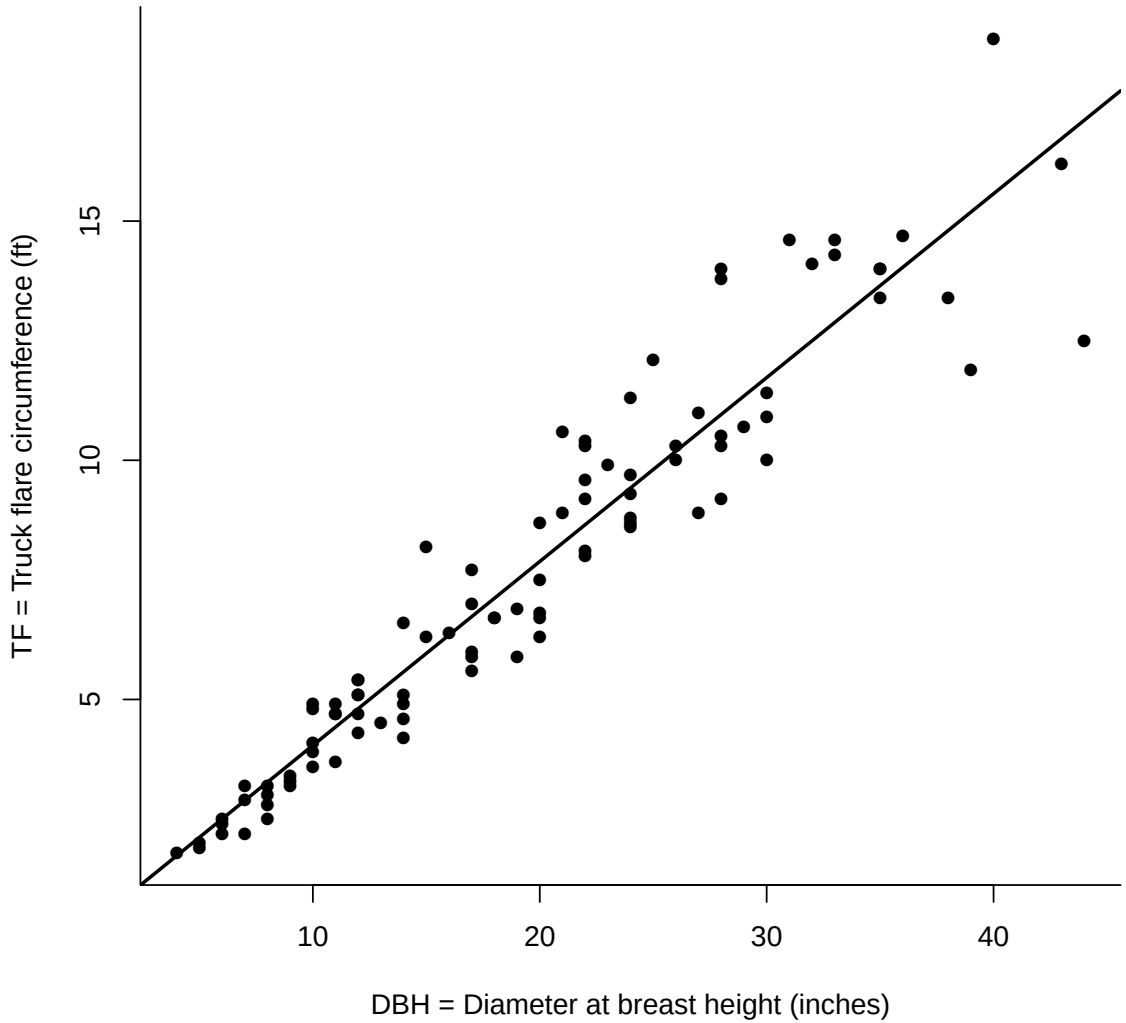
For this class, we will focus on non-constant variance and multiple measurements on the same sample unit [later in the course]

Trunck Flare Diameter


TF = Truck flare circumference (ft)
5
10
15
10
20
30
40
DBH = Diameter at breast height (inches)

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.

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- $\sigma_i^2 = \sigma^2 E[Y_i|X_i]^{2\theta} = \sigma^2(\beta_0 + X_i\beta_1)^{2\theta}$. This one is not in Zuur et al. (2009) and can be fit using: `varPower(form=~fitted(.))`

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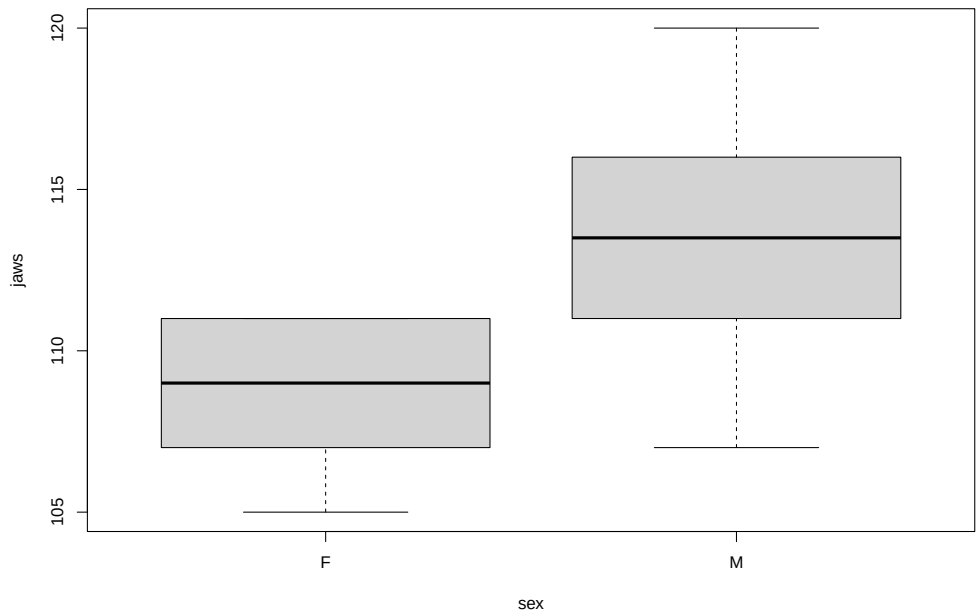
- Some combination of the above + other options (see Ch. 4 of Zuur et al.)

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)
```



T-test with unequal variances: Jaw data

Y_i = jaw length for jackal i

$$Y_i \sim N(\mu_i, \sigma_i^2) \tag{1}$$

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

$$log(\sigma_i) = log(\sigma) + log(\delta)\text{I(sex = female)}_i \tag{3}$$

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

Estimates of regression parameters are obtained by minimizing:

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

Summary output

Variance model:

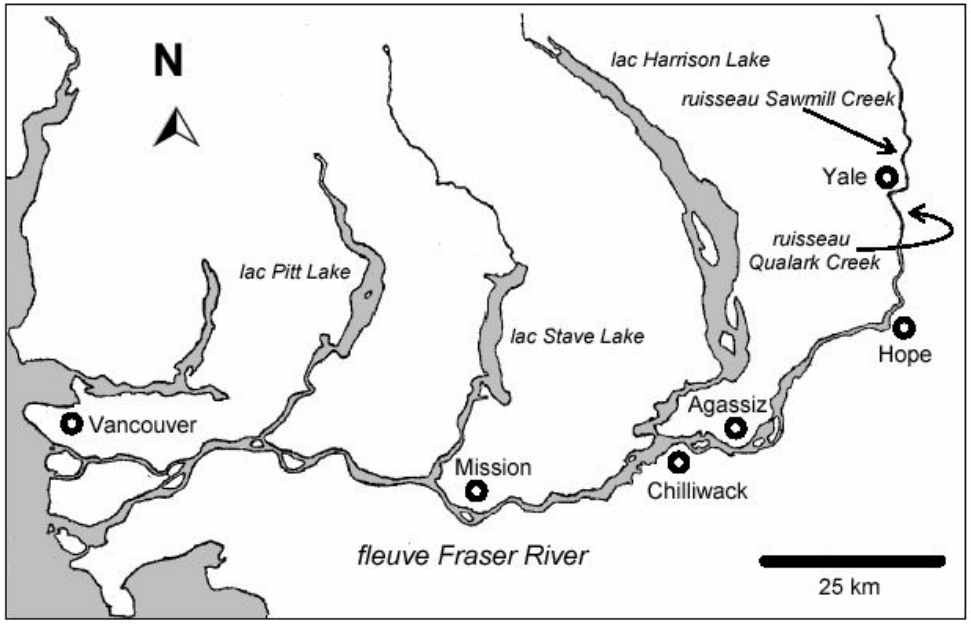
$log(\sigma_i) = log(\sigma) + log(\delta)\text{I(sex = female)}_i$

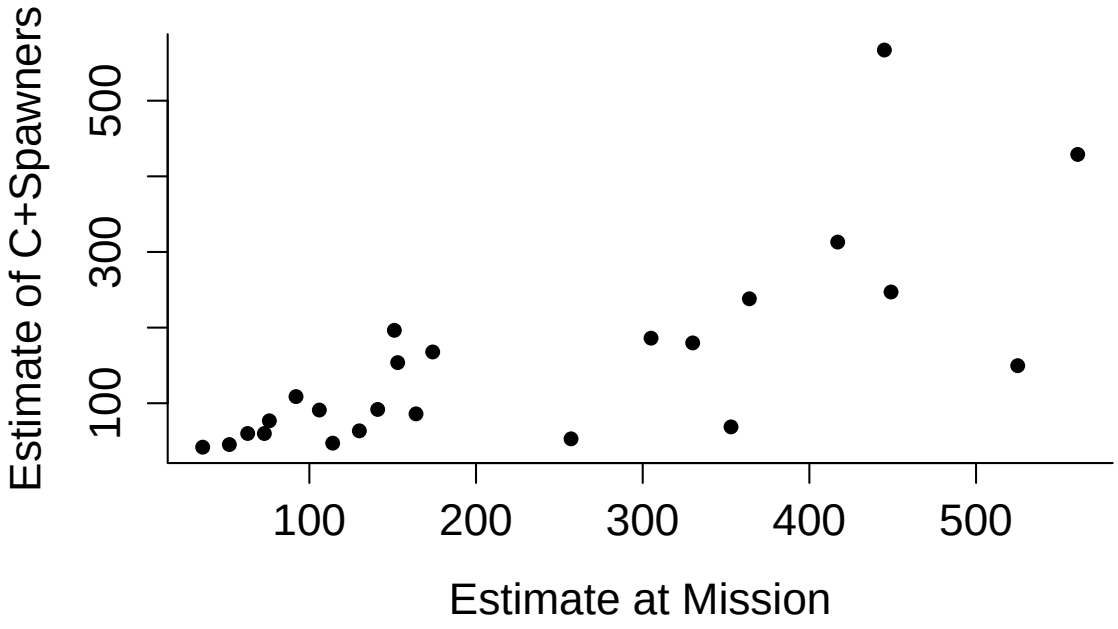
R returns:

- $\hat{\sigma}$
- $\hat{\delta}$ (for females) and $\delta = 1$ for males

See textbook example via this link.

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

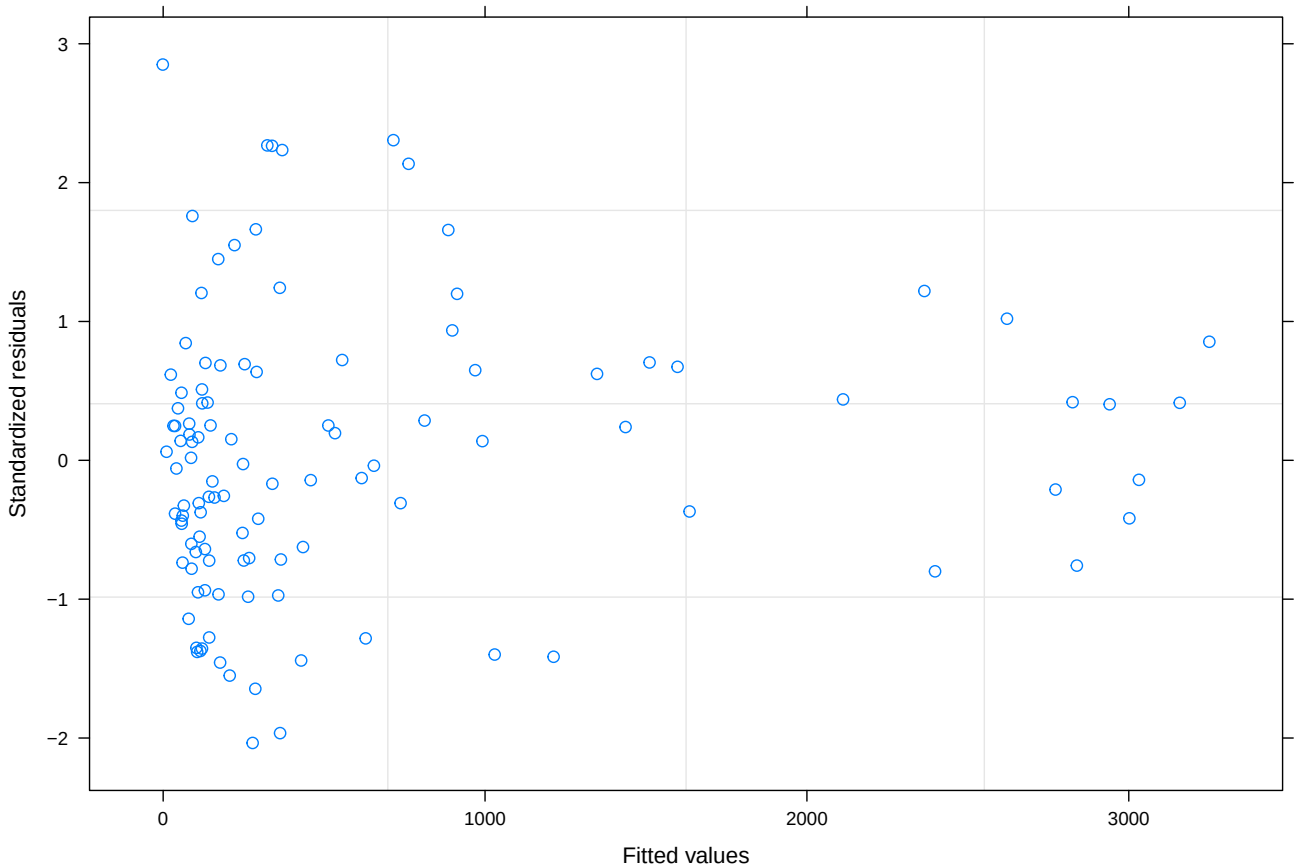
```
varconstp <- gls(SpnEsc ~ MisEsc,
                 weights = varConstPower(form = ~ MisEsc),
                 data = sockeye)
```

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.

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  - Compare models using AIC (after refitting the constant variance model using `gls`)
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- 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

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

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)

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Define:

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

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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 = $\begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{bmatrix}$

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

- `vcov(model)` = $\hat{\Sigma}$ = estimated variance-covariance matrix of $\hat{\beta}$ (works for `lm`, `gls`, maybe others)
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We end up with a matrix that looks something like:

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

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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 $cov(\hat{\sigma}_i^2, \hat{\beta}_0) = cov(\hat{\sigma}_i^2, \hat{\beta}_1) = 0$

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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

$$\mathrm{y}_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
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If these interest you, I highly recommend taking Brian Aukema's class.