Weighted Least Squares and Generalized Least Squares ${ }^{1}$
STA302 Fall 2020
${ }^{1}$ See last slide for copyright information.

## Weighted and Generalized Least Squares

An antidote to unequal variance (of a certain kind)

Example: Aggregated data.Teaching evaluations. Have
■ Mean ratings $\bar{y}_{1}, \ldots, \bar{y}_{m}$
■ Number of students $n_{1}, \ldots, n_{m}$
■ Lots of predictor variables.

$$
\operatorname{Var}\left(\bar{y}_{i}\right)=\frac{\sigma^{2}}{n_{i}}
$$

## Residual Plot

## Residuals by Number of Students in Class



## Model: $\mathbf{y}=\mathbf{X} \boldsymbol{\beta}+\boldsymbol{\epsilon}$

$$
\begin{aligned}
\operatorname{cov}(\boldsymbol{\epsilon}) & =\left(\begin{array}{cccc}
\frac{\sigma^{2}}{n_{1}} & 0 & \cdots & 0 \\
0 & \frac{\sigma^{2}}{n_{2}} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{\sigma^{2}}{n_{m}}
\end{array}\right) \\
& =\sigma^{2}\left(\begin{array}{cccc}
\frac{1}{n_{1}} & 0 & \cdots & 0 \\
0 & \frac{1}{n_{2}} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{1}{n_{m}}
\end{array}\right)
\end{aligned}
$$

Unknown $\sigma^{2}$ times a known matrix.

## Generalize

- $\mathbf{y}=\mathbf{X} \boldsymbol{\beta}+\boldsymbol{\epsilon}$
- $\operatorname{cov}(\boldsymbol{\epsilon})=\sigma^{2} \mathbf{V}$
- $\mathbf{V}$ is a known symmetric positive definite matrix.
- A good estimate of $\mathbf{V}$ can be substituted and everything works out for large samples.


## Generalized Least Squares

Transform the data.

$$
\begin{aligned}
\mathbf{y} & =\mathbf{X} \boldsymbol{\beta}+\boldsymbol{\epsilon}, \text { with } \operatorname{cov}(\boldsymbol{\epsilon})=\sigma^{2} \mathbf{V} \\
\Longrightarrow \mathbf{V}^{-\frac{1}{2}} \mathbf{y} & =\mathbf{V}^{-\frac{1}{2}} \mathbf{X} \boldsymbol{\beta}+\mathbf{V}^{-\frac{1}{2}} \boldsymbol{\epsilon} \\
\mathbf{y}^{*} & =\mathbf{X}^{*} \boldsymbol{\beta}+\boldsymbol{\epsilon}^{*}
\end{aligned}
$$

Same $\boldsymbol{\beta}$.

$$
\begin{aligned}
\operatorname{cov}\left(\boldsymbol{\epsilon}^{*}\right) & =\operatorname{cov}\left(\mathbf{V}^{-\frac{1}{2}} \boldsymbol{\epsilon}\right) \\
& =\mathbf{V}^{-\frac{1}{2}} \operatorname{cov}(\boldsymbol{\epsilon}) \mathbf{V}^{-\frac{1}{2}} \\
& =\mathbf{V}^{-\frac{1}{2}}\left(\sigma^{2} \mathbf{V}\right) \mathbf{V}^{-\frac{1}{2}} \\
& =\sigma^{2} \mathbf{I}
\end{aligned}
$$

## Least Squares Estimate for the * Model is B.L.U.E. $\mathbf{y}^{*}=\mathbf{X}^{*} \boldsymbol{\beta}+\boldsymbol{\epsilon}^{*}$

- By Gauss-Markov, $\widehat{\boldsymbol{\beta}}^{*}$ will beat any other linear combination of the $\mathbf{y}^{*}$.
- $\mathbf{y}^{*}=\mathbf{V}^{-1 / 2} \mathbf{y}$.
- So any linear combination of the $\mathbf{y}$ is a linear combination of the $\mathbf{y}^{*}$.

$$
\begin{aligned}
\mathbf{c}^{\prime} \mathbf{y} & =\mathbf{c}^{\prime} \mathbf{V}^{1 / 2} \mathbf{V}^{-1 / 2} \mathbf{y} \\
& =\mathbf{c}^{\prime} \mathbf{V}^{1 / 2} \mathbf{y}^{*} \\
& =\mathbf{c}_{2}^{\prime} \mathbf{y}^{*}
\end{aligned}
$$

- And $\widehat{\boldsymbol{\beta}}^{*}$ beats it. It's B.L.U.E. for the original problem.


## Generalized Least Squares

$\mathbf{y}^{*}=\mathbf{X}^{*} \boldsymbol{\beta}+\boldsymbol{\epsilon}^{*}$

$$
\begin{aligned}
\widehat{\boldsymbol{\beta}}^{*} & =\left(\mathbf{X}^{*} \mathbf{X}^{*}\right)^{-1} \mathbf{X}^{* \prime} \mathbf{y}^{*} \\
& =\left(\left(\mathbf{V}^{-\frac{1}{2}} \mathbf{X}\right)^{\prime}\left(\mathbf{V}^{-\frac{1}{2}} \mathbf{X}\right)\right)^{-1}\left(\mathbf{V}^{-\frac{1}{2}} \mathbf{X}\right)^{\prime} \mathbf{V}^{-\frac{1}{2}} \mathbf{y}^{*} \\
& =\left(\mathbf{X}^{\prime} \mathbf{V}^{-\frac{1}{2}} \mathbf{V}^{-\frac{1}{2}} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{V}^{-\frac{1}{2}} \mathbf{V}^{-\frac{1}{2}} \mathbf{y} \\
& =\left(\mathbf{X}^{\prime} \mathbf{V}^{-1} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{V}^{-1} \mathbf{y}
\end{aligned}
$$

- So it is not necessary to literally transform the data.
- Convenient expressions for tests and confidence intervals are only a homework problem away.
- $\widehat{\boldsymbol{\beta}}^{*}$ is called the "generalized least squares" estimate of $\boldsymbol{\beta}$.

■ If $\mathbf{V}$ is diagonal, it's called"weighted least squares."

Variance Proportional to $x_{i}$

$$
y_{i}=\beta_{0}+\beta_{1} x_{i}+\epsilon_{i}
$$

$$
\operatorname{cov}(\boldsymbol{\epsilon})=\sigma^{2}\left(\begin{array}{cccc}
x_{1} & 0 & \cdots & 0 \\
0 & x_{2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & x_{n}
\end{array}\right)
$$

## First-order Autoregressive Time Series

Estimate $\rho$ with the first-order sample autocorrelation

$$
\operatorname{cov}(\boldsymbol{\epsilon})=\sigma^{2}\left(\begin{array}{cccccc}
1 & \rho & \rho^{2} & \rho^{3} & \cdots & \rho^{n-1} \\
\rho & 1 & \rho & \rho^{2} & \cdots & \rho^{n-2} \\
\rho^{2} & \rho & 1 & \rho & \cdots & \rho^{n-3} \\
\rho^{3} & \rho^{2} & \rho & 1 & \cdots & \rho^{n-4} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \rho^{n-4} & \cdots & 1
\end{array}\right)
$$

## An amazing scalar example with no independent variables

■ $y_{i j} \stackrel{i . i . d .}{\sim} ?\left(\mu, \sigma^{2}\right)$.
■ Have $\bar{y}_{1}, \ldots, \bar{y}_{m}$ based on $n_{1}, \ldots, n_{m}$.
■ $\bar{y}_{j} \sim N\left(\mu, \frac{\sigma^{2}}{n_{j}}\right)$ by the Central Limit Theorem.

- Want to estimate $\mu$.
- A natural estimator is the mean of means: $\widehat{\mu}_{1}=\frac{1}{m} \sum_{j=1}^{m} \bar{y}_{j}$.
- $E\left(\widehat{\mu}_{1}\right)=\mu$, so it's unbiased.
- $\operatorname{Var}\left(\widehat{\mu}_{1}\right)=\frac{\sigma^{2}}{m^{2}} \sum_{j=1}^{m} \frac{1}{n_{j}}$. Can we do better?
- Noting that $\widehat{\mu}_{1}=\sum_{j=1}^{m} \frac{1}{m} \bar{y}_{j}$ is a linear combination of the $\bar{y}_{j}$ with the weights adding to one ...


## Try Weighted Least Squares

$$
\bar{y}_{j}=\mu+\epsilon_{j} \text { with } E\left(\epsilon_{j}\right)=0 \text { and } \operatorname{Var}\left(\epsilon_{j}\right)=\frac{\sigma^{2}}{n_{j}}
$$

It's a regression with $\beta_{0}=\mu$ and no explanatory variables.

$$
\operatorname{cov}(\boldsymbol{\epsilon})=\sigma^{2}\left(\begin{array}{cccc}
\frac{1}{n_{1}} & 0 & \cdots & 0 \\
0 & \frac{1}{n_{2}} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{1}{n_{m}}
\end{array}\right)=\sigma^{2} \mathbf{V}
$$

## Scalar Calculation

$$
\begin{aligned}
\bar{y}_{j} & =\mu+\epsilon_{j} \\
\Longrightarrow \sqrt{n_{j}} \bar{y}_{j} & =\sqrt{n_{j}} \mu+\sqrt{n_{j}} \epsilon_{j} \\
y_{j}^{*} & =x_{j}^{*} \beta_{1}^{*}+\epsilon_{j}^{*}
\end{aligned}
$$

- It's another regression model.

■ This time there is no intercept, and $\mu$ is the slope.

$$
\begin{aligned}
\operatorname{Var}\left(\epsilon_{j}^{*}\right) & =\operatorname{Var}\left(\sqrt{n_{j}} \epsilon_{j}\right) \\
& =n_{j} \operatorname{Var}\left(\epsilon_{j}\right) \\
& =n_{j} \frac{\sigma^{2}}{n_{j}} \\
& =\sigma^{2}
\end{aligned}
$$

## Least Squares for Simple Regression through the Origin

 $y_{j}^{*}=x_{j}^{*} \beta_{1}^{*}+\epsilon_{j}^{*}$, with $\beta_{1}^{*}=\mu, y_{j}^{*}=\sqrt{n_{j}} \bar{y}_{j}$ and $x_{j}^{*}=\sqrt{n_{j}}$$$
\begin{aligned}
\widehat{\beta}_{1}^{*} & =\frac{\sum_{j=1}^{m} x_{j}^{*} y_{j}^{*}}{\sum_{j=1}^{m} x_{j}^{* 2}} \\
& =\frac{\sum_{j=1}^{m} \sqrt{n_{j}} \sqrt{n_{j}} \bar{y}_{j}}{\sum_{j=1}^{m}{\sqrt{n_{j}}}^{2}} \\
& =\frac{\sum_{j=1}^{m} n_{j} \bar{y}_{j}}{\sum_{j=1}^{m} n_{j}} \\
& =\sum_{j=1}^{m}\left(\frac{n_{j}}{\sum_{\ell=1}^{m} n_{\ell}}\right) \bar{y}_{j}
\end{aligned}
$$

- A linear combination of the $\bar{y}_{j}$; the weights add to one.
- B.L.U.E.


## And not only that, but ...

$$
\begin{aligned}
\widehat{\beta}_{1}^{*} & =\frac{\sum_{j=1}^{m} n_{j} \bar{y}_{j}}{\sum_{j=1}^{m} n_{j}} \\
& =\frac{\sum_{j=1}^{m} n_{j} \frac{\sum_{i=1}^{n_{j}} y_{i j}}{n_{j}}}{\sum_{j=1}^{m} n_{j}} \\
& =\frac{\sum_{j=1}^{m} \sum_{i=1}^{n_{j}} y_{i j}}{\sum_{j=1}^{m} n_{j}}=\frac{\sum_{j=1}^{m} \sum_{i=1}^{n_{j}} y_{i j}}{n}
\end{aligned}
$$

- So the B.L.U.E. of $\mu$ is just the sample mean of all the data.
- One more comment is that $\widehat{\boldsymbol{\beta}}^{*}=\left(\mathbf{X}^{\prime} \mathbf{V}^{-1} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{V}^{-1} \mathbf{y}$ yields the same expression.


## Copyright Information

This slide show was prepared by Jerry Brunner, Department of Statistics, University of Toronto. It is licensed under a Creative Commons Attribution - ShareAlike 3.0 Unported License. Use any part of it as you like and share the result freely. The $\mathrm{LA}_{\mathrm{E}} \mathrm{X}$ source code is available from the course website: http://www.utstat.toronto.edu/~brunner/oldclass/302f20

