Variance models and generalized least squares

Peter Hoff

STAT 423

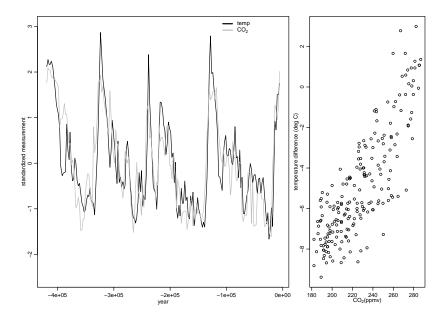
Applied Regression and Analysis of Variance

University of Washington

Vostok ice core data

Ice core data from East Antarctica:

- year year at which ice was frozen (-5000 to -420000 years)
 - co2 CO₂ concentration from ice sample (ppm)
 - tmp temperature estimate (difference from current), 1000 years after co2



 $\mathsf{tmp} = \beta_0 + \beta_1 \times \mathsf{co}_2 + \epsilon$

fit<-lm(tmp ~ co2 , data=VostokIce)</pre>

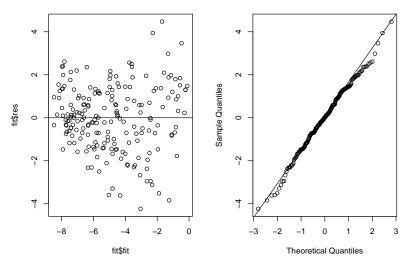
summary(fit)\$coef

 ##
 Estimate
 Std. Error
 t value
 Pr(>|t|)

 ## (Intercept)
 -23.02414043
 0.879542928
 -26.17739
 3.272183e-66

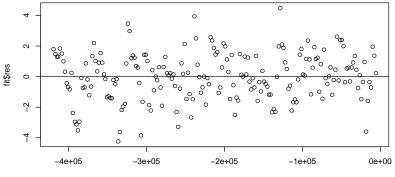
 ## co2
 0.07985291
 0.003833728
 20.82905
 8.766508e-52





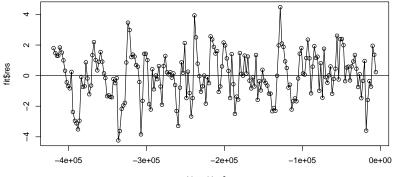
plot(fit\$res~VostokIce\$year)

abline(h=0)



VostokIce\$year

plot(fit\$res~VostokIce\$year)
lines(fit\$res~VostokIce\$year)
abline(h=0)



VostokIce\$year

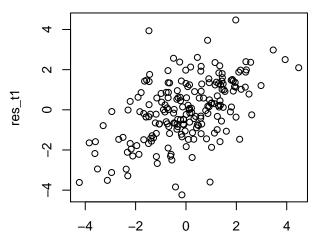
```
res_t1<-fit$res[-1]
res_t0<-fit$res[-length(fit$res)]
cbind( res_t0 , res_t1 )[1:4,]
## res_t0 res_t1
## 1 1.796974 1.474342
## 2 1.474342 1.296136
## 3 1.296136 1.306136
## 4 1.306136 1.839503</pre>
```

```
res_t1<-fit$res[-1]
res_t0<-fit$res[-length(fit$res)]
cbind( res_t0 , res_t1 )[1:4,]
## res_t0 res_t1
## 1 1.796974 1.474342
## 2 1.474342 1.296136
## 3 1.296136 1.306136
## 4 1.306136 1.839503</pre>
```

cor(cbind(res_t0 , res_t1))

res_t0 res_t1
res_t0 1.0000000 0.5183877
res_t1 0.5183877 1.0000000

plot(res_t0, res_t1)



res_t0

Estimation

A1: $E[y|X] = X\beta$

Estimation

A1: $E[y|X] = X\beta$ R1: $E[\hat{\beta}] = \beta$.

Estimation

A1: $E[y|X] = X\beta$ R1: $E[\hat{\beta}] = \beta$.

Inference

A2: Var[y] = $\sigma^2 \mathbf{I}$

Estimation

A1: $E[y|X] = X\beta$ R1: $E[\hat{\beta}] = \beta$.

Inference

A2: Var[**y**] = $\sigma^2 \mathbf{I}$

R2:

- standard errors: $\widetilde{\operatorname{Var}[\hat{\boldsymbol{\beta}}]} = \hat{\sigma}^2 (\mathbf{X}^T \mathbf{X})^{-1}$
- hypothesis tests
- confidence intervals

Estimation

A1: $E[y|X] = X\beta$ R1: $E[\hat{\beta}] = \beta$.

Inference

A2: Var[**y**] = $\sigma^2 \mathbf{I}$

R2:

- standard errors: $\widetilde{\operatorname{Var}[\hat{\beta}]} = \hat{\sigma}^2 (\mathbf{X}^T \mathbf{X})^{-1}$
- hypothesis tests
- confidence intervals

If we assume $Var[\mathbf{y}] = \sigma^2 \mathbf{I}$ and it is not, our SEs, CIs and HTs could be misleading.

For the VostokIce data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \mathbf{\Sigma} = \sigma^2 \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \vdots & & & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1 \end{pmatrix}$$

where $ho\in(-1,1)$ is an unknown quantity, to be estimated.

For the VostokIce data, it might be more reasonable to assume

$$\operatorname{Var}[\mathbf{y}] = \Sigma = \sigma^{2} \begin{pmatrix} 1 & \rho & \rho^{2} & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \vdots & & & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1 \end{pmatrix}$$

where $\rho \in (-1, 1)$ is an unknown quantity, to be estimated.

This covariance model is said to have first-order autoregressive structure.

For the VostokIce data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^{2} \begin{pmatrix} 1 & \rho & \rho^{2} & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \vdots & & & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1 \end{pmatrix}$$

where $\rho \in (-1, 1)$ is an unknown quantity, to be estimated.

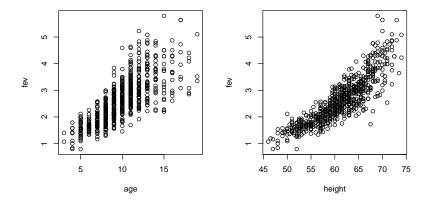
This covariance model is said to have first-order autoregressive structure.

Q:

- What are the SEs of the OLS estimates for autocorrelated data?
- Are the OLS estimates appropriate if we have autocorrelated data?

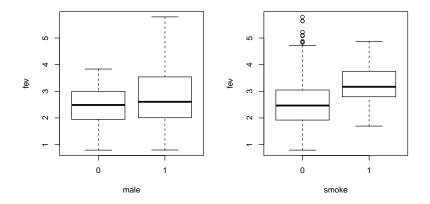
FEV data

Data on lung capacity by age, height, sex and smoking status

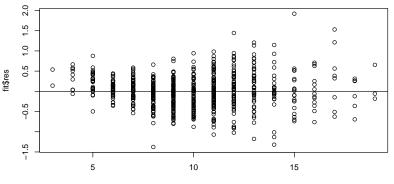


FEV data

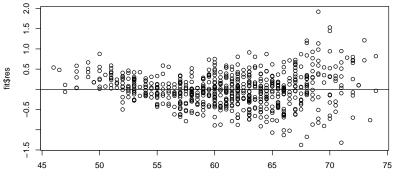
Data on lung capacity by age, height, sex and smoking status



```
fit<-lm( fev ~ age + height + male + smoke, data=fev)</pre>
summary(fit)
##
## Call:
## lm(formula = fev ~ age + height + male + smoke, data = fev)
##
## Residuals:
## Min 10 Median 30 Max
## -1.37656 -0.25033 0.00894 0.25588 1.92047
##
## Coefficients:
##
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -4.456974 0.222839 -20.001 < 2e-16 ***
## age 0.065509 0.009489 6.904 1.21e-11 ***
## height 0.104199 0.004758 21.901 < 2e-16 ***
## male 0.157103 0.033207 4.731 2.74e-06 ***
## smoke -0.087246 0.059254 -1.472 0.141
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.4122 on 649 degrees of freedom
## Multiple R-squared: 0.7754, Adjusted R-squared: 0.774
## F-statistic: 560 on 4 and 649 DF, p-value: < 2.2e-16
```



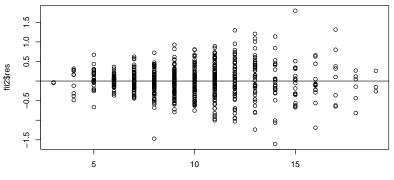
age



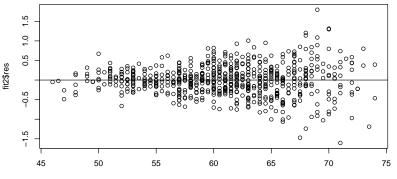
height

fit2<-lm(fev~ age+I(age^2) + height+I(height^2) + male + smoke, data=fev)
summary(fit2)\$coef</pre>

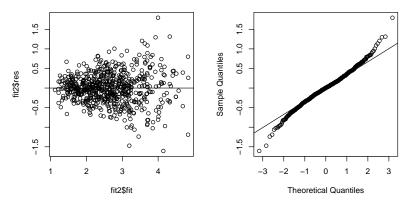
##		Estimate	Std. Error	t value	Pr(> t)
##	(Intercept)	5.92227124	1.7832742991	3.3210097	9.473601e-04
##	age	0.02800588	0.0421609352	0.6642614	5.067597e-01
##	I(age^2)	0.00176656	0.0017540528	1.0071304	3.142486e-01
##	height	-0.23734507	0.0617263805	-3.8451156	1.324046e-04
##	I(height^2)	0.00284376	0.0004949071	5.7460481	1.407141e-08
##	male	0.09515148	0.0328666266	2.8950790	3.918433e-03
##	smoke	-0.13959064	0.0574575045	-2.4294588	1.539252e-02



age



height



Normal Q-Q Plot

For the fev data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} v_1 & 0 & 0 & \cdots & 0\\ 0 & v_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & v_n \end{pmatrix}$$

where v_i is increasing in $\mathbf{x}_i^T \boldsymbol{\beta}$.

For the fev data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \mathbf{\Sigma} = \sigma^2 \begin{pmatrix} v_1 & 0 & 0 & \cdots & 0\\ 0 & v_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & v_n \end{pmatrix}$$

where v_i is increasing in $\mathbf{x}_i^T \boldsymbol{\beta}$.

This covariance model is said to have *mean-variance relationship*.

For the fev data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} v_1 & 0 & 0 & \cdots & 0\\ 0 & v_2 & 0 & \cdots & 0\\ \vdots & & & & \vdots\\ 0 & 0 & 0 & \cdots & v_n \end{pmatrix}$$

where v_i is increasing in $\mathbf{x}_i^T \boldsymbol{\beta}$.

This covariance model is said to have *mean-variance relationship*.

Q:

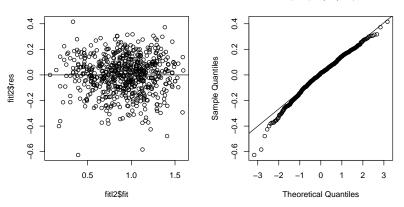
- What are the SEs of the OLS estimates for heteroscedastic data?
- Are the OLS estimates appropriate if we have heteroscedastic data?

Alternative approach: variance stabilizing transformation

fitl2<-lm(log(fev)~age+I(age^2)+height+I(height^2)+male+smoke,data=fev)</pre>

summary(fitl2)\$coef

##			Std. Error		
##	(Intercept)	-2.403151e+00	0.6571994572	-3.65665425	0.0002762954
##	age	2.466185e-02	0.0155377912	1.58721748	0.1129519557
##	I(age^2)	-6.163316e-05	0.0006464303	-0.09534385	0.9240712320
##	height	5.794673e-02	0.0227483477	2.54729422	0.0110864759
##	I(height^2)	-1.259285e-04	0.0001823907	-0.69043290	0.4901695920
##	male	3.201560e-02	0.0121125108	2.64318464	0.0084119141
##	smoke	-4.384840e-02	0.0211751164	-2.07075125	0.0387780566

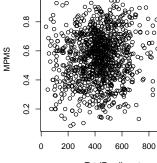


Normal Q–Q Plot

Educational testing

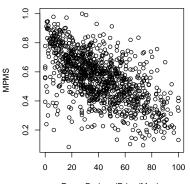
colnames(WASL)

- ## [1] "County"
- ## [2] "School"
- ## [3] "MathMetStandard"
- ## [4] "ReadingMetStandard"
- ## [5] "WritingMetStandard"
- ## [6] "ScienceMetStandard"
- ## [7] "MathTotalTested"
- ## [8] "ReadingTotalTested"
- ## [9] "WritingTotalTested"
- ## [10] "ScienceTotalTested"
- ## [11] "TotalEnrollment"
- ## [12] "PercentWhite"
- ## [13] "StudentsPerClassroomTeacher"
- ## [14] "FreeorReducedPricedMeals"
- ## [15] "AvgYearsEducationalExperience"
- ## [16] "PercentTeachersWithAtLeastMasterDegree"

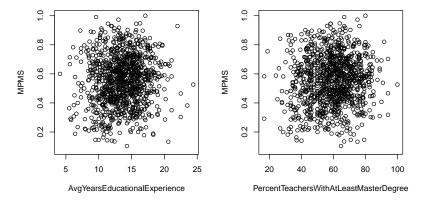


1.0

TotalEnrollment



FreeorReducedPricedMeals



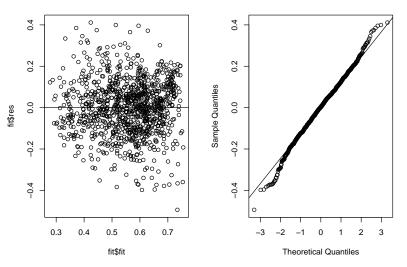
##	Estimate Std. Error
## (Intercept)	6.968472e-01 3.160130e-02
## TotalEnrollment	-3.928079e-06 2.771583e-05
## FreeorReducedPricedMeals	-4.589542e-03 1.828598e-04
<pre>## AvgYearsEducationalExperience</pre>	2.474453e-03 1.425301e-03
## PercentTeachersWithAtLeastMasterDegree	2.919762e-04 3.080947e-04
##	t value Pr(> t)
## (Intercept)	22.0512212 1.293163e-88
## TotalEnrollment	-0.1417269 8.873234e-01
## FreeorReducedPricedMeals	-25.0986867 6.373824e-109
<pre>## AvgYearsEducationalExperience</pre>	1.7360918 8.284576e-02
<pre>## PercentTeachersWithAtLeastMasterDegree</pre>	0.9476831 3.435125e-01

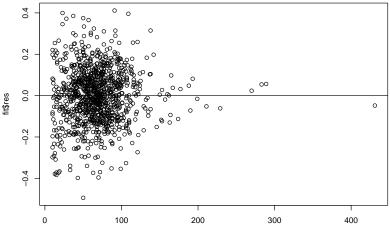
fit<-lm(MPMS~FreeorReducedPricedMeals+AvgYearsEducationalExperience,data=WASL)

```
summary(fit)$coef
```

##		Estimate	Std. Error	t value
##	(Intercept)	0.711660884	0.0210808699	33.758611
##	FreeorReducedPricedMeals	-0.004595451	0.0001793026	-25.629590
##	AvgYearsEducationalExperience	0.002556806	0.0013908766	1.838269
##	# Pr(> t)			
##	(Intercept)	3.737758e-169	9	
##	FreeorReducedPricedMeals	1.274005e-112	2	
##	${\tt AvgYearsEducationalExperience}$	6.630862e-02	2	

Normal Q-Q Plot





WASL\$MathTotalTested[obsdata]

For these data

```
y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}
```

Let p_i be the probability a student tested in school i will meet standard.
E[y_i] =

For these data

$$y_i$$
 = percent met standard_i = $\frac{\text{total met standard}_i}{\text{number tested}_i}$

Let p_i be the probability a student tested in school *i* will meet standard.

$$\models \mathsf{E}[y_i] = p_i$$

• Var $[y_i] =$

For these data

$$y_i$$
 = percent met standard_i = $\frac{\text{total met standard}_i}{\text{number tested}_i}$

Let p_i be the probability a student tested in school *i* will meet standard.

•
$$E[y_i] = p_i$$

• $Var[y_i] = p_i(1 - p_i)/n_i$.

For these data

$$y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}$$

Let p_i be the probability a student tested in school *i* will meet standard.

$$\blacktriangleright \mathsf{E}[y_i] = p_i$$

•
$$\operatorname{Var}[y_i] = p_i(1-p_i)/n_i$$
.

Thus we expected that the errors in a linear model will be heteroscedastic because

- the variance depends on p_i, and
- the variance depends on n_i .

For these data

$$y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}$$

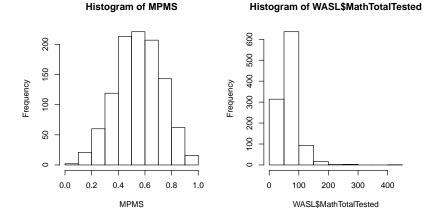
Let p_i be the probability a student tested in school *i* will meet standard.

$$\blacktriangleright \mathsf{E}[y_i] = p_i$$

•
$$\operatorname{Var}[y_i] = p_i(1-p_i)/n_i$$
.

Thus we expected that the errors in a linear model will be heteroscedastic because

- the variance depends on p_i, and
- the variance depends on n_i .



For the WASL data, it might be more reasonable to assume

$$Var[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

For the WASL data, it might be more reasonable to assume

$$\operatorname{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

This covariance is a result of the responses being sample means with different sample sizes.

For the WASL data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

This covariance is a result of the responses being sample means with different sample sizes.

Q:

- What are the SEs of the OLS estimates for heteroscedastic data?
- Are the OLS estimates appropriate if we have heteroscedastic data?

Alternative model for the data

Logistic regression:

$$p_i = \frac{\exp(\beta^T x_i)}{1 + \exp(\beta^T x_i)}$$
$$\log \frac{p_i}{1 - p_i} = \beta^T x_i$$

$\ensuremath{\mathsf{OLS}}$ and $\ensuremath{\mathsf{GLS}}$

OLS:
$$\hat{\boldsymbol{\beta}}_{OLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

 $\blacktriangleright E[\hat{\boldsymbol{\beta}}_{OLS}] = \boldsymbol{\beta}$
 $\blacktriangleright Var[\hat{\boldsymbol{\beta}}_{OLS}] = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \boldsymbol{\Sigma} \mathbf{X}) (\mathbf{X}^T \mathbf{X})^{-1}$

$\ensuremath{\mathsf{OLS}}$ and $\ensuremath{\mathsf{GLS}}$

OLS:
$$\hat{\boldsymbol{\beta}}_{OLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

 $\models \mathbf{E}[\hat{\boldsymbol{\beta}}_{OLS}] = \boldsymbol{\beta}$
 $\models \operatorname{Var}[\hat{\boldsymbol{\beta}}_{OLS}] = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \boldsymbol{\Sigma} \mathbf{X}) (\mathbf{X}^T \mathbf{X})^{-1}$

GLS:
$$\hat{\boldsymbol{\beta}}_{GLS} = (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1} \mathbf{X}^T \Sigma^{-1} \mathbf{y}$$

 $\blacktriangleright E[\hat{\boldsymbol{\beta}}_{GLS}] = \boldsymbol{\beta}$
 $\blacktriangleright Var[\hat{\boldsymbol{\beta}}_{GLS}] = (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1}$

OLS and GLS

OLS:
$$\hat{\boldsymbol{\beta}}_{OLS} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

 $\models \mathbf{E}[\hat{\boldsymbol{\beta}}_{OLS}] = \boldsymbol{\beta}$
 $\models \operatorname{Var}[\hat{\boldsymbol{\beta}}_{OLS}] = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \boldsymbol{\Sigma} \mathbf{X}) (\mathbf{X}^T \mathbf{X})^{-1}$

GLS:
$$\hat{\boldsymbol{\beta}}_{GLS} = (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{y}$$

 $\models \mathbf{E}[\hat{\boldsymbol{\beta}}_{GLS}] = \boldsymbol{\beta}$
 $\models \operatorname{Var}[\hat{\boldsymbol{\beta}}_{GLS}] = (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1}$

 $\mathsf{Var}[\hat{\boldsymbol{\beta}}_{\mathit{GLS}}] < \mathsf{Var}[\hat{\boldsymbol{\beta}}_{\mathit{OLS}}], \quad \text{in a matrix sense}.$

If we use $\hat{\boldsymbol{\beta}}_{OLS}$ to infer $\boldsymbol{\beta}$, we need $\boldsymbol{\Sigma}$ to compute standard errors.

- Typically, some aspect of Σ is unknown.
- In practice, we estimate Σ from the data.

If we use $\hat{\beta}_{OLS}$ to infer β , we need Σ to compute standard errors.

- Typically, some aspect of Σ is unknown.
- In practice, we estimate Σ from the data.

We can't even compute $\hat{oldsymbol{eta}}_{GLS}$ without knowledge of Σ

- For WLS, we know "enough" to obtain $\hat{oldsymbol{eta}}_{GLS}$.
- For other problems, we might iteratively estimate Σ and $\hat{\beta}_{GLS}$.

This later approach is called *feasible GLS*.

If we use $\hat{\beta}_{OLS}$ to infer β , we need Σ to compute standard errors.

- Typically, some aspect of Σ is unknown.
- In practice, we estimate Σ from the data.

We can't even compute \hat{eta}_{GLS} without knowledge of Σ

- For WLS, we know "enough" to obtain $\hat{oldsymbol{eta}}_{GLS}$.
- For other problems, we might iteratively estimate Σ and $\hat{\beta}_{GLS}$.

This later approach is called *feasible GLS*.

Feasible GLS: Letting $\hat{m{eta}}_{GLS}^{(0)}=\hat{m{eta}}_{OLS}$, iterate as follows:

1. Estimate
$$\hat{\Sigma}_{(k+1)}$$
 from $\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}_{GLS}^{(k)}$;

2. Let
$$\hat{\boldsymbol{\beta}}_{GLS}^{(k+1)} = (\mathbf{X}^T \hat{\boldsymbol{\Sigma}}_{(k+1)}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \hat{\boldsymbol{\Sigma}}_{(k+1)}^{-1} \mathbf{y}$$

OLS for ice core data with corrected SEs

```
fit<-lm( tmp ~ co2 , data=VostokIce )
s2<-sum(fit$res^2)/(n-2)
e1<-fit$res[-1]
e0<-fit$res[-n]
rho<-cor(e1,e0)
c( s2, rho )
## [1] 2.3498446 0.5183877</pre>
```

```
Sig<- s2* ( rho<sup>abs</sup>(outer( 1:n , 1:n , "-" ) ) )
```

Sig[3,8]

[1] 0.08796556

s2*rho⁵

[1] 0.08796556

OLS for ice core data with corrected SEs

$$\mathsf{Var}[\hat{\boldsymbol{\beta}}_{OLS}] = (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} (\mathbf{X}^{\mathsf{T}} \boldsymbol{\Sigma} \mathbf{X}) (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1}$$

```
X<-cbind(1,VostokIce$co2)</pre>
```

tXX<-t(X)%*%X

itXX<-solve(tXX)</pre>

VBols<- itXX %*% (t(X)%*%Sig%*%X) %*% itXX

VBols

[,1] [,2]
[1,] 2.081738848 -0.0089660853
[2,] -0.008966085 0.0000393115

OLS for ice core data with corrected SEs

```
se_b1<-sqrt( VBols[2,2] )
se_b1
## [1] 0.006269889
t_b1<-fit$coef[2]/se_b1
t_b1
## co2
## 12.73594</pre>
```

```
summary(fit)$coef
```

 ##
 Estimate
 Std. Error
 t value
 Pr(>|t|)

 ## (Intercept)
 -23.02414043
 0.879542928
 -26.17739
 3.272183e-66

 ## co2
 0.07985291
 0.003833728
 20.82905
 8.766508e-52

```
y<-VostokIce$tmp
beta <- solve( t(X)%*%X )%*%t(X)%*%y
Theta<-NULL
for(iter in 1:15)
  ## update Sigma
  e<-y-X%*%beta
  s2<-sum(e^2)/(n-2)
  rho < -cor(e[-1], e[-n])
  Sig<- s2* ( rho^abs(outer( 1:n , 1:n , "-" ) ) )</pre>
  ## update beta
  beta - solve( t(X) * solve(Sig) * X ) * t(X) * solve(Sig) * y
  ## save parameter estimates
  Theta<-rbind(Theta, c(beta,s2,rho) )</pre>
```

Theta

##		[,1]	[,2]	[,3]	[,4]
##	[1,]	-18.83769	0.06155813	2.349845	0.5183877
##	[2,]	-16.55915	0.05163925	2.620561	0.6257848
##	[3,]	-14.79284	0.04398281	2.994345	0.6927016
##	[4,]	-13.44266	0.03816190	3.393018	0.7395576
##	[5,]	-12.52059	0.03421227	3.761456	0.7708074
##	[6,]	-11.96593	0.03185155	4.044637	0.7896868
##	[7,]	-11.66375	0.03057188	4.227341	0.8000821
##	[8,]	-11.50913	0.02991926	4.330819	0.8054454
##	[9,]	-11.43274	0.02959743	4.384851	0.8081085
##	[10,]	-11.39568	0.02944142	4.411819	0.8094040
##	[11,]	-11.37785	0.02936645	4.424970	0.8100278
##	[12,]	-11.36932	0.02933056	4.431309	0.8103267
##	[13,]	-11.36524	0.02931341	4.434347	0.8104695
##	[14,]	-11.36330	0.02930523	4.435799	0.8105376
##	[15,]	-11.36237	0.02930133	4.436493	0.8105702

Inference based on GLS

```
\operatorname{Var}[\hat{\boldsymbol{\beta}}_{GLS}] = (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1}
```

```
VBgls<-solve( t(X)%*%solve(Sig)%*%X )</pre>
```

```
se_b1<-sqrt( VBgls[2,2] )</pre>
```

se_b1

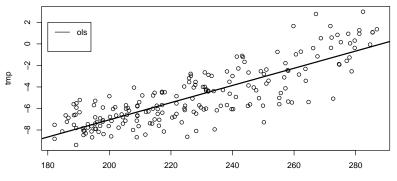
[1] 0.006986359

t_b1<-beta[2]/se_b1

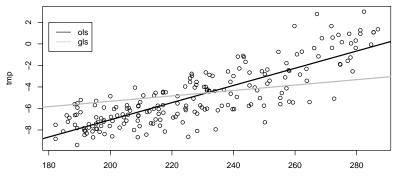
t_b1

[1] 4.194077

```
library(nlme)
fit_gls <- gls(tmp~co2, correlation=corARMA(p=1),data=VostokIce)</pre>
summary(fit_gls)
## Generalized least squares fit by REML
## Model: tmp ~ co2
## Data: VostokIce
##
        AIC BIC logLik
## 664.8527 678.0058 -328.4264
##
## Correlation Structure: AR(1)
## Formula: ~1
## Parameter estimate(s):
##
       Phi
## 0.8470009
##
## Coefficients:
                  Value Std.Error t-value p-value
##
## (Intercept) -10.355955 1.7231321 -6.009960 0e+00
## co2 0.025119 0.0070807 3.547493 5e-04
##
## Correlation:
      (Intr)
##
## co2 -0.947
##
## Standardized residuals:
        Min
                    Q1 Med Q3 Max
##
## -1.7007966 -0.7472771 -0.3278727 0.4786885 2.7789435
##
## Residual standard error: 2.312641
## Degrees of freedom: 200 total; 198 residual
```



co2



co2

Q: Why does the OLS fit seem more visually reasonable?

Q: Why does the OLS fit seem more visually reasonable? **A**: Recall what $\hat{\beta}_{OLS}$ and $\hat{\beta}_{GLS}$ are minimizing.

$$\hat{\beta}_{OLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$
$$\hat{\beta}_{GLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T \hat{\Sigma}^{-1} (\mathbf{y} - \mathbf{X}\beta)$$

Q: Why does the OLS fit seem more visually reasonable? **A:** Recall what $\hat{\beta}_{OLS}$ and $\hat{\beta}_{GLS}$ are minimizing.

$$\hat{\beta}_{OLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$
$$\hat{\beta}_{GLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T \hat{\Sigma}^{-1} (\mathbf{y} - \mathbf{X}\beta)$$

By definition, $\hat{\beta}_{\textit{OLS}}$ will provide a better fit to the observed data.

Q: Why does the OLS fit seem more visually reasonable? **A**: Recall what $\hat{\beta}_{OLS}$ and $\hat{\beta}_{GLS}$ are minimizing.

$$\hat{\beta}_{OLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$
$$\hat{\beta}_{GLS} = \arg\min(\mathbf{y} - \mathbf{X}\beta)^T \hat{\Sigma}^{-1} (\mathbf{y} - \mathbf{X}\beta)$$

By definition, $\hat{\beta}_{OLS}$ will provide a better fit to the observed data. Do you believe that β_{GLS} is closer to the truth?

Simulation study

IDEA:

- Simulate data under a particular correlation ρ ;
- Compare OLS and GLS estimates.

Simulation study

IDEA:

- Simulate data under a particular correlation *ρ*;
- Compare OLS and GLS estimates.

```
beta_true<-c(-11,.05) ; s2_true<-4 ; rho_true<-.85
hSig_true<- mhalf( s2_true* ( rho_true^abs(outer( 1:n , 1:n , "-" ) ) ) )</pre>
```

Simulation study

IDEA:

- Simulate data under a particular correlation *ρ*;
- Compare OLS and GLS estimates.

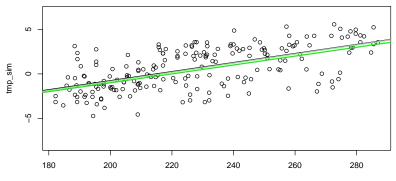
```
beta_true<-c(-11,.05) ; s2_true<-4 ; rho_true<-.85</pre>
```

hSig_true<- mhalf(s2_true* (rho_true^abs(outer(1:n , 1:n , "-"))))

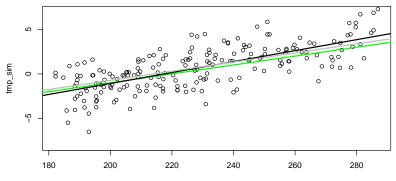
```
tmp_sim<- beta_true[1] + beta_true[2]*co2 + hSig_true%*%rnorm(n)</pre>
```

```
beta_ols<-lm(tmp_sim~co2)$coef</pre>
```

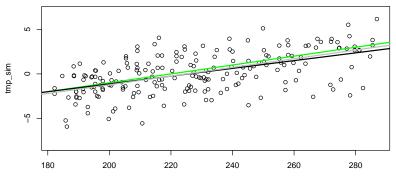
```
beta_gls<-gls(tmp_sim~co2, correlation=corARMA(p=1))$coef</pre>
```



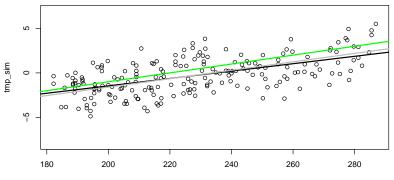
co2



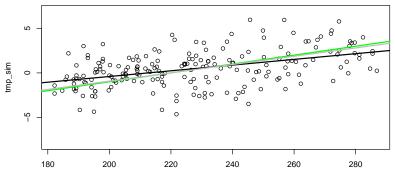
co2



co2

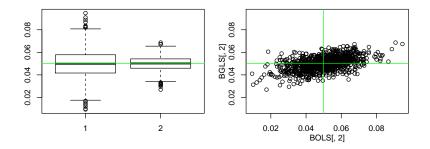


co2

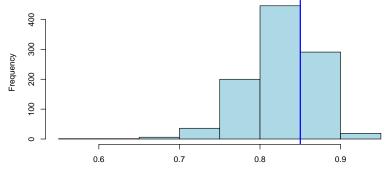


co2

```
BOLS<-BGLS<-NULL
for(s in 1:1000)
{
    set.seed(s)
    tmp_sim<- beta_true[1] + beta_true[2]*co2 + hSig_true%*%rnorm(n)
    BOLS<-rbind(BOLS,lm(tmp_sim~co2)$coef)
    BGLS<-rbind(BGLS,gls(tmp_sim~co2,correlation=corARMA(p=1))$coef)
}</pre>
```



Estimates of ρ



RHO

Abundance of caution

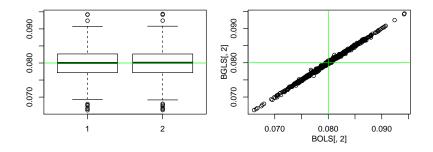
What if the data are not correlated, but we use GLS?

Abundance of caution

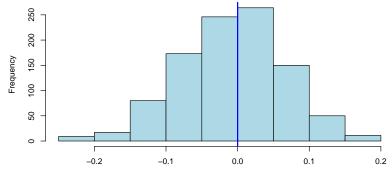
What if the data are not correlated, but we use GLS?

- Both estimators are still unbiased.
- Which will have lower variance?

```
beta_true<-c(-23,.08) ; s2_true<-2.5 ; rho_true<-0
hSig_true<- mhalf( s2_true* ( rho_true^abs(outer( 1:n , 1:n , "-" ) ) ) )
BOLS<-BGLS<-NULL
for(s in 1:1000)
{
    set.seed(s)
    tmp_sim<- beta_true[1] + beta_true[2]*co2 + hSig_true%*%rnorm(n)
BOLS<-rbind(BOLS,lm(tmp_sim~co2)$coef)
BGLS<-rbind(BGLS,gls(tmp_sim~co2,correlation=corARMA(p=1))$coef)
}</pre>
```

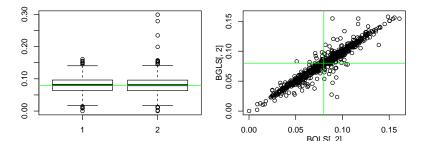


Estimates of ρ

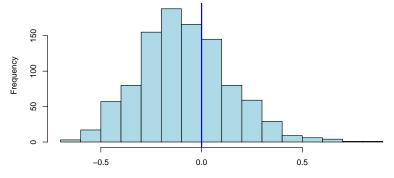


RHO

```
n<-20
co2 < -co2[1:n]
beta_true<-c(-23,.08) ; s2_true<-2.5 ; rho_true<-0</pre>
hSig_true<- mhalf( s2_true* ( rho_true^abs(outer( 1:n , 1:n , "-" ) ) ) ))
BOLS<-BGLS<-NULL
for(s in 1:1000)
  set.seed(s)
  tmp_sim<- beta_true[1] + beta_true[2]*co2 + hSig_true%*%rnorm(n)</pre>
  BOLS<-rbind(BOLS,lm(tmp_sim~co2)$coef)
  BGLS<-rbind(BGLS,gls(tmp_sim~co2,correlation=corARMA(p=1))$coef)</pre>
```



Estimates of ρ



RHO

Summary of GLS for correlated data

- ▶ If there is correlation, GLS is more reliable.
- If there is no correlation, $\hat{\rho} \approx 0$ and $\hat{\beta}_{GLS} \approx \hat{\beta}_{OLS}$.

This latter behavior worked in this example becuase there was plenty of data (n = 200) to get a good estimate of ρ .

Summary of GLS for correlated data

- ▶ If there is correlation, GLS is more reliable.
- If there is no correlation, $\hat{\rho} \approx 0$ and $\hat{\beta}_{GLS} \approx \hat{\beta}_{OLS}$.

This latter behavior worked in this example becuase there was plenty of data (n = 200) to get a good estimate of ρ .

If there is less data, or the correlation model is more complicated, the ability of the GLS estimate to reduce to the OLS estimate is diminished.

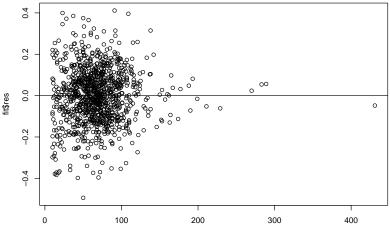
Weighted lest squares

WASL data revisited:

fit<-lm(MPMS~FreeorReducedPricedMeals+AvgYearsEducationalExperience,data=WASL)</pre>

round(summary(fit)\$coef,4)

##	Estimate S	td. Error	t value	Pr(> t)
## (Intercept)	0.7117	0.0211	33.7586	0.0000
## FreeorReducedPricedMeals	-0.0046	0.0002	-25.6296	0.0000
## AvgYearsEducationalExperience	0.0026	0.0014	1.8383	0.0663



WASL\$MathTotalTested[obsdata]

For these data

```
y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}
```

Let p_i be the probability a student tested in school i will meet standard.
E[y_i] =

For these data

$$y_i$$
 = percent met standard_i = $\frac{\text{total met standard}_i}{\text{number tested}_i}$

Let p_i be the probability a student tested in school *i* will meet standard.

$$\models \mathsf{E}[y_i] = p_i$$

• Var $[y_i] =$

For these data

$$y_i$$
 = percent met standard_i = $\frac{\text{total met standard}_i}{\text{number tested}_i}$

Let p_i be the probability a student tested in school *i* will meet standard.

•
$$E[y_i] = p_i$$

• $Var[y_i] = p_i(1 - p_i)/n_i$.

For these data

$$y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}$$

Let p_i be the probability a student tested in school *i* will meet standard.

$$\blacktriangleright \mathsf{E}[y_i] = p_i$$

•
$$\operatorname{Var}[y_i] = p_i(1-p_i)/n_i$$
.

Thus we expected that the errors in a linear model will be heteroscedastic because

- the variance depends on p_i, and
- the variance depends on n_i .

For these data

$$y_i = \text{percent met standard}_i = \frac{\text{total met standard}_i}{\text{number tested}_i}$$

Let p_i be the probability a student tested in school *i* will meet standard.

$$\blacktriangleright \mathsf{E}[y_i] = p_i$$

•
$$\operatorname{Var}[y_i] = p_i(1-p_i)/n_i$$
.

Thus we expected that the errors in a linear model will be heteroscedastic because

- the variance depends on p_i, and
- the variance depends on n_i .

For the WASL data, it might be more reasonable to assume

$$Var[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

For the WASL data, it might be more reasonable to assume

$$\operatorname{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

This covariance is a result of the responses being sample means with different sample sizes.

For the WASL data, it might be more reasonable to assume

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix}$$

where w_i is the number of students tested in school *i*.

This covariance is a result of the responses being sample means with different sample sizes.

Q:

- What does the GLS estimate look like?
- How to implement this in R?

$$\operatorname{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix} = \sigma^2 \mathbf{W}^{-1},$$

where \boldsymbol{W} is a matrix of weights.

$$\mathsf{Var}[\mathbf{y}] = \Sigma = \sigma^2 \begin{pmatrix} 1/w_1 & 0 & 0 & \cdots & 0\\ 0 & 1/w_2 & 0 & \cdots & 0\\ \vdots & & & \vdots\\ 0 & 0 & 0 & \cdots & 1/w_n \end{pmatrix} = \sigma^2 \mathbf{W}^{-1},$$

where \boldsymbol{W} is a matrix of weights.

The GLS estimator is

$$\begin{split} \hat{\beta}_{GLS} &= (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{y} \\ &= (\mathbf{X}^T \mathbf{W} \mathbf{X} / \sigma^2)^{-1} \mathbf{X}^T \mathbf{W} \mathbf{y} / \sigma^2 \\ &= (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{y} \end{split}$$

$\hat{\beta}_{WLS} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{y}$

Note 1: We don't need to know σ^2 , only the weights **W**.

$\hat{\beta}_{\textit{WLS}} = (\mathbf{X}^{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{W}\mathbf{y}$

Note 1: We don't need to know σ^2 , only the weights **W**.

Note 2: The GLS/WLS estimator is basically putting "more weight" on observations with smaller variances, less weight on observations with big variances.

$\hat{\beta}_{\textit{WLS}} = (\mathbf{X}^{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{T}\mathbf{W}\mathbf{y}$

Note 1: We don't need to know σ^2 , only the weights **W**.

Note 2: The GLS/WLS estimator is basically putting "more weight" on observations with smaller variances, less weight on observations with big variances.

This second note is made clear by considering what β_{WLS} is optimizing:

$$\begin{split} \hat{\beta}_{WLS} &= \arg\min_{\beta} (\mathbf{y} - \mathbf{X}\beta)^T \Sigma^{-1} (\mathbf{y} - \mathbf{X}\beta) \\ &= \arg\min_{\beta} (\mathbf{y} - \mathbf{X}\beta)^T \mathbf{W} (\mathbf{y} - \mathbf{X}\beta) \\ &= \arg\min_{\beta} \sum w_i (y_i - \mathbf{x}_i^T \beta)^2 \end{split}$$

WLS implementation

fit_ols<-lm(MPMS	~	<pre>FreeorReducedPricedMeals + AvgYearsEducationalExperience,</pre>	data=WASL)	
fit_wls<-lm(MPMS	~	FreeorReducedPricedMeals + AvgYearsEducationalExperience,	weights=MathTotalTested,	dat

WLS implementation

round(summary(fit_ols)\$coef,4)

##	Estimate St	d. Error	t value	Pr(> t)
## (Intercept)	0.7117	0.0211	33.7586	0.0000
## FreeorReducedPricedMeals	-0.0046	0.0002	-25.6296	0.0000
## AvgYearsEducationalExperience	0.0026	0.0014	1.8383	0.0663

```
round(summary(fit_wls)$coef,4)
```

##	Estimate	Std. Error	t value	Pr(> t)
## (Intercept)	0.7304	0.0206	35.4357	0.0000
## FreeorReducedPricedMeals	-0.0048	0.0002	-28.3886	0.0000
<pre>## AvgYearsEducationalExperience</pre>	0.0021	0.0014	1.5162	0.1298