#### STA302 weeks 8-9

Mark Ebden 2018. Continuing Ch 5

With grateful acknowledgment to Alison Gibbs

# What we're doing

- Midterms discussed on Thursday (not Tuesday)
- ▶ §5.2 (Estimation and Inference in MLR) is what we've begun, via the RMA
- ► Chapter 5's matrices



# Fitted values $(\hat{\mathbf{Y}})$ in matrix form



Recall from Weeks 6-7 that our model is:

$$Y = X\beta + e$$

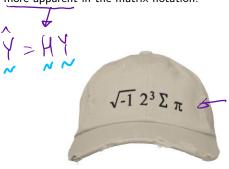
$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{HY}$$

where  $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  is the **hat matrix**, comprised of the  $h_{ij}$  values.

### Re-"cap"

Recall from weeks 4-5 that h in  $h_{ij} = \frac{1}{n} + \frac{(x_i - \bar{x})(x_j - \bar{x})}{S_{xx}}$  stands for "hat". This is because, considering  $\hat{y}_i = \sum_{j=1}^n h_{ij} y_j$ , the h values show how to get from  $y_i$ 's to  $\hat{y}_i$ 's.

This is even more apparent in the matrix notation.





Properties of 
$$\mathbf{H}$$

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

 $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$  is an example of an *idempotent* matrix. Exercise: Show this.

$$HH = X(XX)^{-1}X' \times (X'X)^{-1}X' = X(X'X)^{-1}X' = H$$

**H** is symmetric. **Exercise:** Show this.

$$H = \left[ \underbrace{X(X/X)^{-1}}_{\mathbf{A}} X' \right]$$

$$= \underbrace{X(X/X)^{-1}}_{\mathbf{A}} X' =$$

# Five facts about idempotent matrices

$$\mathcal{I} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad (y = 3)$$

- $\rightarrow$  1. A square matrix **A** is idempotent iff  $\mathbf{A}^2 = \mathbf{A}$ 
  - 2. If **A** is idempotent then  $trace(\mathbf{A}) = rank(\mathbf{A})$
  - **c** 3. **A** is idempotent iff  $\operatorname{rank}(\mathbf{A}) + \operatorname{rank}(\mathbf{I} \mathbf{A}) = n$  where the dimensions of **A** are  $n \times n$  and **I** is the  $n \times n$  identity matrix
- 4. For hat matrix **H** and matrix of all 1's **J**, the following matrices are idempotent:

$$\mathbf{H} = \begin{bmatrix} \mathbf{I} - \mathbf{H} \\ \mathbf{I} \end{bmatrix} \qquad \mathbf{H} - \frac{1}{n} \mathbf{J}$$

- 5. If A, B, and C are idempotent and A = B + C, then rank(A) = rank(B) + rank(C)

# Residuals $(\widehat{\mathbf{e}})$ in matrix form

The residuals are given by

$$\widehat{\mathbf{e}} = \begin{pmatrix} \hat{\mathbf{e}}_1 \\ \vdots \\ \hat{\mathbf{e}}_n \end{pmatrix} = \mathbf{Y} - \widehat{\mathbf{Y}} = \mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}$$

Donning our new hat matrix, this can be rewritten as  $\hat{\mathbf{e}} = \mathbf{Y} - \mathbf{H}\mathbf{Y}$  before determining  $\mathrm{E}(\hat{\mathbf{e}})$  and  $\mathrm{var}(\hat{\mathbf{e}})$ .

To begin, how could we factorize 
$$\hat{\mathbf{e}} = \mathbf{Y} - \mathbf{H}\mathbf{Y}$$
?
$$= \hat{\mathbf{I}} \hat{\mathbf{Y}} - \hat{\mathbf{H}} \hat{\mathbf{Y}}$$

$$= \hat{\mathbf{I}} - \hat{\mathbf{H}} \hat{\mathbf{Y}}$$

# Properties of $\boldsymbol{I}-\boldsymbol{H}$

Is 
$$I - H$$
 idempotent?

Is I - H symmetric?

= (-H

### Continuing:

$$= E(Y-X\beta) = E(Y-E(X\beta))$$

$$= X\beta - XE(\beta)$$

$$= X\beta - XB$$

$$= 0$$

$$var(\hat{e}) = Van [(I-H)Y] = (I-H) Van(Y) (I-H)'$$

$$= (I-H) \sigma^{2}I(I-H)$$

$$= \sigma^{2}(I-H)(I-H)$$

$$= \sigma^{2}(I-H) = 0$$

### Recap of our recent studies

The SLR model in matrix form is  $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$ , in which:

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \qquad \mathbf{X} = \begin{pmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \vdots \\ 1 & X_n \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \qquad \mathbf{e} = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix}$$

Setting the derivative of RSS( $\beta$ ) to zero yielded  $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$  when rank(X) = 2. This plus the fact that E(e) = 0 gives

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{HY}$$

We can write the residuals in terms of idempotent matrix I - H as

$$\hat{\mathbf{e}} = \mathbf{Y} - \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{H}\mathbf{Y} = (\mathbf{I} - \mathbf{H})\mathbf{Y}$$

 $\widehat{e} = Y - \widehat{Y} = Y - HY = \underbrace{(I - H) \, Y}_{\text{requiring the notion of a}}$  We found  $E(\widehat{e}) = 0$  and were about to try  $var(\widehat{e})$  requiring the notion of a covariance matrix:  $var(\mathbf{X}) = E[(\mathbf{X} - E(\mathbf{X})(\mathbf{X} - E(\mathbf{X}))']]$ 

### Variance of the residuals, in matrix form

$$\begin{aligned} \text{var}(\hat{\mathbf{e}}) &= \mathrm{E}\left\{ \left[\hat{\mathbf{e}} - \mathrm{E}(\hat{\mathbf{e}})\right] \left[\hat{\mathbf{e}} - \mathrm{E}(\hat{\mathbf{e}})\right]' \right\} \\ &= \mathrm{E}\left\{ \left(\mathbf{I} - \mathbf{H}\right) \mathbf{Y} \mathbf{Y}' \left(\mathbf{I} - \mathbf{H}\right) \right\} \\ &= \left(\mathbf{I} - \mathbf{H}\right) \mathrm{E}(\mathbf{Y} \mathbf{Y}') \left(\mathbf{I} - \mathbf{H}\right) \end{aligned}$$

Compare to our previous work:  $var(\hat{e}_i) = \sigma^2(1 - h_{ii})$ . Does the above match?

NB: As before, the " $|\mathbf{X}$ " is implicit — e.g.  $var(\hat{\mathbf{e}}|X)$  is abbreviated as  $var(\hat{\mathbf{e}})$ .

# Variance of the residuals, in matrix form

 $var(\hat{\mathbf{e}}) = \sigma^2 (\mathbf{I} - \mathbf{H})$ 

The middle factor is 
$$E(\mathbf{YY'}) = E\left\{(\mathbf{X}\boldsymbol{\beta} + \mathbf{e})(\mathbf{X}\boldsymbol{\beta} + \mathbf{e})'\right\}$$

$$= E\left\{(\mathbf{X}\boldsymbol{\beta} + \mathbf{e})(\boldsymbol{\beta}'\mathbf{X}' + \mathbf{e}')\right\}$$

$$= E\left\{(\mathbf{X}\boldsymbol{\beta} + \mathbf{e})(\boldsymbol{\beta}'\mathbf{X}' + \mathbf{e}')\right\}$$

$$= E\left\{\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{X}\boldsymbol{\beta}\mathbf{e}' + \mathbf{e}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{e}\mathbf{e}'\right\}$$

$$= E\left\{\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{A}\boldsymbol{\beta}\mathbf{e}' + \mathbf{e}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{e}\mathbf{e}'\right\}$$

$$= E\left\{\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{A}\boldsymbol{\beta}\mathbf{e}' + \mathbf{e}\boldsymbol{\beta}'\mathbf{X}' + \mathbf{e}\mathbf{e}'\right\}$$
Inserting the above into  $var(\mathbf{e})$  gives
$$var(\mathbf{e}) = (\mathbf{I} - \mathbf{H})(\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \sigma^2\mathbf{I})(\mathbf{I} - \mathbf{H})$$

$$= \left[\mathbf{I}(\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \sigma^2\mathbf{I} - \mathbf{H}(\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \sigma^2\mathbf{I})\right](\mathbf{I} - \mathbf{H})$$

$$= \left[\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}' + \sigma^2\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta}\boldsymbol{\beta}'\mathbf{X}') - \sigma^2\mathbf{H}\right](\mathbf{I} - \mathbf{H})$$

$$= \sigma^2(\mathbf{I} - \mathbf{H})(\mathbf{I} - \mathbf{H})$$

What's the rank of 
$$var(\hat{e})$$
? =  $\sigma^2$  (1- $\kappa$ )



Recall the fifth of our Five facts about idempotent matrices:

If 
$$\mathbf{A} = \mathbf{B} + \mathbf{C}$$
, then  $rank(\mathbf{A}) = rank(\mathbf{B}) + rank(\mathbf{C})$ .

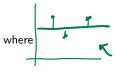
Put another way,  $rank(\mathbf{B}) = rank(\mathbf{A}) - rank(\mathbf{C})$ .

Therefore, for example  $rank(\mathbf{I} - \mathbf{H}) = rank(\mathbf{I}) - rank(\mathbf{H}) = n - 2$ . We'll do other similar calculations when considering ANOVA in matrix terms.

#### ANOVA in matrix terms



Recall from Week 3 that



$$SST = SSReg + RSS$$

$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} y_{i}^2 - n\bar{y}^2$$

Exercise: Show that SST can be re-expressed as

$$SST = \mathbf{Y}'\mathbf{Y} - \frac{1}{n}\mathbf{Y}'\mathbf{J}\mathbf{Y}$$

where **J** is an  $n \times n$  matrix of 1's. This means we can also write

$$\Lambda = 3^{2} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \int \underbrace{\left( \begin{array}{c} \mathbf{y}_{1} - \mathbf{y} \\ \mathbf{y}_{1} - \mathbf{y} \end{array} \right)^{2}}_{\left( \begin{array}{c} \mathbf{y}_{1} - \mathbf{y} \\ \mathbf{y}_{1} - \mathbf{y} \end{array} \right)^{2}} = \underbrace{\left( \begin{array}{c} \mathbf{y}_{1} - \mathbf{y} \\ \mathbf{y}_{1} - \mathbf{y} \end{array} \right)^{2}}_{\left( \begin{array}{c} \mathbf{y}_{1} - \mathbf{y} \\ \mathbf{y}_{2} - \mathbf{y} \end{array} \right)^{2}}$$

- 1. Note that  $I \frac{1}{n}J$  is symmetric. For a vector  $\mathbf{Y}$  and symmetric matrix  $\mathbf{A}$ , you may recall from other courses that  $\mathbf{Y}'\mathbf{A}\mathbf{Y}$  is a *quadratic form* (second-degree polynomial).
- q. form in Irmithle: a y 2

  2 vm's: a y 2 + 6 y 2 + 6 y 4 y 2

  2 vm's: a y 2 + 6 y 2 + 6 y 4 y 2 + 6 y
  - 2. **When I** is idempotent and  $\frac{1}{n}$ **J** is idempotent (from the five facts),  $I = \frac{1}{n}$ **J** is also idempotent.
  - 3. The rank of  $\mathbf{I}-\frac{1}{n}\mathbf{J}$  is  $\mathrm{rank}(\mathbf{I})-\mathrm{rank}\left(\frac{1}{n}\mathbf{J}\right)=n-1.$ 
    - ▶ This is the number of degrees of freedom for SST

# Decomposing SST yi - ŷi +ŷi

Taking the first term of SST = 
$$\underline{Y'Y} - \frac{1}{n}Y'JY$$
, 
$$\underline{Y'Y} = (Y - Xb + Xb)'(Y - Xb + Xb)$$

$$= (Y - Xb)'(Y - Xb) + (Y - Xb)'Xb + (Xb)'(Y - Xb) + (Xb)'(Xb)$$

$$= \hat{e}'\hat{e} + \hat{e}'Xb + (Xb)'\hat{e} + b'X'Xb$$

$$= \hat{e}'\hat{e} + \hat{b}'X'Xb$$
The middle terms were zero because 
$$X'\hat{e} = X'(I - H)Y = X'Y - X'X(X'X)^{-1}X'Y = 0$$
So, 
$$SST = Y'Y - \frac{1}{n}Y'JY$$

$$SST = \hat{e}'\hat{e} + \frac{b'X'Xb - \frac{1}{n}Y'JY}{n}$$

#### A closer look at RSS

$$\mathsf{SST} = \mathsf{SSReg} + \mathsf{RSS}$$

Making use of our expression  $\hat{\mathbf{e}} = (\mathbf{I} - \mathbf{H})\mathbf{Y}$ , we have

RSS = 
$$\hat{e}'\hat{e}$$
  
=  $\mathbf{Y}'(\mathbf{I} - \mathbf{H})'(\mathbf{I} - \mathbf{H})\mathbf{Y}$   
=  $\mathbf{Y}'(\mathbf{I} - \mathbf{H})\mathbf{Y}$ 

This is another quadratic form in  $\mathbf{Y}$ . Also, rank $(\mathbf{I} - \mathbf{H}) = n - 2$  from earlier, the number of degrees of freedom for the error.

# A closer look at SSReg

$$\mathsf{SST} = \mathsf{SSReg} + \mathsf{RSS}$$

Making use of 
$$\hat{\boldsymbol{\beta}} = \mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$
, and slide 16

SSReg = 
$$\mathbf{b}'\mathbf{X}'\mathbf{X}\mathbf{b} - \mathbf{Y}'\frac{1}{n}\mathbf{J}\mathbf{Y}$$
  
=  $\mathbf{Y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} - \mathbf{Y}'\frac{1}{n}\mathbf{J}\mathbf{Y}$   
=  $\mathbf{Y}'\underbrace{\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} - \mathbf{Y}'\frac{1}{n}\mathbf{J}\mathbf{Y}}_{\mathbf{H}}$   
=  $\mathbf{Y}'\left(\mathbf{H} - \frac{1}{n}\mathbf{J}\right)\mathbf{Y}$ 

This is again a quadratic form in **Y**, since the middle matrix is symmetric. Also,  $\operatorname{rank}(\mathbf{H} - \frac{1}{n}\mathbf{J}) = \operatorname{rank}(\mathbf{H}) - \operatorname{rank}(\frac{1}{n}\mathbf{J}) = 2 - 1 = 1$ , the number of degrees of freedom for SSReg.

Result - Rank (K) is generally 2. And from RMA , 26: rank (H) = ... = 2

## Using RSS to estimate $\sigma^2$

In  $S^2 = \text{RSS}/(n-2)$ , we have an unbiased estimator for  $\sigma^2$ . We can show it's unbiased using matrices by showing that  $E(\text{RSS}) = (n-2)\sigma^2$  as we did without matrices — i.e. when we considered  $E(\text{RSS}) = E\left(\sum_{i=1}^n \hat{e}_i^2\right)$ .

 $trace(\mathbf{I} - \mathbf{H}) = trace(\mathbf{I}) - trace(\mathbf{H}) = n - \sum_{i=1}^{n} h_{ii} = n - 2$ .

#### The big picture

We have expressed the ANOVA identity in matrix form:

$$SST = SSReg + RSS$$

$$Y'(I - \frac{1}{n}J)Y = Y'(H - \frac{1}{n}J)Y + Y'(I - H)Y$$

$$SST$$

$$SSReg$$

What does R have to say about this?



SSRy RSS SST

The anova command is one way in R to produce an ANOVA table (of the sort we saw in Week 3), in addition to analysing it. For example, for a 654-point SLR problem:

```
PPC .
 → a2 = read.table("Data .txt", sep=" ", header=T) # Load the data set
--- fev <- a2$fev; age <- a2$age
    m\delta d1 = lm(fev~age)
    anova (mod1)
    ## Analysis of Variance Table
    ##
    ## Response: fev
                  Df Sum Sq Mean Sq F yalue
    ##
                →1 280.92 280.919 872.18 < 2.2e-16 ***
    ## age
    ## Residuals 652_210.00
                               0.322
    ## Signif. codes:
                       0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

#### ANOVA in R

The *p*-value will match that obtained from the summary (lm...) command:

```
summary(mod1)
##
## Call:
## lm(formula = fev ~ age)
##
## Residuals:
                 1Q Median
##
       Min
                                  30
                                          Max
## -1.57539 -0.34567 -0.04989 0.32124 2.12786
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.431648 * 0.077895 5.541 4.36e-08 ***
            _0.222041 * 0.007518 29.533 < 2e-16 ***
## age
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5675 on 652 degrees of freedom
## Multiple R-squared/ 0.5722, Adjusted R-squared:
## F-statistic: 872.2 on 1 and 652 DF, p-value: < 2.2e-16
```

### We hope you have an enjoyable week

- ► Remember that for the Study Break of 5-9 November, there will be a pause in lectures, TA office hours, and instructor office hours
- ▶ No pause in the New College Stats Aid Centre

