9. Additional topics in linear modeling

In the final exam

see lab this week & practice final exam & notes.
Also, look out for collinearity in hw 11.

- Review of random variables.

- Fitting polynomial relationships and other nonlinear trend models using linear models.

- The R^2 statistic to assess model fit.

but figuring out anova (lm1, lm2) might be useful for hw 11. Check what F test this does.

- Multicollinearity: What happens when two or more explanatory variables are highly correlated. How to notice it, and what to do about it.

- More on the linear model formula notation in R: Interactions between explanatory variables.

- Model selection from a large number of possible models.

- More on causation, observational studies and designed experiments.

not directly tested in the final, but perhaps useful context.

For HW11: Material covered in class should be sufficient. If you use other methods, make sure you understand them! KISS : keep it simple, stupid!

Reviewing random variables

- Our definition of a random variable was: **a random variable X is a random number with probabilities assigned to outcomes**.

- A more precise definition: **a random variable is a probability distribution on a range of possible numeric values**.

- This is a simplied mathematical definition of a random variable, sufficient for this course.

  i.e., a probability mass function for a discrete RV or a probability density function for a continuous RV.

- "Random variable" is a problematic name.
  (i) A random variable is not a variable: it is a collection of possible values and their assigned probabilities.
  (ii) A random variable is not random: it is a probability distribution that describes a random phenomenon.

- A single draw of the random variable can only take on one value, but you can think of the random variable itself taking all possible values simultaneously.

Example: Rolling a die

- A die can be considered as a random variable with probability $1/6$ of taking each possible value $1, 2, 3, 4, 5, 6$.

- A single roll of the die is called a draw from the random variable. The roll may take some specific value. Say, we roll the die and it shows 5. However, 5 is not the random variable.

- The random variable is like die while it is in the air. You can think that it simultaneously takes all the possible values $1, 2, 3, 4, 5, 6$ before it lands and only one value is drawn.

Example: the normal distribution

- Let Z be a standard normal random variable.
- We can make a draw from Z using rnorm(1) in R.

```
z <- rnorm(1)
z
## [1] -0.3432662
```

- When we interpret the probability statement $P(Z < 1.5)$. we are not asking whether this particular draw is less than 1.5.
- We think of Z ranging over all its possible values, drawn according to the normal distribution. Then, $P(Z < 1.5)$ asks what proportion of these draws is less than 1.5.

```
pnorm(1.5)
## [1] 0.9331928
z <- rnorm(10000)
sum(z<1.5)/length(z)
## [1] 0.9319
```

Example: $\mathbf{b}$ and $\hat{\boldsymbol{\beta}}$

- The probability model $\mathbf{Y} = \mathbb{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ gives the distribution of all possible outcomes of $\mathbf{Y}$ in terms of the possible outcomes of $\boldsymbol{\epsilon}$.

- $\hat{\boldsymbol{\beta}} = (\mathbb{X}^{\mathrm{T}}\mathbb{X})^{-1}\mathbb{X}^{\mathrm{T}}\mathbf{Y}$ is a random variable that represents all the possible least squares coefficient vectors and their associated probabilities under the probability model.

- The random variable $\hat{\boldsymbol{\beta}}$ is constructed using $\mathbf{Y}$ which is in turn constructed using $\boldsymbol{\epsilon} \sim \mathrm{MVN}(\mathbf{0}, \sigma^2\mathbb{I})$.

- When we construct one random variable as a function of another, we don't necessarily know its probability distribution.

- In this case, we have worked out the distributions:
    $$\mathbf{Y} \sim \mathrm{MVN}(\mathbb{X}\boldsymbol{\beta}, \sigma^2\mathbb{I})$$
    $$\hat{\boldsymbol{\beta}} \sim \mathrm{MVN}(\boldsymbol{\beta}, \sigma^2(\mathbb{X}^{\mathrm{T}}\mathbb{X})^{-1})$$

- By contrast, $\mathbf{b}$ is one specific vector derived from the data, and $\boldsymbol{\beta}$ is an unknown constant vector which plays a role in the probability model.

- When we look at a probability statement like $\mathrm{P}(\hat{\beta}_1 > b_1)$ we are asking what proportion of the possible outcomes of the random variable $\hat{\beta}_1$ are larger than the specific number b_1.
- This probability must be defined under some specific probability model, usually corresponding to a null hypothesis H_0.
- To make sense of a probability statement like this, it is helpful to keep track of which quantities are random variables and which are constants.

Keeping track of random variables

Question 9.1. Which of the following make sense, for data $y_1, \ldots, y_n$

these belong to a probability model, not data.

1. A simple model is $y_1, \ldots, y_n \sim \text{normal}(\mu, \sigma)$.

   Nonsense. *data, not a random variable.* *distribution of a random variable*

2. $\text{Var}(y_1) = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - \bar{y})^2$ for $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.

   $= \text{Var}(y_1, \ldots, y_n)$ *Sample variance.*

   Nonsense. *variance of a random variable.* *Sample variance of $y_1, \ldots, y_n$. Formally, $\text{Var}(y_1) = 0$ since y_1 is constant.*

3. If **y** follows the usual linear model, $\text{E}[\mathbf{b}] = \boldsymbol{\beta}$. *$y_1$ is constant.*

   Nonsense. $E[\hat{\beta}] = \beta$ ✓ *constant.* $E[\beta] = b$ ✗ *not a random variable, so we shouldn't take its expectation.*

4. Because $\hat{\beta}_1 \pm 1.96 \, \text{SD}(\hat{\beta}_1)$ covers β_1 with probability 0.95, we call $b_1 \pm 1.96 \, \text{SE}(b_1)$ a 95% confidence interval for β_1.

   Sense. This is essentially the definition of a 95% C.I. The probability statement in a CI refers to the random variable $\hat{\beta}_1$ defined according to the probability model.

Keeping track of random variables: summary

- If you compute a probability, or an expectation, or a variance/covariance (not to be confused with the sample variance/covariance of data) then make sure you are working with random variables.

- If you say that a quantity has a probability distribution, such as the normal distribution, then that quantity should be a random variable.

- If the histogram of data, or residuals, follows a normal curve we are tempted to say that the data are normally distributed. Resist this temptation. It conflicts with our definition, according to which only a random variable can have a distribution. Say that the histogram shows that a normal model for the data, or measurement errors, is appropriate.

Using linear models to fit polynomial relationships

- Recall the basic linear trend model from Chapter 1 for data $y_1, \ldots, y_n$ with y_i measured at time t_i,

  [M1] $y_i = b_0 + b_1 t_i + e_i, \quad i = 1, \ldots, n$

- What if the data have a trend that is not linear?

- The next thing we might consider is a quadratic trend model,

  [M2] $y_i = b_0 + b_1 t_i + b_2 t_i^2 + e_i, \quad i = 1, \ldots, n$

- M1 and M2 are both linear models, with respective design matrices

$$
\mathbb{X}^{[1]} = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_n \end{bmatrix}
\qquad
\mathbb{X}^{[2]} = \begin{bmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ \vdots & \vdots \\ 1 & t_n & t_n^2 \end{bmatrix}
$$

*both are linear in the coefficient vector b.*

• When the explanatory variable for y_i is the time of measurement, t_i, then we call the linear model a trend.

• When we fit y_i using a function of an arbitrary explanatory variable x_i we say we are **smoothing**.

• We can choose any p in the general order p polynomial smoothing model,

[M3] $y_i = b_0 + b_1 x_i + b_2 x_i^2 + b_3 x_i^3 + \cdots + b_p x_i^p + e_i, \quad i = 1, \dots, n$

• This is a linear model with design matrix

$$\mathbb{X}^{[3]} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^p \\ 1 & x_2 & x_2^2 & \dots & x_2^p \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^p \end{bmatrix}$$

Here, it is natural to call the intercept b_0 to correspond to x_i^0

smooth curve via polynomial smoothing.
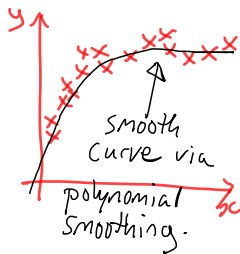
Question 9.2. How would you decide what order p to use when applying the polynomial smoothing model,

$$y_i = b_0 + b_1 x_i + b_2 x_i^2 + b_3 x_i^3 + \cdots + b_p x_i^p + e_i, \quad i = 1, \ldots, n$$

(i) Make residual plots for different values of p. For example, a time plot of residuals, or plotting e_i vs e_{i-1} (a lag plot).

(ii) Run an F-test, to test formally if p is sufficient or $p+1$ is a significantly better explanation of the data.

Suggestions ① look at data and estimate by eye the number of local maxima / inflection points. To have R local maxima, need $p = R+1$.

② look at R^2 the correlation² between $y_1, \ldots, y_n$ and the fitted values $\hat{y}_1, \ldots, \hat{y}_n$.

Cubic polynomial smoothing of life expectancy

Einstein: "A model should be as simple as possible, but no simpler" (attributed)

```
L_poly3 <- lm(Total~Year+I(Year^2)+I(Year^3),data=L)
```
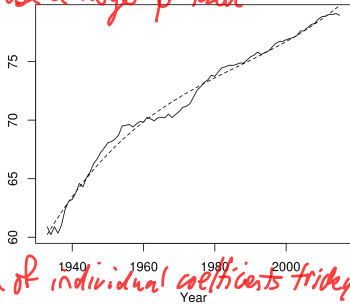
Note: Occam's razor says if a simple model is good enough, we should stick with it. So, we don't use a larger p then necessary.

```
plot(L$Year,L$Total,
    type="line",
    xlab="Year",
    ylab="Life expectancy")

lines(L$Year,fitted(L_poly3),
    lty="dashed")
```


Note: powers of x can be highly correlated. This can make interpretation of individual coefficients tricky.

Question 9.3. Why do we need to write I(Year^2) not just Year^2 to fit a polynomial smoothing model in the R formula notation?

This is a technical issue. Year^2 has a special meaning in R's model formula notation. I() tells R to evaluate Year^2 and use this as a covariate.

Question 9.4. How would you check that the R model formula we wrote is correct for the cubic polynomial we intend to fit?

Check the design matrix, via model.matrix (L~poly3)

Suggestion: plot the data & plot the curve. We did this & the curve looked good, so likely things are not too far wrong.

Question 9.5. If we have done a good job of modeling the trend, we might hope that the residuals look like independent measurement errors. How would you check if this is the case?

Make a time plot of the residuals, or a lag plot.

Repeating diagnostic tests for life expectancy vs unemployment using cubic detrending

```
L_detrended <- L_poly3$residuals
U_annual <- apply(U[,2:13],1,mean)
U_detrended <- lm(U_annual~Year+I(Year^2)+I(Year^3),
  data=U)$residuals
L_detrended <- subset(L_detrended,L$Year %in% U$Year)
lm_poly3 <- lm(L_detrended~U_detrended)
n <- length(resid(lm_poly3))
e <- resid(lm_poly3)[2:n] ; lag_e <- resid(lm_poly3)[1:(n-1)]
```
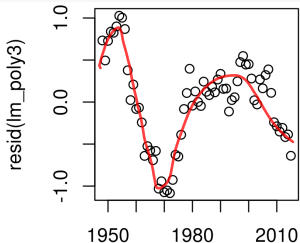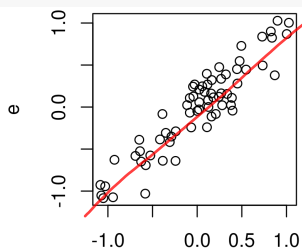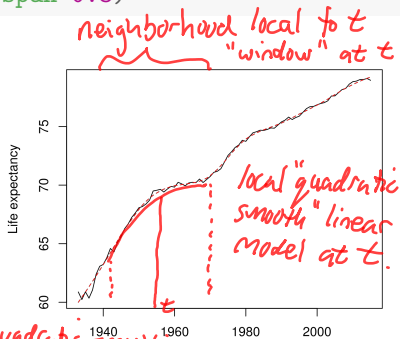
Local linear smoothing of life expectancy

the computer moves the window across the full dataset.

```
L_loess <- loess(Total~Year,data=L,span=0.3)
```

```
plot(L$Year,L$Total,
  type="line",
  xlab="Year",
  ylab="Life expectancy")

lines(L$Year,fitted(L_loess),
  lty="dashed",col="red")
```


neighborhood local to t
"window" at t

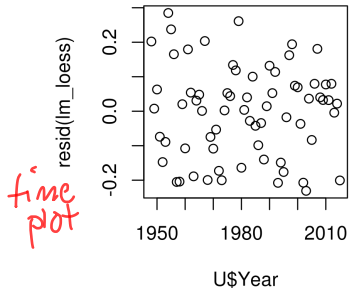*local "quadratic smooth" linear model at t.*

local quadratic smoothing

- `loess()` is a **smoother** that fits a local linear model. This means that, at each point x_i, the smoother predicts y_i fitting a linear model that ignores all the data except for points close to x_i.

- Setting span=0.3 means that the closest 30% of the points are used.

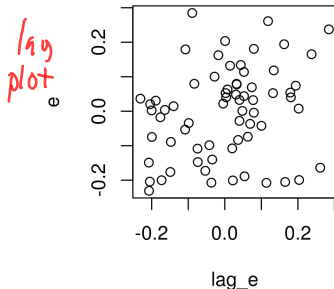# Repeating diagnostic tests for life expectancy vs unemployment using a smoother

```
L_detrended <- resid(L_loess)
U_annual <- apply(U[,2:13],1,mean)
U_detrended <- resid(loess(U_annual~Year,data=U,span=0.3))
L_detrended <- subset(L_detrended,L$Year %in% U$Year)
lm_loess <- lm(L_detrended~U_detrended)
n <- length(resid(lm_loess))
e <- resid(lm_loess)[2:n] ; lag_e <- resid(lm_loess)[1:(n-1)]
```

```
coef(summary(lm_loess))
```

```
##                   Estimate Std. Error   t value      Pr(>|t|)
## (Intercept) 0.007138079 0.01613621 0.4423641 0.6596720450
## U_detrended 0.067235405 0.01628394 4.1289394 0.0001045733
```

- Recall that linear detrending gave a statistically signficant association between life expectancy and unemployment.

- This suggested that mortality is **pro-cyclical**, meaning it increases when the business cycles is in economic expansion and unemployment is low.

- We found the residuals in this regression had a strong pattern, casting doubt on the validity of our linear model and its unintuitive conclusion.

Question 9.6. Re-assess the evidence based on this new analysis.

With appropriate nonlinear detrending, giving no clear pattern to the residuals, the positive coefficent is still present, and its significance even increases. This strengthens the evidence for pro-cyclical mortality.

The R-squared statistics to assess goodness of fit

- R^2 is the square of the correlation between the data and the fitted values.

- It can also be computed as

$$R^2 = 1 - \frac{\text{RSS}}{\text{SST}} = \frac{\text{SST} - \text{RSS}}{\text{SST}}$$

where RSS is the residual sum of squares and SST is the total sum of squares, defined as

SST is the residual sum of squares for a model with intercept only.

$$\text{SST} = \sum_{i=1}^{n} \left(y_i - \bar{y} \right)^2, \quad \text{where } \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i.$$

- R^2 is sometimes described as the fraction of the variation in the data explained by the linear model.

- $1 - R^2$ is the fraction of the variation in the data left unexplained by the model.

Uses and abuses of R-squared

Note: The F test may be worse than R^2 for looking at practical significance rather than statistical significance for a large sample.

- A low R^2 sends a clear signal: the fitted model doesn't describe the data much better than the sample mean. *: If the sample is big, the F test may reject the null hypothesis of iid: $Y_i = \mu + \varepsilon_i$ when the effect of the covariate is very small.*
- Sometimes a small, but statistically significant, correlation is of interest. If you are monitoring data on the operation of an aircraft jet engine, you want to know about evidence suggesting a malfunction as soon as it is statistically significant. **Interpretation of R-squared depends on context**. *① $p < 0.05$ is arbitrary; ② confounding can lead to an appearance of significance without a causal link.*
- The R^2 statistic compares the residual sum of squares under the full model with the residual sum of squares under a model with a constant mean. By contrast, the F test compares the full model with a model that omits specific selected explanatory variables. The F test is more appropriate for assessing whether a variable, or group of variables, should be included in the model. *** When the sample size is big, SEs are often small, so even small effects of no practical significance can show up as statistically significant ***

Question 9.7. Explain why R^2 cannot decrease when you add an extra explanatory variable into a linear model. (Explanations for questions like this should involve some math notation, not just words.)

Recall that $R^2 = 1 - \dfrac{RSS}{SST}$ ← residual sum of squares
← sum of squares of difference from the sample mean.

SST doesn't change when we add an explanatory variable

RSS can only decrease with a new explanatory variable; the least squares can only be less than the value with the constraint that the coefficient for the new variable is zero. Therefore, R^2 can only increase.

- Simplicity in a model is a good thing. The fact that any added model complexity makes R^2 seem "better" requires caution in interpretation.

Adjusted R-squared

- One approach to penalize R^2 for a more complex model is to divide each sum of squares by its degrees of freedom. This gives the **adjusted R-squared**,

  nested models occur when all variables in the null hypothesis are also in the alternative: the alternative includes the null.

$$R_{\text{adj}}^2 = 1 - \frac{\text{RSS}/(n-p)}{\text{SST}/(n-1)}.$$

- Dividing by the degrees of freedom in R_{adj}^2 is like what we do in the F statistic.

- The F statistic takes advantage of the nice mathematical property that $\text{SST} - \text{RSS}$ and RSS are independent random variables for the probability model with normally distributed measurement error.

- For comparing two **nested** models (when the larger model consists of adding variables to the smaller model) an F test is a clearer statistical argument than comparing R_{adj}^2.

- When the models are (not nested) the F test is not applicable. Comparing R_{adj}^2 values gives one way to assess the models, though not a formal test.

- Now we've studied R_{adj}^2, we understand everything in `summary(lm())`.

```
## Call:
## lm(formula = GPA ~ ACT + High_School, data = gpa)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.10265 -0.29862  0.07311  0.40355  1.31336
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 1.292793   0.136725   9.455  < 2e-16 ***
## ACT         0.037210   0.005939   6.266 6.48e-10 ***
## High_School 0.010022   0.001279   7.835 1.74e-14 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5672 on 702 degrees of freedom
## Multiple R-squared:  0.2033,Adjusted R-squared:  0.2011
## F-statistic: 89.59 on 2 and 702 DF,  p-value: < 2.2e-16
```

Handwritten annotations:

It is better to plot the data, do a histogram of residuals, or plot residuals than rely on this 5 number summary.

This gives some indication of skew & outliers.

this is quite large compared to the inter-quartile range
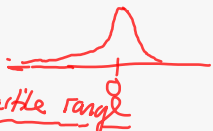
This is the F test comparing the full model (3 parameters) to just the average (1 parameter)

= R^2

Collinear explanatory variables in a linear model

- Let $\mathbb{X} = [x_{ij}]_{n \times p}$ be an $n \times p$ design matrix.

- If there is a nonzero vector $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$ such that $\mathbb{X}\boldsymbol{\alpha} = \mathbf{0}$ then the columns of $\mathbb{X}$ are **collinear**.

- Here, $\mathbf{0}$ is the zero vector, $(0, 0, \ldots, 0)$.

- We can write $\mathbf{x}_j = (x_{1j}, x_{2j}, \ldots, x_{nj})$ for the jth column of $\mathbb{X}$. Then,

$$\mathbb{X}\boldsymbol{\alpha} = \alpha_1 \mathbf{x}_1 + \alpha_2 \mathbf{x}_2 + \cdots + \alpha_j \mathbf{x}_j.$$

the expanded Matrix form of $\mathbb{X} \underset{\sim}{\alpha}$

We see that $\mathbb{X}\boldsymbol{\alpha}$ can be thought of as a **linear combination of the columns** of $\mathbb{X}$. *Collinear $\Leftrightarrow$ there is a linear combination that is zero.*

- Collinearity of explanatory variables has important consequences for fitting a linear model to data.

- It can also be useful to notice whether the variables are close to collinear, meaning that $\mathbb{X}\boldsymbol{\alpha}$ is small but nonzero.
For example, close to zero & exactly zero are the same to a computer.

Example: an intercept with a coefficient for each factor

- Recall the mouse weight dataset. Consider a sample linear model,

$$y_{ij} = \overset{M}{\mu} + \overset{M}{\mu_j} + e_{ij}, \qquad Y_{ij} = \mu + \mu_j + \varepsilon_{ij}$$

- Suppose that we don't set the $\mu_1 = 0$ so we try to estimate both μ_1 and μ_2 at the same time as the intercept, μ.

- Let's work with just 3 mice in each treatment group, so $i = 1, 2, 3$ and $j = 1, 2$. The design matrix is therefore

```
X <- cbind(rep(1,6),rep(c(1,0),each=3),rep(c(0,1),each=3)) ; X
##       [,1] [,2] [,3]
## [1,]    1    1    0
## [2,]    1    1    0
## [3,]    1    1    0
## [4,]    1    0    1
## [5,]    1    0    1
## [6,]    1    0    1
```

We know from a previous chapter that this model is over-parameterized. Here, we see that collinearity is another way to understand unidentifiability.

- For $\boldsymbol{\alpha} = (1, -1, -1)$, we have $\mathbb{X}\boldsymbol{\alpha} = \underset{\sim}{0}$

The least squares fit with collinear predictors

- Suppose that $\mathbf{b}$ is a least squares coefficient vector, so that the fitted value vector $\hat{\mathbf{y}} = \mathbb{X}\mathbf{b}$ minimizes $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$.

- Suppose that $\mathbb{X}$ is collinear, with $\mathbb{X}\boldsymbol{\alpha} = \mathbf{0}$.

- Since

$$\mathbb{X}(\mathbf{b} + \boldsymbol{\alpha}) = \mathbb{X}\mathbf{b} + \mathbb{X}\boldsymbol{\alpha} = \mathbb{X}\mathbf{b} + \mathbf{0} = \mathbb{X}\mathbf{b},$$

we see that $\mathbf{b} + \boldsymbol{\alpha}$ is also a least squares coefficient vector.

- **When $\mathbb{X}$ is collinear, a least squares coefficient still exists, but it is not unique.** *Collinearity is equivalent to parameter unidentifiability.*

Question 9.8. Let c be any number. Recall multiplication of a vector by a scalar: $c\boldsymbol{\alpha} = (c\alpha_1, \ldots, c\alpha_p)$. Show that $\mathbf{b} + c\boldsymbol{\alpha}$ is also a least squares fit.

$$\mathbb{X}(\mathbf{b} + c\boldsymbol{\alpha}) = \mathbb{X}\mathbf{b} + \mathbb{X}c\boldsymbol{\alpha} = \mathbb{X}\mathbf{b} + c\mathbb{X}\boldsymbol{\alpha} = \mathbb{X}\mathbf{b} + c\mathbf{0} = \mathbb{X}\mathbf{b}.$$

distributive property of matrix multiplication

commutative property of matrix × scalar multiplication

Standard errors for collinear variables

Question 9.9. Any variable that is part of a collinear combination of variables has infinite standard error. Why?

The least squares fit can be achieved by any equivalent set of parameters. By changing c in Question 9.8, we can choose parameters heading off to infinity as c heads to infinity.

A proper finite confidence interval (corresponding to finite standard errors) would have to rule out extreme values of the parameters with high probability. Due to unidentifiability, we cannot be sure the parameter is in any finite region when there is collinearity.

What does R do if you give it collinear variables?

formally, if R fitted this model, all the SEs would be infinite. R fixes this by fitting some model different from what you ask!

```
mice <- read.table("femaleMiceWeights.csv",header=T,sep=",")
chow=rep(c(1,0),each=12)
hf=rep(c(0,1),each=12)
lm1 <- lm(Bodyweight~chow+hf,data=mice)
coef(summary(lm1))

##               Estimate  Std. Error  t value     Pr(>|t|)
## (Intercept)  26.834167   1.039353  25.818139  6.045435e-18
## chow         -3.020833    1.469867  -2.055174  5.192480e-02
```

- R noticed that the three explanatory variables are collinear, and refused to fit the third

Note: When there is collinearity, we have to be extra careful about causal interpretations. If two variables are collinear, the data cannot inform which (if any) might be causal

```
model.matrix(lm1)

##    (Intercept) chow hf
## 1            1    1  0
## 2            1    1  0
## 3            1    1  0
## 4            1    1  0
## 5            1    1  0
## 6            1    1  0
## 7            1    1  0
## 8            1    1  0
## 9            1    1  0
## 10           1    1  0
## 11           1    1  0
## 12           1    1  0
## 13           1    0  1
## 14           1    0  1
## 15           1    0  1
## 16           1    0  1
## 17           1    0  1
## 18           1    0  1
## 19           1    0  1
```

Collinear variables and the determinant of $\mathbb{X}^\mathrm{T}\mathbb{X}$

easy to calculate, so a simple check for collinearity. `det( t(X) %*% X )`

- Recall that the variance of $\hat{\beta}$ in the usual linear model is $\sigma^2(\mathbb{X}^\mathrm{T}\mathbb{X})^{-1}$.

- Collinearity means the variance is infinite, a matrix version of dividing by zero.

- Recall that a square matrix is invertible if its determinant is nonzero.

- We can check that collinearity means $\det(\mathbb{X}^\mathrm{T}\mathbb{X}) = 0$.

```
X <- model.matrix(lm1)
t(X)%*%X

##              (Intercept) chow hf
## (Intercept)          24   12 12
## chow                 12   12  0
## hf                   12    0 12

det(t(X)%*%X)
## [1] 0
```

Linearly independent vectors and matrix rank

note: linear independence is entirely different from independence of random variables.

- Columns of a matrix that are not collinear are said to be **linearly independent**.

- The **rank** of $\mathbb{X}$ is the number of linearly independent columns.

- $\mathbb{X}$ has **full rank** if all the columns are linearly independent. In this case, we expect the least squares coefficient to be uniquely defined and so $\mathbb{X}^{\mathrm{T}}\mathbb{X}$ has non-zero determinant and is invertible.

- If $\mathbb{X}$ does not have full rank, we can drop **linearly dependent** columns until the remaining columns are linearly independent. This is a practical approach to handling collinearity.

Example: reducing a design matrix to full rank

```
X <- model.matrix(lm1)
det(t(X)%*%X)

## [1] 0

X2 <- X[,1:2]
det(t(X2)%*%X2)

## [1] 144
```

• Dropping the third column of X has given us a full-rank design matrix.

Question 9.10. The least squares fitted values are the same using the predictor matrix X2 as X. Why does dropping the last column not change the fitted values? The column we dropped is linearly dependent. The least squares coefficient is not unique. We can compensate for dropping column 3 by using columns 1 & 2, since the 3 columns are redundant.

Almost collinear variables

normally, large SEs is easier to assess than a small determinant.

e.g. HW11.

- If the determinant of $\mathbb{X}^T\mathbb{X}$ is close to zero, the variance of the model-generated least squares coefficient vector becomes large.

you can standardize all the covariates to have mean=0, sample SD=1

- This can happen when multiple explanatory variables are included in a model which all model similar things.

Question 9.11. Recall our data analysis using unemployment to explain life expectancy. What would happen if we added total employment as an additional explanatory variable? (Being unemployed is not the only alternative to being employed, since only adults currently looking for work are counted as unemployed.)

together with an intercept

We think unemployment and employment should be close to collinear, since #unemployed + #employed = #workforce

# of people who want to work.

roughly constant.

putting both unemployment & employment should give large standard errors for both — in a linear model, the data can't tell which of two approximately collinear variables is better.

More on the R model formula notation

• A **model formula** in `lm()` is something that looks like `y~x`.

• The R formula notation has various conventions that are designed to make it easy to specify useful models.

• `?formula` tells you everything you need to know, and more.

• You can think of the R formula for `lm()` is a way of constructing a design matrix. *Models central to conclusions.*

• Inspect the resulting design matrix using `model.matrix()` and check you understand what R has produced. If you can do this, you can safely use the power of the formula notation.

Question 9.12. In a report, the (model) should be written in mathematical notation, not as an R formula. Why? *(i) well-written scientific reports should be independent of a specific software choice; (ii) math is more precise and forces you to write out all your model details; (iii) writing the model in math cross-checks against your R code.*

Experimenting with the R formula notation

- Consider the freshman GPA data

```
gpa <- read.table("gpa.txt",header=T); head(gpa,3)

##   ID  GPA High_School ACT Year
## 1  1 0.98          61  20 1996
## 2  2 1.13          84  20 1996
## 3  3 1.25          74  19 1996
```

- We can play the game of trying out various things in R formula notation, inspecting the resulting design matrix, and figuring out how to write the model efficiently in mathematical notation.

- You can also think about whether the different models give any new insights into the data.

```
lm1 <- lm(GPA~ACT+High_School*Year,data=gpa)
coef(summary(lm1))[,1:2]
```
this is not just multiplication

```
##                       Estimate   Std. Error
## (Intercept)      -4.722613e+01 1.350854e+02
## ACT               3.708961e-02 5.946966e-03
## High_School       3.460100e-01 1.702035e+00
## Year              2.428369e-02 6.760800e-02
## High_School:Year -1.681424e-04 8.518297e-04
```

- The $*$ here denotes inclusion of an **interaction** between `High_School` and `Year`, written in the R output as `High_School:Year`.

Question 9.13. Conceptually, what do you think an interaction between two variables is, and why might it be needed?

- Maybe high school & year have only one coefficient?
- the slope of high school depends on year & vice versa.
- maybe the effect of high school & year is not additive.

- To find out exactly what R thinks an interaction is, we can check the design matrix.

```
head(model.matrix(lm1))
```
the interaction of high school & year

```
##   (Intercept) ACT High_School Year High_School:Year
## 1           1  20          61 1996           121756
## 2           1  20          84 1996           167664
## 3           1  19          74 1996           147704
## 4           1  23          95 1996           189620
## 5           1  28          77 1996           153692
## 6           1  23          47 1996            93812
```

Question 9.14. Write out the sample model that R has computed in `lm1` using subscript notation.

Let y_i be GPA for student i, a_i be ACT score, h_i be high school rank, t_i the year of freshman standing.

$$y_i = b_1 + b_2 a_i + b_3 h_i + b_4 t_i + b_5 h_i t_i + e_i,$$
$$i = 1, \ldots, 705.$$

Note: the word interaction makes natural sense when one or more of the variables is a factor.

Interactions and additivity

```
lm2 <- lm(GPA~ACT+High_School+Year+High_School:Year,data=gpa)
head(model.matrix(lm2),4)

##   (Intercept) ACT High_School Year High_School:Year
## 1           1  20          61 1996           121756
## 2           1  20          84 1996           167664
## 3           1  19          74 1996           147704
## 4           1  23          95 1996           189620
```

- `lm2` has the same design matrix as `lm1`.
- We see that, in R formula notation, `y~u*v` is the same as `y~u+v+u:v`.
- In the model `y~u+v` the effects of the variables are said to be **additive**.
- In a causal interpretation of an additive model, the result of increasing `u` by one unit and increasing `v` by one unit is the sum of the marginal effect of increasing `u` plus the marginal effect of increasing `v`.
- The interaction term `u:v` breaks additivity: we can't know the consequence of changing `u` unless we know the value of `v`.

• We have not (yet) found any interesting effect of year. Let's drop year out of the model and look for whether there is an interaction between ACT and high school percentile for predicting freshman GPA.

```
lm3 <- lm(GPA~ACT*High_School,data=gpa)
```

Question 9.15. Write out the fitted sample linear model in subscript form, letting y_i, a_i, h_i and e_i be the freshman GPA, ACT score, high school percentile and residual error respectively for the ith student.

$$y_i = b_1 a_i + b_2 h_i + b_3 a_i h_i + e_i, \quad i = 1, \ldots, 705.$$

Interpreting a discovered interaction

```
coef(summary(lm3))[,1:2]
```

Note: a priori, there may be no particular reason to suppose that ACT and High School rank are additive.

```
##                     Estimate    Std. Error
## (Intercept)      3.157679842  0.4788067771
## ACT             -0.046067744  0.0213355076
## High_School     -0.014405030  0.0061479608
## ACT:High_School  0.001071326  0.0002638611
```

← *this coef. is >> 2 SEs from zero.*

Question 9.16. Explain in words to the admissions director what you have found about the interaction under investigation here.

Note: now we have the interaction, the marginal effects are less significant than before, and gone negative.

If your ACT & High school are consistent, you have a higher predicted 1st year GPA than predicted by an additive model.

There are not many people with low HS rank & high ACT. ACT. Those with high HS rank and low ACT underperform. Perhaps these correspond to weaker high schools.
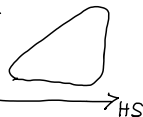
Marginal effects when there is an interaction

- Notice in 'lm3' that the coefficients for ACT score and high school percentile are negative. That is surprising!

Centering means removing the sample mean.

```
ACT_centered <- gpa$ACT-mean(gpa$ACT)
HS_centered <- gpa$Hi - mean(gpa$Hi)
lm3b <- lm(GPA~ACT_centered*HS_centered,data=gpa)
signif(coef(summary(lm3b))[,c(1,2,4)],3)
```

```
##                         Estimate Std. Error Pr(>|t|)
## (Intercept)              2.94000   0.022900 0.00e+00
## ACT_centered             0.03640   0.005880 1.04e-09
## HS_centered              0.01190   0.001350 8.23e-18
## ACT_centered:HS_centered 0.00107   0.000264 5.46e-05
```

Question 9.17. After centering the variables, the interaction effect stays the same, but the marginal effects change sign. What is happening? Why?

Centering does not affect an additive model much. For example, centering x in a simple model $y_i = ax_i + b + e_i$ just changes the intercept to compensate.

with an interaction, centering reduces colinearity between the product term & the linear terms. This gives smaller standard errors.

Quantifying the improvement in the model

```
s3 <- summary(lm3)$sigma
lm4 <- lm(GPA~ACT+High_School,data=gpa)
s4 <- summary(lm4)$sigma
lm5 <- lm(GPA~1,data=gpa)
s5 <- summary(lm5)$sigma
cat("s3 =",s3,"; s4 =",s4,"; s5 =",s5)
```

residual standard deviations for 3 models. These measure the predictability under the different models.

with interaction *w/o interaction* *modeling using just a mean (intercept only).*

```
## s3 = 0.5610067 ; s4 = 0.5671605 ; s5 = 0.6345278
```

Question 9.18. Comment on both **statistical significance** and **practical significance** of the interaction between a prediction of freshman GPA.

s3 and s4 are not very different. There is a statistically significant interaction, but it is not very practically important. This divergence occurs when the dataset is large [big data → small standard errors → statistical significance of small effects). Here, it seems n = 705 is "big".

s5 is not so much bigger either. GPA is only weakly predicted by High school rank & ACT.

An interaction involving a factor

• Let's go back to the football field goal data.

```
goals <- read.table("FieldGoals2003to2006.csv",header=T,sep=",")
goals[1,c("Name","Teamt","FGt","FGtM1")]

##               Name Teamt  FGt FGtM1
## 1 Adam Vinatieri    NE 73.5    90

lm6 <- lm(FGt~FGtM1*Name,data=goals)
```

→ sample double subscript form.

Question 9.19. What model do you think is being fitted here? Write it in subscript form, where y_{ij} is the field goal average for the jth year of kicker i, with $i = 1, \ldots, 19$ and $j = 1, 2, 3, 4$. Let e_{ij} be the residual error, and let x_{ij} be the previous year's average. Check your answer against the design matrix shown on the next slide.

$$y_{ij} = a + a_i + bx_{ij} + b_i x_{ij} + e_{ij}$$

the "usual" additive effects

the "interaction" is a kicker-specific slope.

with $a_1 = 0$, $b_1 = 0$, $i = 1, \ldots, 19$, $j = 1, 2, 3, 4$.

```
X<-model.matrix(lm6) ; colnames(X)<-1:38 ; X[1:17,c(1:8,21:26)]
```

```
##      1  X  2 3 4 5 6 7 8    21    22    23 24 25 26
## 1  1 90.0 0 0 0 0 0 0   0.0   0.0   0.0  0  0  0
## 2  1 73.5 0 0 0 0 0 0   0.0   0.0   0.0  0  0  0
## 3  1 93.9 0 0 0 0 0 0   0.0   0.0   0.0  0  0  0
## 4  1 80.0 0 0 0 0 0 0   0.0   0.0   0.0  0  0  0
## 5  1 88.2 1 0 0 0 0 0  88.2   0.0   0.0  0  0  0
## 6  1 82.7 1 0 0 0 0 0  82.7   0.0   0.0  0  0  0
## 7  1 84.3 1 0 0 0 0 0  84.3   0.0   0.0  0  0  0
## 8  1 72.7 1 0 0 0 0 0  72.7   0.0   0.0  0  0  0
## 9  1 72.2 0 1 0 0 0 0   0.0  72.2   0.0  0  0  0
## 10 1 87.0 0 1 0 0 0 0   0.0  87.0   0.0  0  0  0
## 11 1 85.2 0 1 0 0 0 0   0.0  85.2   0.0  0  0  0
## 12 1 75.0 0 1 0 0 0 0   0.0  75.0   0.0  0  0  0
## 13 1 82.1 0 0 1 0 0 0   0.0   0.0  82.1  0  0  0
## 14 1 95.6 0 0 1 0 0 0   0.0   0.0  95.6  0  0  0
## 15 1 85.7 0 0 1 0 0 0   0.0   0.0  85.7  0  0  0
## 16 1 79.1 0 0 1 0 0 0   0.0   0.0  79.1  0  0  0
## 17 1 80.0 0 0 0 1 0 0   0.0   0.0   0.0 80  0  0
```

Question 9.20. Interpret the ANOVA table below.

```
anova(lm6)

## Analysis of Variance Table
##
## Response: FGt
##             Df  Sum Sq Mean Sq F value   Pr(>F)
## FGtM1        1   87.20  87.199  1.9008 0.176047
## Name        18 2252.47 125.137  2.7279 0.004565 **
## FGtM1:Name  18  417.75  23.209  0.5059 0.938592
## Residuals   38 1743.20  45.874
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

(handwritten annotations) model with kicker-specific intercepts.

(handwritten annotation) ← model with interactions i.e., kicker-specific slopes

(handwritten notes)
The p-value of 0.939 says that the 18 d.f. needed to add a slope for each kicker is _not_ justified by the data.

The p-value of 0.0046 corresponds to an F test for kicker-specific intercept vs shared intercept. This does justify modeling using kicker-specific intercept.

The causal interpretation of observational studies

- Consider a simple least-squares linear model $y_i = ax_i + b + e_i$ for $i = 1, \ldots, n$. The usual corresponding probability model is $Y_i = \alpha x_i + \beta + \epsilon_i$ with $\epsilon_1, \ldots, \epsilon_n$ being independent $N[0, \sigma]$ random variables.

- The coefficient α for x_i, $i = 1, \ldots, n$ is commonly called the **effect** of x_i on y_i.

- Sometimes a is called the effect, but it is more properly an **estimated effect**.

- The **causal interpretation** of the linear model is that, if we manipulated x_i to increase it by one unit for individual i, keeping everything else fixed, we would expect y_i to increase by a units.

- The use of the word "effect" has a causal meaning in common usage.

- We should think carefully about when this meaning is justified.

Does coffee cause heart attacks?

- Coffee has relatively high levels of caffeine, a commonly consumed drug. Many studies have been done to see if it has adverse (or positive) health effects.

- A typical observational study will model a health outcome (say, a measure of heart health) and investigate linear models based on available explanatory variables.

- If higher levels of coffee consumption are associated with lower heart health scores, beyond what can be explained by chance variation in our sample, we will be suspicious about drinking coffee.

Question 9.21. Suggest important confounding variable(s) in the causal interpretation of this model. What would you do to help make a convincing argument for or against coffee?

Which surgeon do you choose?

- Cost effectiveness of medical treatment is a major current issue. You are advising a health insurance program, and your boss gives you data on success rates for a certain heart surgery, together with the salary of the surgeon performing the operation.

Question 9.22. Suppose you find the estimated effect is negative and statistically significant: higher salaries are associated with lower success rates. How would you interpret this result? What are possible confounding factors?

When can we infer causation from observational data?

The following considerations may add weight to the causal interpretation of an association

- There is a plausible mechanism.
- There are no un-measured variables considered plausible mechanisms.
- The effect is consistent across population subgroups.
- For data collected though time, the proposed cause precedes the consequence.
- Consistency with available experimental evidence.
- A consistent gradient between increases in the proposed cause and its consequence.

The ideas were developed in the 1950s while tracking down the case against cigarettes (Wikipedia: Bradford Hill criteria) and continue to be debated.

- There is risk of **selection bias** if the individuals are not selected randomly from the population they are supposed to represent.

- Selection bias is a type of confounding. The confounder is a variable that explains the selection process.

Question 9.23. In World War II, the US Airforce was suffering heavy losses in bombing raids over Germany. To decide where to add extra armor, engineers studied bullet holes on returning planes to see which parts were exposed to most gunfire. A prominent statistician, Abraham Wald, provided a different interpretation. What was it?

- Any observations study can and should be examined for confounding and selection bias issues.

Question 9.24. Consider the field goal percentage data. Recall that we analyzed the 19 NFL kickers who made at least ten field goal attempts in each of 2002, 2003, 2004, 2005 and 2006 seasons. We found a slope of -0.504 when predicting field goal percentage in year t using field goal percentage in year t-1, with a separate intercept for each kicker. Comment on the possible roles of selection bias and/or confounding for interpreting this result.

Randomized experiments and random samples

- The huge difficulties interpreting observational studies motivate avoiding them whenever possible

- Random assignment to treatment in a controlled experiment removes the possibility of confounding, and ensures that any statistically significan effect can legitimately be given a causal interpretation.

- A **randomized experiment** occurs when individual i is randomly assigned a **treatment**. A treatment is a set of explanatory variables corresponding to a row of $\mathbb{X}$.

- In a randomized experiment the independence assumption on the errors is reasonable: we can view the errors as coming from differences between individuals drawn independently from a large population.

- Random sampling removes selection bias, apart from missing data.

Selecting from many possible models

• Suppose we have a large number ℓ of potential explanatory variables in our dataset.

• The total number of possible linear models is 2^ℓ since each of the ℓ variables can be either in or out of the model.

• If we allow for the possiblity of interactions, things are even worse.

• For two variables x_{i1} and x_{i2} on each individual $i = 1, 2, \ldots, n$, modeling an **interaction** can be viewed as including a new variable $x_{i3} = x_{i1}x_{i2}$.

Question 9.25. If there are ℓ explanatory variables, considered as **main effects**, and any pair of them could give rise to an **interaction effect**, how many possible models are there? For simplicity, allow for the possibility of including interactions without the main effects.

Practical considerations for model selection

- Sometimes, you build models based on specific hypotheses about the system you are investigating.

- In this case, our tools for hypothesis testing work well. You work through a process of starting with a basic model and considering a relatively small sequence of alternative hypotheses to build up an understanding of the data.

- A different scenario occurs when you explore a very large number of different models.

- If you consider 1000 alternative models and each one is tested at significance level 0.01 then you expect to find 10 models that would formally let you reject the null hypothesis at a "high" level of significance for random variables generated under the null model.

- Similar issues arise if you consider many variables in a single linear model and look to identify significant ones.

Question 9.26. Suppose that you consider $\ell = 100$ variables by placing them all in a linear model and reporting the variables whose t statistic is significant at the 0.05 level. How many "significant" variables would you expect to report under a null probability model where all the coefficients are zero?

Confidence intervals after model selection

Question 9.27. Suppose you have $\ell = 100$ explanatory variables and you consider $\ell = 100$ different models, each with only one of the explanatory variables in the model. You pick as your favorite model the one with the highest R^2 statistic, which is equivalent to picking the one with the smalles p-value for its t statistic. You report a 95% confidence interval for the coefficient in this linear model. What is the chance that a corresponding model-generated confidence interval will cover the true parameter value, for the null probability model where all the coefficients for all the explanatory variables are zero? You can suppose that, under this null probability model, the model-generated p-values for each explanatory variable are independent.

Dealing with multiple testing

- The difficulty of properly evaluating statistical significance when investigating very many hypotheses is called the **multiple testing** situation.

- Dealing with multiple testing is a current scientific concern. It is related to the so-called crisis in scientific reproducibility.

- Advances in data acquisition and computation increasingly lead to large datasets to be investigated.

- One principle: report all the tests you make, not just the nominally significant ones. This lets the reader assess the hazard of multiple testing bias.

- Another principle: any result not yet confirmed by an independent experiment is suspicious.