9. Additional topics in linear modeling

- Review of random variables.
- Fitting polynomial relationships and other nonlinear trend models using linear models.
- The R^2 statistic to assess model fit.
- 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.

Reviewing random variables

- Our definition of a random variable was **A random variable X is a random number with probabilities assigned to outcomes**.
- For the purposes of this course, a random variable is equivalent to the probability distribution of its possible values.
- "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.
- Let's investigate some consequences of these ideas.

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 $\mathrm{P}(Z < 1.5)$. 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, $\mathrm{P}(Z < 1.5)$ 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.

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

- 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

- Which of the following make sense, for data $y_1, \ldots, y_n$

A. A simple model is $y_1, \ldots, y_n \sim \mathrm{normal}(\mu, \sigma)$.
No. On the left of $\sim$ we have data, on the right a probability distribution.
B. $\mathrm{Var}(y_1) = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2$ for $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.
No. y_1 is a single constant. It doesn't have a variance. $y_1, \ldots, y_n$ does have a sample variance
C. In a linear model, $\mathrm{E}[\mathbf{b}] = \boldsymbol{\beta}$.
No. $\mathbf{b}$ is a constant so $\mathrm{E}[\mathbf{b}] = \mathbf{b}$.
D. Because $\hat{\beta}_1 \pm 1.96\mathrm{SD}\hat{\beta}_1$ covers β_1 with probability 0.95, we call $b_1 \pm 1.96\mathrm{SE}b_1$ a 95% confidence interval.
Yes. The probability statement in a confidence interval refers to the random variable $\hat{\beta}_1$ 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] $\quad y_i = b_0 + b_1 t_i + e_i, \quad i = 1, \ldots, n$

- What if the data have a trend that is not linear?
- The next thing we might consider is a quadratic trend model,

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

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

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

Question 9.1. How would you decide what order p to use when applying the polynomial smoothing model,

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

Ideas: (i) look for which coefficients are statistically significant in the probability model

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \cdots + \beta_p x_i^p + \epsilon_i,$$

with $\epsilon_i \sim \text{iid normal}(0, \sigma)$ and $i = 1, \ldots, n$. (ii) make F tests to compare models with two different values of p under this probability model. (iii) look at the fitted line and see if you like it.

The order p polynomial smoothing model

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

- This is a linear model with design matrix

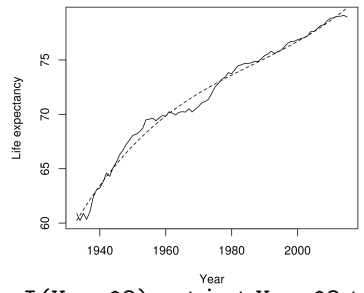
$$\mathbb{X}^{[3]} = \begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^p \\ 1 & x_2 & x_2^2 & \ldots & x_2^p \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \ldots & x_n^p \end{bmatrix}$$

Cubic polynomial smoothing of life expectancy

```
L_poly3 <- lm(Total~Year+I(Year^2)+I(Year^3),data=L)
```

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

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



Question 9.2. 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 consideration. `Year^2` happens to denote an interaction term in R's model formula language, so we have to tell R we just want the squared variable.

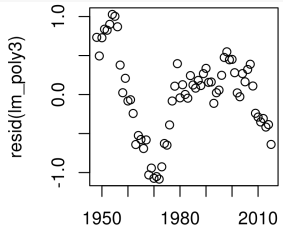
Checking the cubic smoothing calculation

Question 9.3. How would you check that the R model formula we wrote is correct for the cubic polynomial we intend to fit?
Look at the design matrix!
Question 9.4. 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 timeplot and/or a plot of the residuals against the lagged residuals.

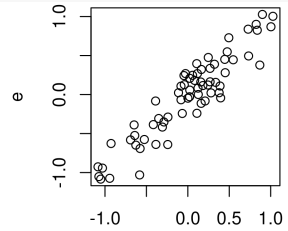
Repeating diagnostic tests for life expectancy vs unemployment using cubic detrending

```
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)]
```

```
plot(U$Year,resid(lm_poly3))
```




```
plot(lag_e,e)
```

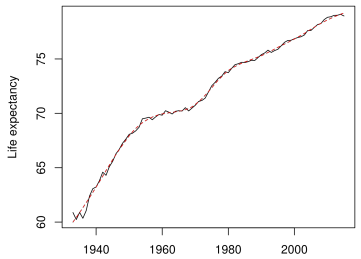


Local linear smoothing of life expectancy

```
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")
```

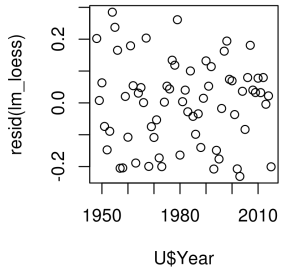


- `loess()` is a **smoother** that fits a local linear model. This means that, at each point x_j, the smoother predicts y_i fitting a linear model that ignores all the data except for points close to x_i.
- Setting `span=0.3` means that the closest 30% of the points are used.

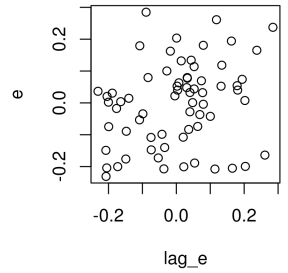
Repeating diagnostic tests for life expectancy vs unemployment using a smoother

```
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)]
```

```
plot(U$Year,resid(lm_loess))
```




```
plot(lag_e,e)
```



Revisiting the evidence for pro-cyclical mortality

```
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 9.5. Re-assess the evidence based on this new analysis.

With appropriate nonlinear detrending, the residuals show no pattern and the p-value is smaller. 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

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

- 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

- A low R^2 sends a clear signal: the fitted model doesn't describe the data much better than the sample mean.
- 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**.
- 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.

Question 9.6. 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

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

Adding an extra explantory variable does not change SST and cannot increase RSS. As we noted before, adding a new explanatory can only reduce the residual sum of squared error in the least squares fit.

- 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**,

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

- Dividing by the degrees of freedom in R^2_{adj} 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^2_{adj}.
- When the models are not nested, the F test is not applicable. Comparing R^2_{adj} values gives one way to assess the models, though not a formal test.
- Now we've studied R^2_{adj}, 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
```

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,

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

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

- 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.

Example: an intercept with a coefficient for each factor

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

$$y_{ij} = \mu + \mu_j + e_{ij}.$$

- 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
```

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

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 $\sum_{i=1}^{n} \left(y_i - \hat{y}_i\right)^2$.
- 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 coefficent still exists, but it is not unique.**

Question 9.7. 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.

What does R do if give it collinear variables?

```
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

Standard errors for collinear variables

Question 9.8. Any variable that is part of a collinear combination of variables has infinite standard error. Why?
The same least squares fit can be achieved with any set of equivalent variables. These equivalent variables fall on a line or plane heading off to infinity.

```
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 $\mathbb{X}^T\mathbb{X}$

- Recall that the variance of $\hat{\beta}$ in the usual linear model is $\sigma^2\left(\mathbb{X}^T\mathbb{X}\right)^{-1}$.
- 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 $\det\left(\mathbb{X}^T\mathbb{X}\right) = 0$.

```
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

- 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 $\mathbb{X}^T\mathbb{X}$ 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 9.9. 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?

All fitted values achievable using the last column can be replaced by a different rule using only the first two. For example, the row vector $\mathbf{x}^* = (x_1, x_2, x_3)$ gives the same prediction as $\mathbf{x}^{**} = (x_1 + x_3, x_2 - x_3, 0)$

Almost collinear variables

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

Question 9.10. 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.)

Fluctuations around the trend in total employment are highly negatively correlated with fluctuations in unemployment. Since these variables are close to collinear, the fitted values would change little and the standard errors on each one would become large. Likely, the data could not tell us whether employment or unemployment is better as an explanatory variable for understanding cyclical mortality fluctuations.

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.
- 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 9.11. In a report, the model should be written in mathematical notation, not as an R formula. Why?
(i) well written scientific reports should be independ of a specific software choice; (ii) math is more precise and it requires you to check you understand your model; (iii) writing the model in math cross-checks against your R code.

```
lm1 <- lm(GPA~ACT+High_School*Year,data=gpa)
coef(summary(lm1))[,1:2]

##                      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 9.12. Conceptually, what do you think an interaction between two variables is, and why might it be needed?
This interaction allows the effect of high school rank on GPA to vary over time. All relationships change somewhat over time. A priori, it is unclear whether a change will be big enough to have a substantial effect.

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

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.

```
head(model.matrix(lm1))

##   (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 9.13. Write out the sample model that R has computed in `lm1` using subscript notation.
Let a_i be ACT score for student i, h_i be high school rank and t_i the year in which the student was a college freshman. The model is

$$y_i = b_1 + b_2 a_i + b_3 h_i + b_4 t_i + b_5 h_i t_i + e_i$$

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 increading `u` by one unit and increading `v` by one unit is the sum of the marginal effect of increading `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`.

The interaction between ACT and high school percentile

- 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 9.14. 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.

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

Interpreting a discovered interaction

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

##                     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
```

Question 9.15. Explain in words to the admissions director what you have found about the interaction under investigation here.
There is strong statistical evidence for a positive interaction. This leads to increased predicted GPA scores when the product term $a_i h_i$ is large. After centering the variables, we see this is the case when both a_i and h_i are either above or below average. Students with inconsistent ACT and high school scores (one high, one low) statistically perform less well than would be expected without consideration of the interaction.

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!

```
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 9.16. After centering the variables, the interaction effect stays the same, but the marginal effects change sign. What is happening? Why?
Recentering trades off between the variables and the intercept: subtracting a constant to any covariate can be counterbalanced by a corresponding addition to the intercept. Centering therefore doesn't change the least squares fitted values.

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)

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

Question 9.17. Comment on both **statistical significance** and **practical significance** of the interaction between a prediction of freshman GPA. Looking at the numbers, we see that adding interaction does not substantially decrease the estimated measurement error. We also see that these models are only a small amount better at prediction than a simple averagre.

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

##    1    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
```

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)
```

Question 9.18. 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.

$$y_{ij} = a + a_i + bx_{ij} + b_i x_{ij} + e_{ij}, \quad a_1 = 0, \quad b_1 = 0$$

for $i = 1, \ldots, 19$ and $j = 1, 2, 3, 4$.

Question 9.19. 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
```

There is no evidence supporting different slopes for each player. Having different intercepts for each player continues to be supported. This supplementary analysis reinforces our previous choice of model

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 9.20. 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?
Smoking is the main confounder. You could restrict your study to non-smokers.

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 9.21. 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?
Likely, the highest qualified and highest paid surgeons deal with the sickest cases. These are also the patients most likely to have complications with surgery.

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.

How did the observations get into the study?

- 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 9.22. 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?
These were the planes that came back. You should put armor exactly where the bullet holes are not present on these planes.

Revisiting the fieldgoal kicker data

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

Question 9.23. 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.
If the kickers had a really bad season they might retire or be fired, and therefore not end up in the dataset. Consequently, 2006 might be expected to have lower success rate for this dataset, since kickers with a poor 2006 season can still stay in the dataset. Possibly, kickers who appear to be highly capable (due to a lucky season) are asked to take kicks from a longer distance the next year - this is not confounding or selection bias but is a different causal interpretation. Any ideas?

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 9.24. 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.
There are $\ell(\ell-1)/2$ possible interactions and ℓ main effects, so $\ell(\ell+1)/2$ possible explanatory variables. Each can be in or out of the model, giving a total of

$$2^{\ell(\ell+1)/1}$$

possible models. This get big quickly as ℓ increases.

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.

The expected number of false discoveries

Question 9.25. 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?
If all coefficients are zero, then the chance of a p-value for each variable being significant at the 5% level (if the null hypothesis is correct) is 5%. So, the expected number of significant variables is $0.05 \times 100 = 5$.

Confidence intervals after model selection

Question 9.26. 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 this confidence interval will cover the truth, under the null probability model where all the coefficients for all the explanatory variables are zero?
The 95% CI covers zero exactly when we fail to reject the null hypothesis that zero is the true value. Thus, the CI for the parameter with the smallest p-value covers the true value of zero only when all p-values are greater than 0.05. The chance that all p-values are greater than 0.05 under the null mypothesis is $0.95^{100} = 0.0059$.

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.