We can think of ANOVA and the two-sample *t*-test as applicable to situations where there is a response variable which is quantitative, and another variable that indicates group membership, which we might think of a as categorical predictor variable.

In the slides on categorical data, all varaibles are categorical, and we keep track of the counts of observation in each category or combination of categories.

In this section, we analyze cases where we have multiple quantitative variables.



In the simplest case, there are two quantitative variables. Examples include the following:

- heights of fathers and sons (this is a famous example from Galton, Darwin's cousin)
- ages of husbands and wifes
- systolic versus diastolic pressure for a set of patients
- high school GPA and college GPA
- college GPA and GRE scores
- MCAT scores before and after a training course

In the past, we might have analyzed pre versus post data using a two-sample *t*-test to see whether there was a difference. It is also possible to try to quantify the relationship—instead of just asking whether the two sets of scores are different, or getting an interval for the average difference, we can also try to predict the new score based on the old score, and the amount of improvmenet might depend on the old score.

Here is some example data for husbands and wives. Heights are in mm.

Couple	HusbandAge	HusbandHeight	: WifeAge	WifeHeight
1	49	1809	43	1590
2	25	1841	28	1560
3	40	1659	30	1620
4	52	1779	57	1540
5	58	1616	52	1420
6	32	1695	27	1660
7	43	1730	52	1610
8	47	1740	43	1580
9	31	1685	23	1610
10	26	1735	25	1590
11	40	1713	39	1610
12	35	1736	32	1700

## Correlation: Husband and wife ages

Correlation is 0.88.



## Correlation: Husband and wife heights

Correlation is 0.18 with outlier, but -0.54 without outlier.



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# Correlation: scatterplot matrix

pairs(x[,2:5]) allows you to look at all data simultaneously.



```
library(ggplot2)
library(GGally)
p1 <- ggpairs(x[,2:5])
print(p1)</pre>
```

# Correlation: scatterplot matrix



For a data set like this, you might not expect age to be significantly correlated with height for either men or women (but you could check). You could also check whether differences in couples ages are correlated with differences in their heights. The correlation between two variables is done as follows:

cor(x\$WifeAge,x\$HusbandAge)

Note that the correlation is looking at something different than the t test. A t-test for this data might look at whether the husbands and wives had the same average age. The correlation looks at whether younger wives tend to have younger husbands and older husbands tend to have older wives, whether or not there a difference in the ages overall. Similarly for height. Even if husbands tend to be taller than wives, that doesn't necessarily mean that there is a relationship between the heights for couples.

The pairwise correlations for an entire dataset can be done as follows. What would it mean to report the correlation between the Couple variable and the other variables? Here I only get the correlations for variables other than the ID variable.

<pre>options(digits=4) # done so that the output fits #on the screen! cor(x[.2:5])</pre>							
,	HusbandAge	HusbandHeight	WifeAge	WifeHeight			
HusbandAge	1.0000	-0.24716	0.88003	-0.5741			
HusbandHeight	-0.2472	1.00000	0.02124	0.1783			
WifeAge	0.8800	0.02124	1.00000	-0.5370			
WifeHeight	-0.5741	0.17834	-0.53699	1.0000			

The correlation measures the linear relationship between variables X and Y as seen in a scatterplot. The sample correlation between  $X_1, \ldots, X_n$  and  $Y_1, \ldots, Y_n$  is denoted by r has the following properties

- ►  $-1 \le r \le 1$
- if  $Y_i$  tends to increase linearly with  $X_i$ , then r > 0
- if  $Y_i$  tends to decrease linearly with  $X_i$ , then r < 0
- ▶ if there is a perfect linear relationship between X and Y, then r = 1 (points fall on a line with positive slope)
- if there is a perfect negative relationship between X and Y, then r = -1 (points fall on a line with negative slope)
- ► the closer the points (X<sub>i</sub>, Y<sub>i</sub>) are to a straight line, the closer r is to 1 or -1
- r is not affected by linear transformations (i.e., converting from inches to centimeters, Fahrenheit to Celsius, etc.
- ► the correlation is symmetric: the correlation between X and Y is the same as the correlation between Y and X

For n observations on two variables, the sample correlation is calculated by

$$r = \frac{S_{XY}}{S_X S_Y} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 \sum_{i=1}^{n} (y_i - \bar{y})^2}}$$

Here  $S_X$  and  $S_Y$  are the sample standard deviations and

$$S_{XY} = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{n - 1}$$

is the sample covariance. All the (n-1) terms cancel out from the numerator and denominator when calculating r.





Cls and hypothesis tests can be done for correlations using cor.test(). The test is usually based on testing whether the population correlation  $\rho$  is equal to 0, so

$$H_0: \rho = 0$$

and you can have either a two-sided or one-sided alternative hypothesis. We think of r as a sample estimate of  $\rho$ , the Greek letter for r. The test is based on a *t*-statistic which has the formula

$$t_{obs} = r \sqrt{\frac{n-2}{1-r^2}}$$

and this is compared to a t distribution with n - 2 degrees of freedom. As usual, you can rely on R to do the test and get the CI.

The *t* distribution derivation of the p-value and CI assume that the joint distribution of X and Y follow what is called a bivariate normal distribution. A sufficient condition for this is that X and Y each individually have normal distributions, so you can do usual tests or diagnostics for normality. Similar to the *t*-test, the correlation is sensitive to outliers. For the husband and wife data, the sample sizes are small, making it difficult to detect outliers. However, there is not clear evidence of non-normality.



Shairpo-Wilk's tests for normality would all be not rejected, although the sample sizes are quite small for detecting deviations from normality:

```
> shapiro.test(x$HusbandAge)$p.value
[1] 0.8934
> shapiro.test(x$WifeAge)$p.value
[1] 0.2461
> shapiro.test(x$WifeHeight)$p.value
[1] 0.1304
> shapiro.test(x$HusbandHeight)$p.value
[1] 0.986
```

## Correlation

Here we test whether ages are significantly correlated and also whether heights are positively correlated.

```
> cor.test(x$WifeAge,x$HusbandAge)
```

```
Pearson's product-moment correlation
```

```
data: x$WifeAge and x$HusbandAge
t = 5.9, df = 10, p-value = 2e-04
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
0.6185 0.9660
```

# Correlation

Here we test whether ages are significantly correlated and also whether heights are positively correlated.

> cor.test(x\$WifeHeight,x\$HusbandHeight)

```
Pearson's product-moment correlation
```

```
data: x$WifeHeight and x$HusbandHeight
t = 0.57, df = 10, p-value = 0.6
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
   -0.4407   0.6824
sample estimates:
    cor
0.1783
```

We might also test the heights with the bivariate outlier removed:

```
> cor.test(x$WifeHeight[x$WifeHeight>1450],x$HusbandHeight[x
Pearson's product-moment correlation
data: x$WifeHeight[x$WifeHeight > 1450] and x$HusbandHeight
t = -1.9, df = 9, p-value = 0.1
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 -0.8559 0.1078
sample estimates:
    cor
-0.5261
```

Removing the outlier changes the direction of the correlation (from positive to negative). The result is still not significant at the  $\alpha = 0.05$  level, although the p-value is 0.1, suggesting slight evidence against the null hypothesis of no relationship between heights of husbands and wives. Note that the negative correlation here means that, with the one outlier couple removed, taller wives tended to be associated with shorter husbands and vice versa.

A nonparametric approach for dealing with outliers or otherwise nonnormal distributions for the variables being correlated is to rank the data within each sample and then compute the usual correlation on the ranked data. Note that in the Wilcoxon two-sample test, you pool the data first and then rank the data. For the Spearman correlation, you rank each group separately.

The idea is that large observations will have large ranks in both groups, so that if the data is correlated, large ranks will tend to get paired with large ranks, and small ranks will tend to get paired with small ranks if the data is correlated. If the data are uncorrelated, then the ranks will be random with respect to each other.



The Spearman correlation is implemented in cor.test() using the option method=''spearman''. Note that the correlation is negative using the Spearman ranking even with the outlier, but the correlation was positive using the usual (Pearson) correlation. The Pearson correlation was negative when the outlier was removed. Since the results depended so much on the presence of a single observation, I would be more comfortable with the Spearman correlation for this example.

```
cor.test(x$WifeHeight,x$HusbandHeight,method="spearman")
Spearman's rank correlation rho
data: x$WifeHeight and x$HusbandHeight
S = 370, p-value = 0.3
alternative hypothesis: true rho is not equal to 0
sample estimates:
    rho
-0.3034
```

A more extreme example of an outlier. Here the correlation changes from 0 to negative.



Something to be careful of is that if you have many variables (which often occurs), then testing every pair of variables for a significant correlation leads to multiple comparison problems, for which you might want to use a Bonferroni correction, or limit yourself to only testing a small number of pairs of variable that are interesting a priori.



In regression, we try to make a model that predicts the average response of one quantitative variable given one or more predictor variables. We start with the case that there is one predictor variable, X, and one response, Y, which is called simple linear regression.

Unlike correlation, the model depends on which variable is the predictor and which is the response. While the correlation of x and y is the same as the correlation of y and x, the regression of y on x will generally lead to a different model than regressing on x on y. In the phrase "regressing y on x", we mean that y is the response and x is the predictor.



In the basic regression model, we assume that the average value of Y has a linear relationship to X, and we write

$$y = \beta_0 + \beta_1 x$$

Here  $\beta_0$  is the coefficient and  $\beta_1$  is the slope of the line. This is similar to equations of lines from courses like College Algebra where you write

$$y = a + bx$$

or

$$y = mx + b$$

But we think of  $\beta_0$  and  $\beta_1$  as unknown parameters, similar to  $\mu$  for the mean of a normal distribution. One possible goal of a regression analysis is to make good estimates of  $\beta_0$  and  $\beta_1$ .

Review of lines, slopes, and intercepts. The slope is the number of units that y changes for a change of 1 unit in x. The intercept (or y-intercept) is where the line intersects the y-axis.



In real data, the points almost never fall exactly on a line, but there might be a line that describes the overall trend. (This is sometimes even called the trend line). Given a set of points, which line through the points is "best"?



Husband and wife age example.



Husband and wife age example. Here we plot the line y = x. Note that 9 out of 12 points are above the line—for the majority of couples, the husband was older than the wife. The points seem a little shifted up compared to the line.



Now we've added the usual regression line in black. It has a smaller slope but a higher intercept. The lines seem to make similar predictions at higher ages, but the black line seems a better fit to the data for the lower ages. Although this doesn't always happen, exactly half of the points are above the black line.



It is a little difficult to tell visually which line is best. Here is a third line, which is based on regressing the wives' heights on the husbands heights.



It is difficult to tell which line is "best" or even what is meant by a best line through the data. What to do?

One possible solution to the problem is to consider all possible lines of the form

$$y = \beta_0 + \beta_1 x$$

or here

Husband height = 
$$\beta_0 + \beta_1 \times$$
 (Wife height)

In other words, consider all possible choices of  $\beta_0$  and  $\beta_1$  and pick the one that minimizes some criterion. The most common criterion used is the **least squares** criterion—here you pick  $\beta_0$  and  $\beta_1$  that minimize

$$\sum_{i=1}^{n} [y_i - (\beta_0 + \beta_1 x_i)]^2$$

Graphically, this means minimizing the sum of squared deviations from each point to the line.


Rather than testing all possible choices of  $\beta_0$  and  $\beta_1$ , formulas are known for the optimal choices to minimize the sum of squares. We think of these optimal values as estimates of the true, unknown population parameters  $\beta_0$  and  $\beta_1$ . We use  $b_0$  or  $\hat{\beta}_0$  to mean an estimate of  $\beta_0$  and  $b_1$  or  $\hat{\beta}_1$  to mean an estimate of  $\beta_1$ :

$$b_1 = \widehat{\beta}_1 = \frac{\sum_i (x_i - \overline{x})(y_i - \overline{y})}{\sum_i (x_i - \overline{x})^2} = r \frac{S_Y}{S_X}$$
$$b_0 = \widehat{\beta}_0 = \overline{y} - b_1 \overline{x}$$

Here r is the Pearson (unranked) correlation coefficient, and  $S_X$  and  $S_Y$  are the sample standard deviations. Note that if r is positive if, and only if,  $b_1$  is positive. Similarly, if one is negative the other is negative. In other words, r has the same sign as the slope of the regression line.

The equation for the regression line is

$$\widehat{y} = b_0 + b_1 x$$

where x is an value (not just values that were observed), and  $b_0$  and  $b_1$  were defined on the previous slide. The notation  $\hat{y}$  is used to mean the predicted or average value of y for the given x value. You can think of it as meaning the best guess for y if a new observation will have the given x value.

A special thing to note about the regression line is that it necessarily passes through the point  $(\overline{x}, \overline{y})$ .

Options make the dots solid and a bit bigger.

```
plot(WifeAge,HusbandAge,xlim=c(20,60),ylim=c(20,60),xlab=
"Wife Age", ylab="Husband Age", pch=16,
cex=1.5,cex.axis=1.3,cex.lab=1.3)
abline(model1,lwd=3)
```

#### Regression: scatterplot with least squares line

You can always customize your plot by adding to it. For example you can add the point  $(\overline{x}, \overline{y})$ . You can also add reference lines, points, annotations using text at your own specified coordinates, etc.

points(mean(WifeAge),mean(HusbandAge),pch=17,col=''red'')
text(40,30,''r = 0.88'',cex=1.5)
text(25,55,''Hi Mom!'',cex=2)
lines(c(20,60),c(40,40),lty=2,lwd=2)

The points statement adds a red triangle at the mean of both ages, which is the point (37.58, 39.83). If a single coordinate is specified by the points() function, it adds that point to the plot. To add a curve or line to a plot, you can use points() with x and y vectors (just like the original data). For lines(), you specify the beginning and ending x and y coordinates, and R fills in the line. To fit a linear regression model in R, you can use the lm() command, which is similar to aov().

The following assumes you have the file couple.txt in the same directory as your R session:

```
x <- read.table("couples.txt",header=T)
attach(x)
model1 <- lm(HusbandAge ~ WifeAge)
summary(model1)</pre>
```

```
Call:
lm(formula = HusbandAge ~ WifeAge)
Residuals:
   Min 10 Median 30 Max
-8.1066 -3.2607 -0.0125 3.4311 6.8934
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 10.4447 5.2350 1.995 0.073980.
WifeAge 0.7820 0.1334 5.860 0.000159 ***
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 5.197 on 10 degrees of freedom
Multiple R-squared: 0.7745, Adjusted R-squared: 0.7519
F-statistic: 34.34 on 1 and 10 DF, p-value: 0.0001595
```

The lm() command generates a table similar to the ANOVA table generated by aov().

To go through some elements in the table, it first fives the formula used to generate the output. This is useful when you have generated several models, say model1, model2, model3, ... and you can't remember how you generated the model. For example, you might have one model with an outlier removed, another model with one of the variables on a log-transformed scale, etc.

The next couple lines deal with **residuals**. Residuals are the difference between the between and fitted values, That is

$$y_i - \widehat{y}_i = y_i - (b_0 + b_1 x_i)$$

From the web:

www.shodor.org/media/M/T/I/mYzliZjY4ZDc0NjI3YWQ3YWVIM2MzZmUzN2MwOWY.jpg



The next part gives a table similar to ANOVA. Here we get the estimates for the coefficients,  $b_0$  and  $b_1$  in the first quantitative column. We also get standard errors for these, corresponding *t*-values and p-values. The p-values are based on testing the null hypotheses

$$H_0:\beta_0=0$$

and

$$H_0:\beta_1=0$$

The first null hypothesis says that the intercept is 0. For this problem, this is not very meaningful, as it would mean that the husband of 0-yr old woman would also be predicted to be a 0-yr old!

Often the intercept term is not very meaningful in the model. The second null hypothesis is that the slope is 0, which would mean that the wife's age increasing would not be associated with the husband's age increasing.

For this eample, we get a significant result for the wife's age. This means that the wife's age has some statistically significant ability to predict the husband's age. The coefficients give the model

Mean Husband's Age =  $10.4447 + 0.7820 \times (Wife's Age)$ 

The low p-value for the Wife's age, suggest that the coefficient 0.7820 is statistically significantly different from 0. This means that the data show there is evidence that the wife's age is associated with the husband's age. The coefficient of 0.7820 means that for each year of increase in the wife's age, the mean husband's age is predicted to increase by 0.782 years.

As an example, based on this model, a 20-yr old women who was married would be predicted to have a husband who was

$$10.4447 + (0.782)(30) = 33.9$$

or about 34 years old. A 50 yr-old women would be predicted to have husband who was

$$10.4447 + (0.782)(55) = 53.5$$

The fitted values are found by plugging in the observed x values (Wife ages) into the regression equation. This gives the expected husband ages for each wife. They are given automatically using

model1\$fitted.values							
1	2	3	4	5	6		
44.06894	32.33956	33.90348	55.01637	51.10658	31.55760	51.106	
9	10	11	12				
28.42976 29.99368 40.94111 35.46740							
x\$WifeAge	е						
[1] 43 28 30 57 52 27 52 43 23 25 39 32							

For example, if the wife is 43, the regression equation predicts 10.4447 + (0.782)(43) = 44.069 for the husband age.

To see what is stored in model1, type

na	ames	(model1)			
#	[1]	"coefficients"	"residuals"	"effects"	"rank'
#	[5]	"fitted.values"	"assign"	"qr"	"df.re
#	[9]	"xlevels"	"call"	"terms"	"model

The residuals are also stored, which are the observed husband ages minus the fitted values.

$$e_i = y_i - \widehat{y}_i$$

More details about the regression can be obtained using the anova() command on the model1 object:

Here the sum of squared residuals, sum(model1\$residuals<sup>2</sup>) is 270.13.

# Regression: ANOVA table

Other components from the table are (SS means sums of squares):

Residual SS = 
$$\sum_{i=1}^{n} e_i^2$$
  
Total SS =  $\sum_{i=1}^{n} (y_i - \overline{y})^2$   
Regression SS =  $b_1 \sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})$   
Regression SS = Total SS – Residual SS  
 $R^2 = \frac{\text{Regression SS}}{\text{Total SS}} = r^2$ 

The Mean Square values in the table are the SS values divided by the degrees of freedom. The degrees of freedom is n - 2 for the residuals and 1 for the 1 predictor. The *F* statistic is MSR/MSE (Measn square for regression divided by mean square error), and the p-value can be based on the *F* statistic.

ADA1

Note that  $R^2 = 1$  occurs when the Regression SS is equal to the Total SS. This means that the Residual SS is 0, so all of the points fall on the line. In this case, r = 1 and  $R^2 = 1$ .

On the other hand,  $R^2 = 0$  means that the Total SS is equal to the Residual SS, so the Regression SS is 0. We can think of the Regression SS and Residual SS as partitioning the Total SS:

$$\label{eq:started_st$$

If a large proportion of the Total SS is from the Regression rather than from Residuals, then  $R^2$  is high. It is common to say that  $R^2$  is a measure of how much variation is *explained by* the predictor variable(s). This phrase should be used cautiously because it doesn't refer to a causal explanation. For the husband and wife and example for ages, the  $R^2$  value was 0.77. This means that 77% of the variation in husband ages was "explained by" variation in the wife ages. Since  $R^2$  is just the correlation squared, regressing wife ages on husband ages would also result in  $R^2 = 0.77$ , and 77% of the variation in wife ages would be "explained by" variation in husband ages. Typically, you want the  $R^2$  value to be high, since this means you can use one variable (or a set of variables) to predict another variable.

The least-squares line is mathematically well-defined and can be calculated without thinking about the data probabilitistically. However, p-values and tests of significance assume the data follow a probabilistic model with some assumptions. Assumptions for regression include the following:

- each pair  $(x_i, y_i)$  is independent
- ► The expected value of y is a linear function of x: E(y) = β<sub>0</sub> + β<sub>1</sub>x, sometimes denoted µ<sub>Y|X</sub>
- ► the variability of y is the same for each fixed value of x. This is sometimes denoted σ<sup>2</sup><sub>y|x</sub>
- ► the distribution of y given x is normally distributed with mean  $\beta_0 + \beta_1 x$  and variance  $\sigma_{\gamma|x}^2$
- in the model, x is not treated as random

Note that the assumption that the variance is the same regardless of x is similar to the assumption of equal variance in ANOVA.



ADA1

Less formally, the assumptions in their order of importance, are:

- 1. **Validity**. Most importantly, the data you are analyzing should map to the research question you are trying to answer. This sounds obvious but is often overlooked or ignored because it can be inconvenient.
- 2. Additivity and Linearity. The most important mathematical assumption of the regression model is that its deterministic component is a linear function of the separate predictors.
- 3. **Independence of errors** (i.e., residuals). This assumption depends on how the data were collected.
- 4. Equal variance of errors.
- 5. Normality of errors.

It is easy to focus on the last two (especially when teaching) because the first assumptions depend on the scientific context and are not possible to assess just looking at the data in a spreadsheet.

To get back to the regression model, the parameters of the model are  $\beta_0$ ,  $\beta_1$  and  $\sigma^2$  (which we might call  $\sigma_{Y|X}^2$ , but it is the same for every x). Usually  $\sigma^2$  is not directly of interest but is necessary to estimate in order to do hypothesis tests and confidence intervals for the other parameters.

 $\sigma_{Y|X}^2$  is estimated by

$$s_{Y|X}^2 = \text{Residual MS} = rac{\text{Residual SS}}{\text{Residual df}} = rac{\sum_i (y_i - \widehat{y}_i)^2}{n-2}$$

This formula is similar to the sample variance, but we subtract the predicted values for y instead of the mean for y,  $\overline{y}$ , and we divide by n-2 instead of dividing by n-1. We can think of this as two degrees of freedom being lost since  $\beta_0$  and  $\beta_1$  need to be estimated. Usually, the sample variance uses n-1 in the denominator due to one degree of freedom being lost for estimating  $\mu_Y$  with  $\overline{y}$ .

Recall that there are observed residuals, which are observed minus fitted values, and unobserved residuals:

$$e_i = y_i - \hat{y}_i = y_i - (b_0 + b_1)x_i$$
  

$$\varepsilon_i = y_i - E(y_i) = y_i - (\beta_0 + \beta_1)x_i$$

The difference in meaning here is whether the estimated versus unknown regression coefficients are used. We can think of  $e_i$  as an estimate of  $\varepsilon_i$ .

Two ways of writing the regression model are

$$E(y_i) = \beta_0 + \beta_1 x_i$$

 $\mathsf{and}$ 

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

To get a confidence interval for  $\beta_1$ , we can use

$$b_1 \pm t_{crit}SE(b_1)$$

where

$$SE(b_1) = rac{s_{Y|X}}{\sqrt{\sum_i (x_i - \overline{x})^2}}$$

Here  $t_{crit}$  is based on the Residual df, which is n - 2.

To test the null hypothesis that  $\beta_1 = \beta_{10}$  (i.e. a particular value for  $\beta_1$ , you can use the test statistic

$$t_{obs} = \frac{b_1 - \beta_{10}}{SE(b_1)}$$

and then compare to a critical value (or obtain a p-value) using n - 2 df (i.e., the Residual df).

The p-value based on the R output is for testing  $H_0$ :  $\beta_1 = 0$ , which corresponds to a flat regression line. But the theory allows testing any particular slope. For the couples data, you might be interested in testing  $H_0$ :  $\beta_1 = 1$ , which would mean that for every year older that the wife is, the husband's age is expected to increase by 1 year.

Coefficients:

	Estimate	Std.	Error	t	value	Pr(> t )	
(Intercept)	10.4447	5	.2350		1.995	0.073980	•
WifeAge	0.7820	0	.1334		5.860	0.000159	***

To test  $H_0: \beta_1 = 1$ ,  $t_{obs} = (0.782 - 1.0)/(.1334) = -1.634$ . The critical value is qt(.975,10) = 2.22. So comparing |-1.634| to 2.22 for a two-sided test, we see that the observed test statistic is not as extreme as the critical value, so we cannot conclude that the slope is significantly different from 1. For a p-value, we can use pt(-1.634,10)\*2 = 0.133.

Instead of getting values such as the SE by hand from the R output, you can also save the output to a variable and extract the values. This reduces roundoff error and makes it easier to repeat the analysis in case the data changes. For example, from the previous example, we could use

```
model1.values <- summary(model1)
b1 <- model1.values$coefficients[2,1]
b1
#[1] 0.781959
se.b1 <- model1.values$coefficients[2,2]
t <- (b1-1)/se.b1
t
#[1] -1.633918</pre>
```

The object model1.values\$coefficients here is a matrix object, so the values can be obtained from the rows and columns.

For the CI for this example, we have

```
df <- model1.values$fstatistic[3] # this is hard to find
t.crit <- qt(1-0.05/2, df)
CI.lower <- b1 - t.crit * se.b1
CI.upper <- b1 + t.crit * se.b1
print(c(CI.lower,CI.upper))
#[1] 0.4846212 1.0792968
```

Consistent with the hypothesis test, the CI includes 1.0, suggesting we can't be confident that the ages of husbands increase at a different rate from the ages of their wives.

As mentioned earlier, the R output tests  $H_0$ :  $\beta_1 = 0$ , so you need to extract information to do a different test for the slope. We showed using a t-test for testing this null hypothesis, but it is also equivalent to an F test. Here the F statistic is  $t_{obs}^2$  when there is only 1 numerator degree of freedom (one predictor in the regression).

```
t <- (b1-0)/se.b1
t.
#[1] 5.859709
t^2
#[1] 34.33619
```

which matches the F statistic from earlier output.

In addition, the p-value matches that for the correlation using cor.test(). Generally, the correlation will be significant if and only if the slope is significantly different from 0. November 12, 2017 63 / 105

ADA1

Another common application of confidence intervals in regression is for the regression line itself. This means getting a confidence interval for the expected value of y for each value of x. Here the Cl for y given x is

$$b_0 + b_1 x \pm t_{crit} s_{Y|X} \sqrt{rac{1}{n} + rac{(x-\overline{x})^2}{\sum_i (x_i - \overline{x})^2}}$$

where the critical value is based on n-2 degrees of freedom.

In addition to a confidence interval for the mean, you can made **prediction intervals** for a new observation. This gives a plausible interval for a new observation. Here there are two sources of uncertainty: uncertainty about the mean, and uncertainty about how much an individual observation deviates from the mean. As a result, the prediction interval is wider than the CI for the mean.

The prediction interval for y given x is

$$b_0 + b_1 x \pm t_{crit} s_{Y|X} \sqrt{1 + rac{1}{n} + rac{(x - \overline{x})^2}{\sum_i (x_i - \overline{x})^2}}$$

For a particular wife age, such as 40, the CIs and PIs (prediction intervals) are done in R by

```
predict(model1,data.frame(WifeAge=40), interval="confidence",
level=.95)
# fit lwr upr
#1 41.72307 38.30368 45.14245
predict(model1,data.frame(WifeAge=40), interval="prediction",
level=.95)
# fit lwr upr
#1 41.72307 29.6482 53.79794
```

Here the predicted husband's age for a 40-yr old wife is 41.7 years. A Cl for the mean age for the husband is (38.3,45.1), but a prediction interval is that 95% of husbands for a wife this age would be between 29.6 and 53.8 years old. There is quite a bit more uncertainty for an individual compared to the population average.

To plot the CIs at each point, here is some R code:

```
library(ggplot2)
p <- ggplot(x, aes(x = WifeAge, y = HusbandAge))
p <- p + geom_point()
p <- p + geom_smooth(method = lm, se = TRUE)
p <- p + theme(text = element_text(size=20))
print(p)</pre>
```



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Note that the confidence bands are narrow in the middle of the data. This is how these bands usually look. There is less uncertainty near the middle of the data than there is for more extreme values. You can also see this in the formula for the SE, which has  $(x - \overline{x})^2$  inside the square root. This is the only place where x occurs by itself. The further it is from  $\overline{x}$ , the larger this value is, and therefore the larger the SE is.



There is a large literature on regression diagnostics. This involves checking the assumptions of the regression model. Some of the most important assumptions, such as that observations are independent observations from a single population (e.g., the population of married couples), cannot be checked just by looking at the data. Consequently, regression diagnostics often focus on what can be checked by looking at the data.

To review, the model is  $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$  where

- 1. the observed data are a random sample
- 2. the average y value is linearly related to x
- 3. the variation in y given x is independent of x (the variability is the same for each level of x
- 4. the distribution of responses for each x is normally distributed with mean  $\beta_0 + \beta_1 x$  (which means that  $\varepsilon$  is normal with mean 0)

The following plots show examples of what can happen in scatterplots:

- (a) Model assumptions appear to be satisfied
- (b) The relationship appears linear, but the variance appears nonconstant
- (c) The relationship appears nonlinear, althought the variance is appears to be constant
- (d) The relationship is nonlinear and the variance is not constant



ADA1


Regression diagnostics are often based on examinging the residuals:

$$e_i = y_i - \widehat{y}_i = y_i - (b_0 + b_1 x_i)$$

Based on the model assumptions, the residuals should be normally distributed with mean 0 and some variance  $\sigma^2$ . To standardize the residuals, they are often divided by their standard error. Here  $r_i$  is called the **studentized residual**:

$$r_i = \frac{e_i}{SE(e_i)} = \frac{e_i}{s_{Y|X}\sqrt{\frac{1}{n} + \frac{(x_i - \overline{x})^2}{\sum_i (x_i - \overline{x})^2}}}$$

The studentized residuals are standard normal (if the model is correct), so most studentized residuals should be between -2 and +2, just like *z*-scores. Often studentized residuals are plotted against the fitted values,  $\hat{y}_i$ .

For this plot, there is no trend, and you should observed constant variance and no obvious patterns like U-shapes.



Good residual plot.



Bad residual plot (U-shape).



Residual plot with extreme outlier.



Typing plot(model1) (or whatever the name of your model from lm()) and then return several times, R will plot several diagnostic plots. The first is the residuals (not studentized) against the fitted values. This help you look for outliers, nonconstant variance and curvature in the residuals.



Another type of residual is the externally Studentized residual (also called Studentized deleted residual or deleted *t*-residual), which is based on rerunning the analysis without the *i*th observation, then determining what the difference would be between  $y_i$  and  $b_0 + b_1x_i$ , where  $b_0$  and  $b_1$  are estimated with the pair  $(x_i, y_i)$  removed from the model. This could be done by tediously refitting the regression model *n* times for *n* pairs of data, but this can also be done automatically in the software, and there are computational ways to make it reasonably efficient.

The point of doing this is that if an observation is outlier, it might have a large influence on the regression line, making its residual not as extreme as if the regression was fit without the line. The Studentized deleted residuals give a way of seeing which observations have the biggest impact on the regression line. If the model assumptions are correct (without extreme outliers), then the Studentized deleted residual has a t distribution with n-2 degrees of freedom.

Something to be careful of is that if you have different numbers of observations for different values of x, then larger sample sizes will naturally have a larger range. Visually, this can be difficult to distinguish from nonconstant variance. The following examples are simulated.



Residual plot with extreme outlier.



Residual plot with extreme outlier.



Residual plot with extreme outlier.



Residual plot with extreme outlier.



The normality assumption for regression is that the responses are normally distributed for each level of the predictor. Note that it is not assumed that the predictor follows any particular distribution. The predictor can be nonnormal, and can be chosen by the investigator in the case of experimental data. In medical data, the investigator might recruit individuals based on their predictors (for example, to get a certain age group), and then think of the response as random.

It is difficult to tell if the responses are really normal for each level of the predictor, especially if there is only one response for each x value (which happens frequently). However, the model also predicts that the residuals are normally distributed with mean 0 and constant variance. The indvidual values  $y_i$  come from different distributions (because they have different means), but the residuals all come from the same distribution according to the model. Consequently, you can check for normality of the residuals.

As an example, the QQ plot is also generated by typing plot(model1) and hitting return several times. The command plot(model1) will generate four plots. To see them all you might type par(mfrow=c(2,2)) to put them in a 2 × 2 array first. You can also do a formal test on the residuals

```
par(mfrow=c(2,2))
plot(model1)
shapiro.test(model1$residual)
# Shapiro-Wilk normality test
#
#data: model1$residual
#W = 0.95602, p-value = 0.7258
```

QQ plot



Studentized residuals, i.e., residuals divided by their standard errors so that they look like *z*-scores, can be obtained from R using rstudent(model1). It helps to sort them to see which ones are most extreme.

rstudent(model1)								
sort(rstudent	<pre>sort(rstudent(model1))</pre>							
# 7	2	10	4	1	1			
#-2.02038876	-1.65316857	-0.83992238	-0.69122350	-0.179870	25			
# 6	9	8	1		З			
# 0.08799631	0.54099532	0.57506585	1.00173208	1.292578	24			

The biggest outlier based on the residuals has a z-score of -2.02, which is not very extreme for 12 observations from a normal distribution. This corresponds to observation 7, which is

>	x[7,]					
	Couple	${\tt HusbandAge}$	${\tt Husband}{\tt Height}$	WifeAge	WifeHeight	
7	7	43	1730	52	1610	

The negative number is due to the husband being younger than expected given the wife's age.

If there are outliers in the data, you have to be careful about how to analyze them. If an outlier is due to an incorrect measurement or error in the data entry, then it makes sense to remove it. For a data entry error, you might be able to correct the entry by consulting with the investigators, for example if a decimal is put in the wrong place. This is preferable to simply removing the data altogether.

If an outlier corresponds to genuine data but is removed, I would typically analyze the data both with and without the outlier to see how much of a difference it makes. In some cases, keeping an outlier might not change conclusions in the model. Removing the outlier will tend to decrease variability in the data, which might make you underestimate variances and standard errors, and therefore incorrect conclude that you have significance or greater evidence than you actually have. Removing an outlier that is a genuine observation also makes it less clear what population your sample represents. For the husband and wife example, if we removed a couple that appeared to be an outlier, we would be making inferences about the population of couples that do not have unusual ages or age combinations, rather than inferences about the more general population, which might include unusual ages.



A concept from regression diagnostics is that of **influential observations**. These are observations that can have a large impact on the regression line if they are removed from the data. This is a slightly different concept from that of outliers. An influential observation might or might not be an outlier, and might or might not have a large residual.

In the next slide, the solid line is the regression line with the influential observation and the dotted line is the regression line with the influential observation removed.





Note that in the previous slide, the left plot has an observation with an unusal y value, but that the x value for this observation is not unusual. For the right plot, the outlier is unusual in both x and y values.

Typically, an unusual x value has more potential to greatly alter the regression line, so a measure called **influence** has been developed based on how unusual an observation is in the predictor variable(s), without taking into account the y variable.

To see measures of influence, you can type influence(model1), where model1 is whatever you saved your lm() call to. The leverage values themselves are obtained by influence(model1)\$hat. Leverages are between 0 and 1, where values greater than about 2p/n or 3p/n, where p is the number of predictors, are considered large. If 3p/n is greater than 1, you can use 0.99 as a cutoff.

<pre>&gt; influence(model1)\$hat &gt; influence(model1)\$hat</pre>								
1	2	3	4	5	6	7	8	
0.1027 0.	1439 0.	1212 0.3	3319 0.	2203	0.1572	0.2203	0.1027	
9	10	11	12					
0.2235 0.1877 0.0847 0.1039								

For the husband and wife age data, observation 4 has the highest leverage, and this corresponds to the couple with the highest age for the wife. Recall that for leverage, the y variable (husband's age) is not used. However, the value here is 0.33, which is not high for leverages. Recall that the observation with the greatest residual was observation 7.

> x[4,]

	Couple	HusbandAge	HusbandHeight	WifeAge	WifeHeight
4	4	52	1779	57	1540

The formula for the leverage is somewhat complicated (it is usually defined in terms of matrices), but to give some intuition, note that the z-scores for the wife's ages also give observation 4 as the most unusual, with a z-score of 1.65:

> (x\$WifeAge-mean(x\$WifeAge))/sd(x\$WifeAge)
[1] 0.461 -0.816 -0.646 1.653 1.228 -0.901 1.228
0.461 -1.242 -1.072 0.121 -0.475

Another measure of influence is **Cook's distance** or Cook's D. An expression for Cook's D is

$$D_j \propto \sum_i (\widehat{y}_i - \widehat{y}_{i[-j]})^2$$

Here  $\hat{y}_{i[-j]}$  is the predicted value of the *i*th observation when the regression line is computed with the *j*th observation removed from the data set. This statistic is based on the idea of recomputing the regression line *n* times, each time removing observation *j*, j = 1, ..., n to get a statistic for how much removing the *j*th observation changes the regression line for the remaining.

The symbol  $\propto$  means that the actual value is a multiple of the value that doesn't depend on j. There are different interpretations for what counts as a large value of  $D_j$ . One is values of  $D_j > 1$ . Another approach is to see if  $D_j$  is large for some j compared to other Cook's distances in the data.

<pre>&gt; cooks.distance(model1)</pre>							
1	2	3	4	5	6		
0.057390	0.195728	0.108014	0.125200	0.318839	0.000802		
7	8	9	10	11	12		
0.440936	0.020277	0.045336	0.083990	0.001656	0.000523		

Cook's distance depend's on an observation being unusual for both x and y and having an influence on the regression line. In this case, observation 7 has the highest Cook's D, but it is not alarming. In the following example, an artificial data set with 101 observations has an outlier that is fairly consistent with the overall trend of the data with the outlier removed. However, Cook's D still picks out the outlier. As before, the solid line is with the outlier included.





a <- lm(y ~ x) hist(cooks.distance(a))



Note that with one predictor we can pretty easily plot the data and visually see unusual observations. In multiple dimensions, with multiple predictor variables, this becomes more difficult, which makes these diagnostic techniques more valuable when there are multiple predictors. This will be explored more next semester.

The following is a summary for analyzing regression data.



- 1. **Plot the data**. With multiple predictors, a scatterplot matrix is the easiest way to do this.
- 2. Consider transformations of the data, such as logarithms. For count data, square roots are often used. Different transformations will be explored more next semester.
- 3. Fit the model, for example using aov() or lm()
- 4. Examine residual plots. Here you can look for
  - curvature in the residuals or other nonrandom patterns
  - nonconstant variance
  - outliers
  - normality of residuals

- 5. Check Cook's D values
- 6. If there are outliers or influential observations, consider redoing the analysis with problematic points removed

