Introduction to regression

Regression

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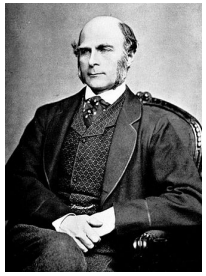
A famous motivating example



(Perhaps surprisingly, this example is still relevant)

http://www.nature.com/ejhg/journal/v17/n8/full/ejhg20095a.html

Predicting height: the Victorian approach beats modern genomics

Questions for this class

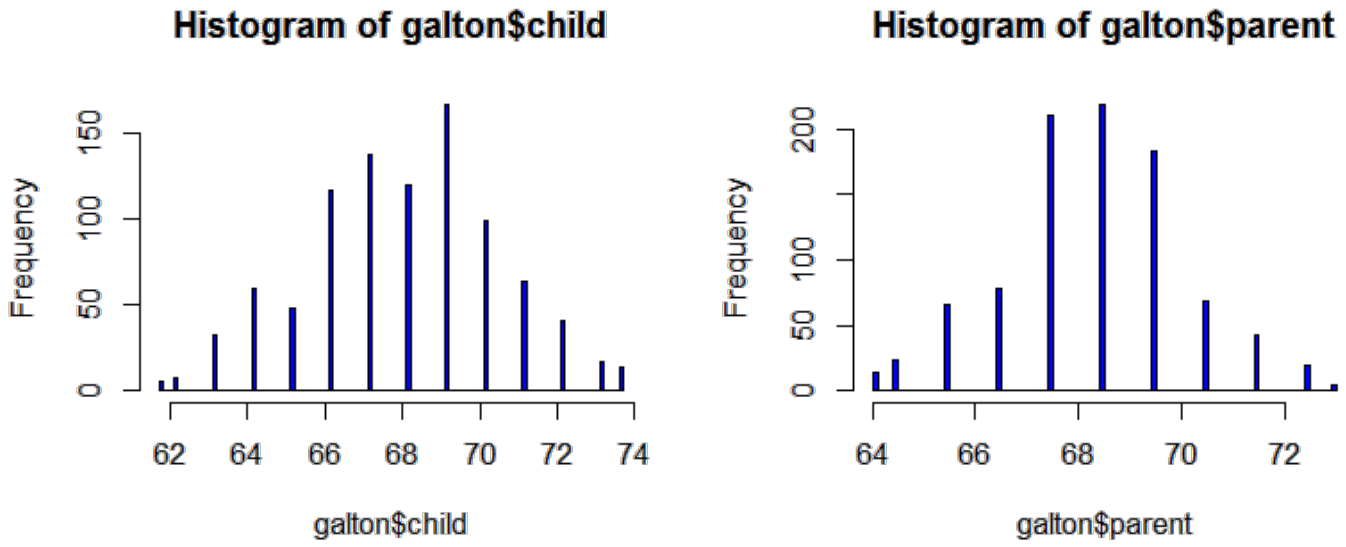
- Consider trying to answer the following kinds of questions:
  - To use the parents' heights to predict childrens' heights.
  - To try to find a parsimonious, easily described mean relationship between parent and children's heights.
  - To investigate the variation in childrens' heights that appears unrelated to parents' heights (residual variation).
  - To quantify what impact genotype information has beyond parental height in explaining child height.
  - To figure out how/whether and what assumptions are needed to generalize findings beyond the data in question.
  - Why do children of very tall parents tend to be tall, but a little shorter than their parents and why children of very short parents tend to be short, but a little taller than their parents? (This is a famous question called 'Regression to the mean'.)

Galton's Data

- Let's look at the data first, used by Francis Galton in 1885.
- Galton was a statistician who invented the term and concepts of regression and correlation, founded the journal Biometrika, and was the cousin of Charles Darwin.
- You may need to run `install.packages("UsingR")` if the `UsingR` library is not installed.
- Let's look at the marginal (parents disregarding children and children disregarding parents) distributions first.
    - Parent distribution is all heterosexual couples.
    - Correction for gender via multiplying female heights by 1.08.
    - Overplotting is an issue from discretization.

Code

```
library(UsingR); data(galton)
par(mfrow=c(1,2))
hist(galton$child,col="blue",breaks=100)
hist(galton$parent,col="blue",breaks=100)
```



Finding the middle via least squares

- Consider only the children's heights.
  - How could one describe the "middle"?
  - One definition, let Y_i be the height of child i for $i = 1, \ldots, n = 928$, then define the middle as the value of μ that minimizes

$$\sum_{i=1}^{n} (Y_i - \mu)^2$$

- This is physical center of mass of the histrogram.
- You might have guessed that the answer $\mu = \bar{X}$.

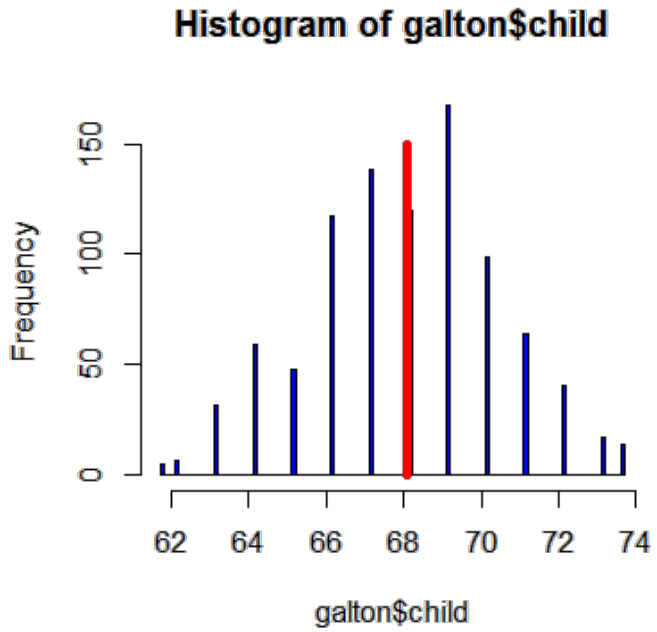
Experiment

Use R studio's manipulate to see what value of μ minimizes the sum of the squared deviations.

```
library(manipulate)
myHist <- function(mu){
  hist(galton$child,col="blue",breaks=100)
  lines(c(mu, mu), c(0, 150),col="red",lwd=5)
  mse <- mean((galton$child - mu)^2)
  text(63, 150, paste("mu = ", mu))
  text(63, 140, paste("MSE = ", round(mse, 2)))
}
manipulate(myHist(mu), mu = slider(62, 74, step = 0.5))
```

The least squares estimate is the empirical mean

```
hist(galton$child,col="blue",breaks=100)
meanChild <- mean(galton$child)
lines(rep(meanChild,100),seq(0,150,length=100),col="red",lwd=5)
```

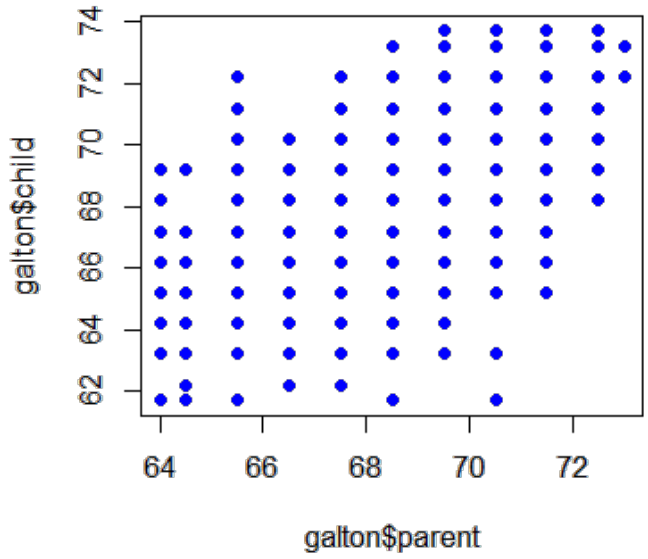


The math follows as:

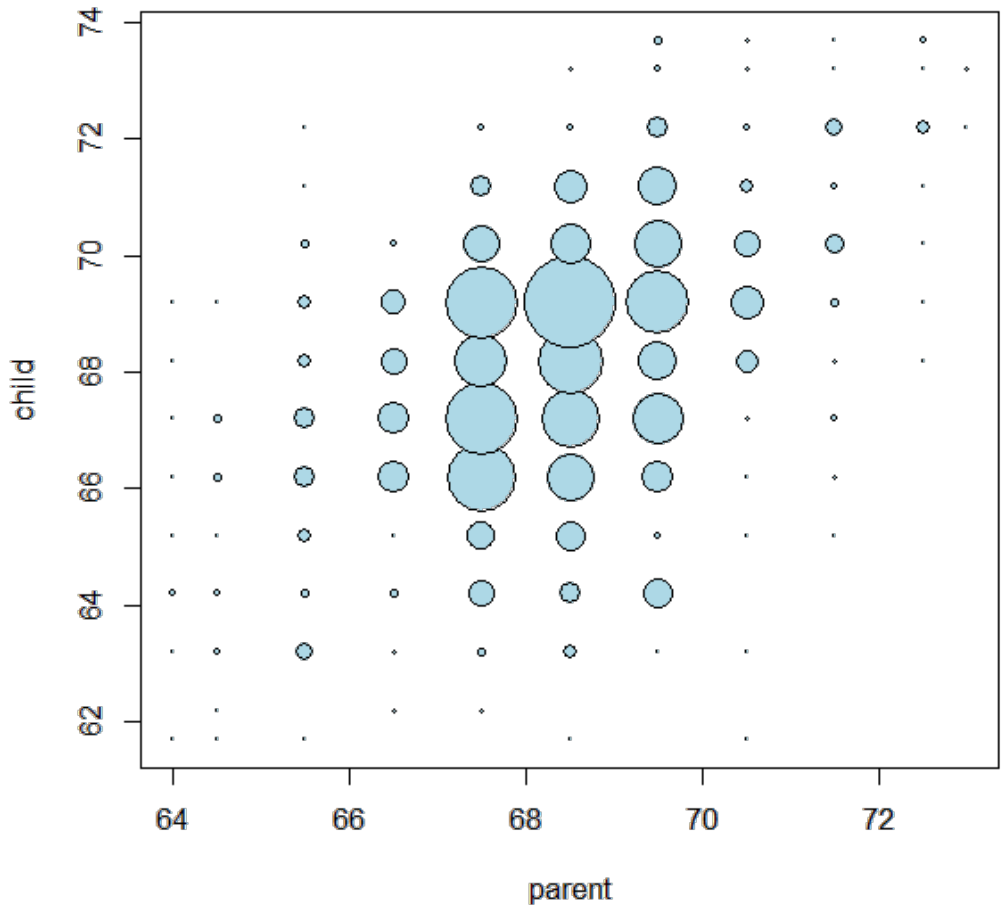
$$
\begin{aligned}
\sum_{i=1}^{n}(Y_i - \mu)^2 &= \sum_{i=1}^{n}(Y_i - \bar{Y} + \bar{Y} - \mu)^2 \\
&= \sum_{i=1}^{n}(Y_i - \bar{Y})^2 + 2\sum_{i=1}^{n}(Y_i - \bar{Y})(\bar{Y} - \mu) + \sum_{i=1}^{n}(\bar{Y} - \mu)^2 \\
&= \sum_{i=1}^{n}(Y_i - \bar{Y})^2 + 2(\bar{Y} - \mu)\sum_{i=1}^{n}(Y_i - \bar{Y}) + \sum_{i=1}^{n}(\bar{Y} - \mu)^2 \\
&= \sum_{i=1}^{n}(Y_i - \bar{Y})^2 + 2(\bar{Y} - \mu)(\sum_{i=1}^{n} Y_i - n\bar{Y}) + \sum_{i=1}^{n}(\bar{Y} - \mu)^2 \\
&= \sum_{i=1}^{n}(Y_i - \bar{Y})^2 + \sum_{i=1}^{n}(\bar{Y} - \mu)^2 \\
&\geq \sum_{i=1}^{n}(Y_i - \bar{Y})^2
\end{aligned}
$$

Comparing childrens' heights and their parents' heights

```
plot(galton$parent,galton$child,pch=19,col="blue")
```



Size of point represents number of points at that (X, Y) combination (See the Rmd file for the code).



Regression through the origin

- Suppose that X_i are the parents' heights.
- Consider picking the slope β that minimizes

$$\sum_{i=1}^{n} (Y_i - X_i \beta)^2$$

- This is exactly using the origin as a pivot point picking the line that minimizes the sum of the squared vertical distances of the points to the line
- Use R studio's manipulate function to experiment
- Subtract the means so that the origin is the mean of the parent and children's heights

```r
myPlot <- function(beta){
  y <- galton$child - mean(galton$child)
  x <- galton$parent - mean(galton$parent)
  freqData <- as.data.frame(table(x, y))
  names(freqData) <- c("child", "parent", "freq")
  plot(
    as.numeric(as.vector(freqData$parent)),
    as.numeric(as.vector(freqData$child)),
    pch = 21, col = "black", bg = "lightblue",
    cex = .15 * freqData$freq,
    xlab = "parent",
    ylab = "child"
    )
  abline(0, beta, lwd = 3)
  points(0, 0, cex = 2, pch = 19)
  mse <- mean( (y - beta * x)^2 )
  title(paste("beta = ", beta, "mse = ", round(mse, 3)))
}
manipulate(myPlot(beta), beta = slider(0.6, 1.2, step = 0.02))
```

The solution

In the next few lectures we'll talk about why this is the solution

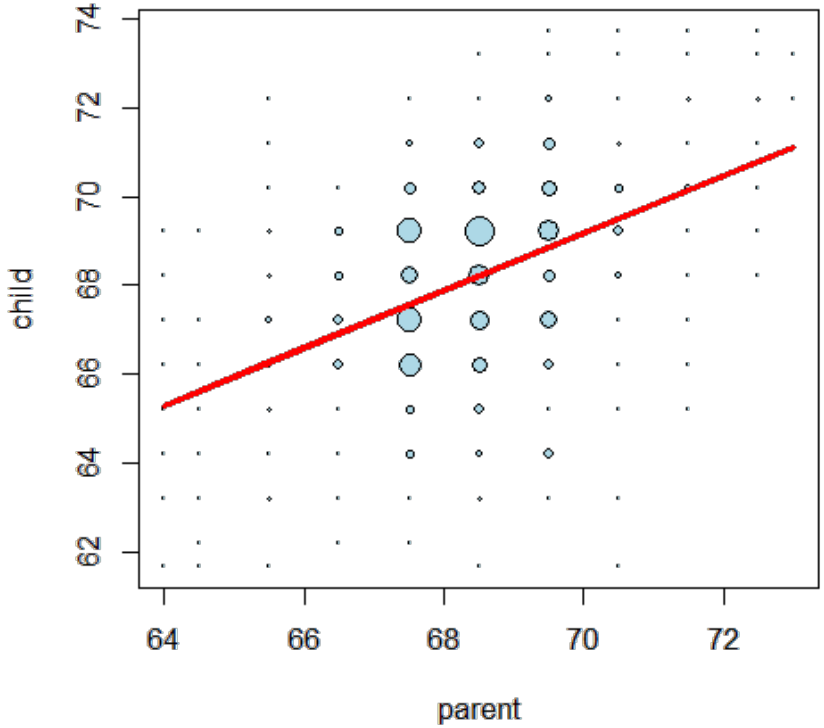
```
lm(I(child - mean(child))~ I(parent - mean(parent)) - 1, data = galton)
```

```
Call:
lm(formula = I(child - mean(child)) ~ I(parent - mean(parent)) -
    1, data = galton)

Coefficients:
I(parent - mean(parent))
                   0.646
```

Visualizing the best fit line

Size of points are frequencies at that X, Y combination



Some basic notation and background

Regression

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Some basic definitions

- In this module, we'll cover some basic definitions and notation used throughout the class.
- We will try to minimize the amount of mathematics required for this class.
- No caclculus is required.

Notation for data

- We write $X_1, X_2, \ldots, X_n$ to describe n data points.
- As an example, consider the data set $\{1, 2, 5\}$ then
  - $X_1 = 1$, $X_2 = 2$, $X_3 = 5$ and $n = 3$.
- We often use a different letter than X, such as $Y_1, \ldots, Y_n$.
- We will typically use Greek letters for things we don't know. Such as, μ is a mean that we'd like to estimate.
- We will use capital letters for conceptual values of the variables and lowercase letters for realized values.
  - So this way we can write $P(X_i > x)$.
  - X_i is a conceptual random variable.
  - x is a number that we plug into.

The empirical mean

- Define the empirical mean as

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

- Notice if we subtract the mean from data points, we get data that has mean 0. That is, if we define

$$\tilde{X}_i = X_i - \bar{X}.$$

  The the mean of the $\tilde{X}_i$ is 0.

- This process is called "centering" the random variables.
- The mean is a measure of central tendancy of the data.
- Recall from the previous lecture that the mean is the least squares solution for minimizing

$$\sum_{i=1}^{n}(X_i - \mu)^2$$

The emprical standard deviation and variance

- Define the empirical variance as

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i^2 - n\bar{X}^2\right)$$

- The empirical standard deviation is defined as $S = \sqrt{S^2}$. Notice that the standard deviation has the same units as the data.
- The data defined by X_i/s have empirical standard deviation 1. This is called "scaling" the data.
- The empirical standard deviation is a measure of spread.
- Sometimes people divide by n rather than $n-1$ (the latter produces an unbiased estimate.)

Normalization

- The the data defined by

$$Z_i = \frac{X_i - \bar{X}}{s}$$

  have empirical mean zero and empirical standard deviation 1.

- The process of centering then scaling the data is called "normalizing" the data.
- Normalized data are centered at 0 and have units equal to standard deviations of the original data.
- Example, a value of 2 form normalized data means that data point was two standard deviations larger than the mean.

The empirical covariance

- Consider now when we have pairs of data, (X_i, Y_i).
- Their empirical covariance is

$$\mathrm{Cov}(X, Y) = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y}) = \frac{1}{n-1}\left(\sum_{i=1}^{n} X_i Y_i - n\bar{X}\bar{Y}\right)$$

- Some people prefer to divide by n rather than $n-1$ (the latter produces an unbiased estimate.)
- The correlation is defined is

$$\mathrm{Cor}(X, Y) = \frac{\mathrm{Cov}(X, Y)}{S_x S_y}$$

where S_x and S_y are the estimates of standard deviations for the X observations and Y observations, respectively.

Some facts about correlation

- $\text{Cor}(X, Y) = \text{Cor}(Y, X)$
- $-1 \leq \text{Cor}(X, Y) \leq 1$
- $\text{Cor}(X, Y) = 1$ and $\text{Cor}(X, Y) = -1$ only when the X or Y observations fall perfectly on a positive or negative sloped line, respectively.
- $\text{Cor}(X, Y)$ measures the strength of the linear relationship between the X and Y data, with stronger relationships as $\text{Cor}(X, Y)$ heads towards -1 or 1.
- $\text{Cor}(X, Y) = 0$ implies no linear relationship.

Least squares estimation of regression lines

Regression via least squares

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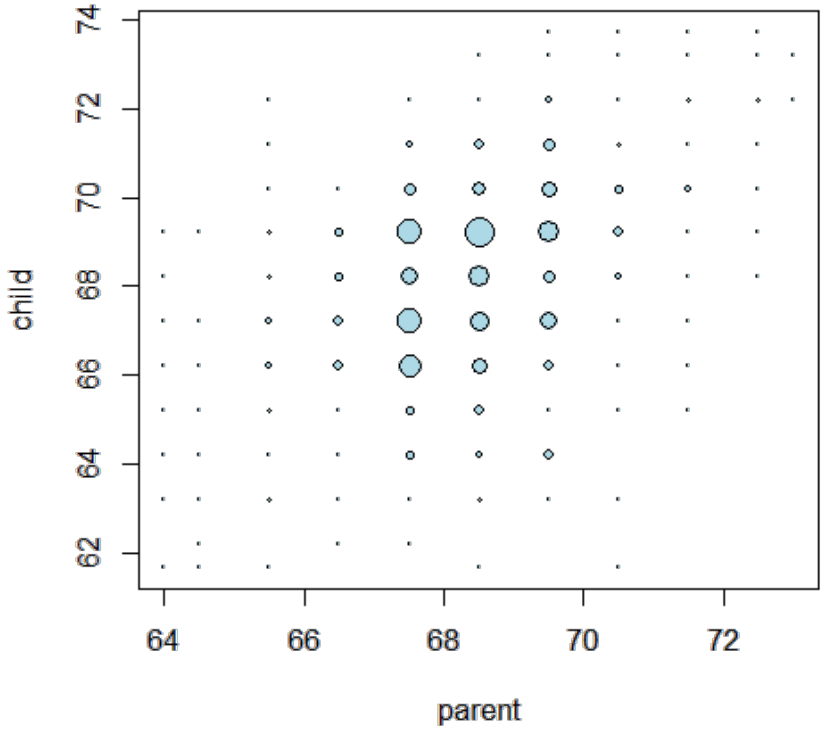
General least squares for linear equations

Consider again the parent and child height data from Galton



Fitting the best line

- Let Y_i be the i^{th} child's height and X_i be the i^{th} (average over the pair of) parents' heights.
- Consider finding the best line
  - Child's Height = β_0 + Parent's Height β_1
- Use least squares

$$\sum_{i=1}^{n} \{Y_i - (\beta_0 + \beta_1 X_i)\}^2$$

- How do we do it?

Let's solve this problem generally

- Let $\mu_i = \beta_0 + \beta_1 X_i$ and our estimates be $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$.
- We want to minimize

$$\dagger \sum_{i=1}^{n} (Y_i - \mu_i)^2 = \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2 + 2 \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) + \sum_{i=1}^{n} (\hat{\mu}_i - \mu_i)^2$$

- Suppose that

$$\sum_{i=1}^{n} (Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

then

$$\dagger = \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2 + \sum_{i=1}^{n} (\hat{\mu}_i - \mu_i)^2 \geq \sum_{i=1}^{n} (Y_i - \hat{\mu}_i)^2$$

Mean only regression

- So we know that if:

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

where $\mu_i = \beta_0 + \beta_1 X_i$ and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$ then the line

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X$$

is the least squares line.

- Consider forcing $\beta_1 = 0$ and thus $\hat{\beta}_1 = 0$; that is, only considering horizontal lines
- The solution works out to be

$$\hat{\beta}_0 = \bar{Y}.$$

Let's show it

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0)(\hat{\beta}_0 - \beta_0)$$

$$= (\hat{\beta}_0 - \beta_0)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0)$$

Thus, this will equal 0 if $\sum_{i=1}^{n}(Y_i - \hat{\beta}_0) = n\bar{Y} - n\hat{\beta}_0 = 0$

Thus $\hat{\beta}_0 = \bar{Y}$.

Regression through the origin

- Recall that if:

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

where $\mu_i = \beta_0 + \beta_1 X_i$ and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$ then the line

$$Y = \hat{\beta}_0 + \hat{\beta}_1 X$$

is the least squares line.

- Consider forcing $\beta_0 = 0$ and thus $\hat{\beta}_0 = 0$; that is, only considering lines through the origin
- The solution works out to be

$$\hat{\beta}_1 = \frac{\sum_{i=1^n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}.$$

Let's show it

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_1 X_i)(\hat{\beta}_1 X_i - \beta_1 X_i)$$

$$= (\hat{\beta}_1 - \beta_1)\sum_{i=1}^{n}(Y_i X_i - \hat{\beta}_1 X_i^2)$$

Thus, this will equal 0 if $\sum_{i=1}^{n}(Y_i X_i - \hat{\beta}_1 X_i^2) = \sum_{i=1}^{n} Y_i X_i - \hat{\beta}_1 \sum_{i=1}^{n} X_i^2 = 0$

Thus

$$\hat{\beta}_1 = \frac{\sum_{i=1^n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}.$$

Recapping what we know

- If we define $\mu_i = \beta_0$ then $\hat{\beta}_0 = \bar{Y}$.
  - If we only look at horizontal lines, the least squares estimate of the intercept of that line is the average of the outcomes.
- If we define $\mu_i = X_i\beta_1$ then $\hat{\beta}_1 = \frac{\sum_{i=1}^{n} Y_i X_i}{\sum_{i=1}^{n} X_i^2}$
  - If we only look at lines through the origin, we get the estimated slope is the cross product of the X and Ys divided by the cross product of the Xs with themselves.
- What about when $\mu_i = \beta_0 + \beta_1 X_i$? That is, we don't want to restrict ourselves to horizontal lines or lines through the origin.

Let's figure it out

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)(\hat{\beta}_0 + \hat{\beta}_1 X_i - \beta_0 - \beta_1 X_i)$$

$$= (\hat{\beta}_0 - \beta_0)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i) + (\beta_1 - \beta_1)\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)X_i$$

Note that

$$0 = \sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i) = n\bar{Y} - n\hat{\beta}_0 - n\hat{\beta}_1\bar{X} \text{ implies that } \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1\bar{X}$$

Then

$$\sum_{i=1}^{n}(Y_i - \hat{\beta}_0 - \hat{\beta}_1 X_i)X_i = \sum_{i=1}^{n}(Y_i - \bar{Y} + \hat{\beta}_1\bar{X} - \hat{\beta}_1 X_i)X_i$$

Continued

$$= \sum_{i=1}^{n} \{(Y_i - \bar{Y}) - \hat{\beta}_1(X_i - \bar{X})\}X_i$$

And thus

$$\sum_{i=1}^{n}(Y_i - \bar{Y})X_i - \hat{\beta}_1 \sum_{i=1}^{n}(X_i - \bar{X})X_i = 0.$$

So we arrive at

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}\{(Y_i - \bar{Y})X_i}{\sum_{i=1}^{n}(X_i - \bar{X})X_i} = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(X_i - \bar{X})}{\sum_{i=1}^{n}(X_i - \bar{X})(X_i - \bar{X})} = \mathrm{Cor}(Y, X)\,\frac{\mathrm{Sd}(Y)}{\mathrm{Sd}(X)}\,.$$

And recall

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1\bar{X}.$$

Consequences

- The least squares model fit to the line $Y = \beta_0 + \beta_1 X$ through the data pairs (X_i, Y_i) with Y_i as the outcome obtains the line $Y = \hat{\beta}_0 + \hat{\beta}_1 X$ where

$$\hat{\beta}_1 = \text{Cor}(Y, X)\frac{\text{Sd}(Y)}{\text{Sd}(X)} \quad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$$

- $\hat{\beta}_1$ has the units of Y/X, $\hat{\beta}_0$ has the units of Y.
- The line passes through the point $(\bar{X}, \bar{Y})$
- The slope of the regression line with X as the outcome and Y as the predictor is $\text{Cor}(Y, X)\text{Sd}(X)/\text{Sd}(Y)$.
- The slope is the same one you would get if you centered the data, $(X_i - \bar{X}, Y_i - \bar{Y})$, and did regression through the origin.
- If you normalized the data, $\{\frac{X_i - \bar{X}}{\text{Sd}(X)}, \frac{Y_i - \bar{Y}}{\text{Sd}(Y)}\}$, the slope is $\text{Cor}(Y, X)$.

Revisiting Galton's data

Double check our calculations using R

```
y <- galton$child
x <- galton$parent
beta1 <- cor(y, x) *  sd(y) / sd(x)
beta0 <- mean(y) - beta1 * mean(x)
rbind(c(beta0, beta1), coef(lm(y ~ x)))
```

```
     (Intercept)      x
[1,]       23.94 0.6463
[2,]       23.94 0.6463
```

Revisiting Galton's data

Reversing the outcome/predictor relationship

```
beta1 <- cor(y, x) *  sd(x) / sd(y)
beta0 <- mean(x) - beta1 * mean(y)
rbind(c(beta0, beta1), coef(lm(x ~ y)))
```

```
     (Intercept)      y
[1,]       46.14 0.3256
[2,]       46.14 0.3256
```

Revisiting Galton's data

Regression through the origin yields an equivalent slope if you center the data first

```
yc <- y - mean(y)
xc <- x - mean(x)
beta1 <- sum(yc * xc) / sum(xc ^ 2)
c(beta1, coef(lm(y ~ x))[2])
```

```
           x
0.6463 0.6463
```

Revisiting Galton's data

Normalizing variables results in the slope being the correlation

```
yn <- (y - mean(y))/sd(y)
xn <- (x - mean(x))/sd(x)
c(cor(y, x), cor(yn, xn), coef(lm(yn ~ xn))[2])
```

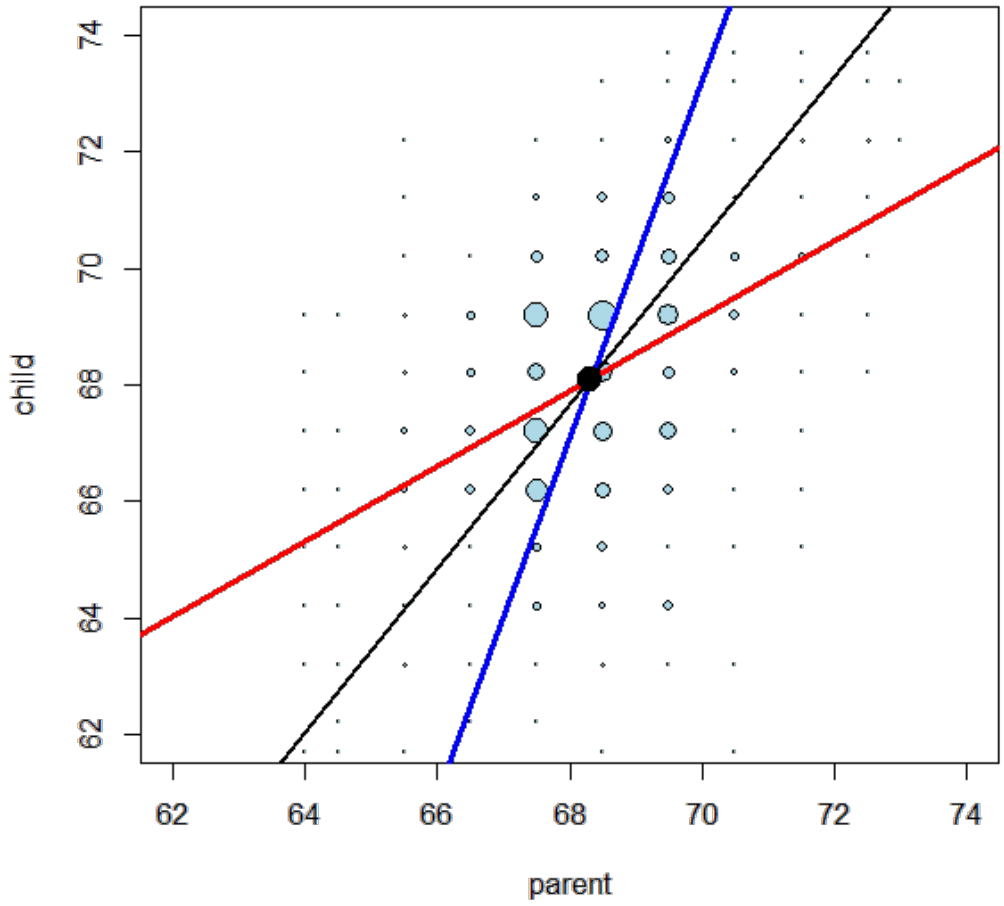
```
                 xn
0.4588 0.4588 0.4588
```

Plotting the fit

- Size of points are frequencies at that X, Y combination.
- For the red lie the child is outcome.
- For the blue, the parent is the outcome (accounting for the fact that the response is plotted on the horizontal axis).
- Black line assumes $\mathrm{Cor}(\mathrm{Y}, \mathrm{X}) = 1$ (slope is $\mathrm{Sd}(\mathrm{Y})/\mathrm{Sd}(\mathrm{x})$).
- Big black dot is $(\bar{\mathrm{X}}, \bar{\mathrm{Y}})$.

The code to add the lines

```
abline(mean(y) - mean(x) * cor(y, x) * sd(y) / sd(x),
  sd(y) / sd(x) * cor(y, x),
  lwd = 3, col = "red")
abline(mean(y) - mean(x) * sd(y) / sd(x) / cor(y, x),
  sd(y) cor(y, x) / sd(x),
  lwd = 3, col = "blue")
abline(mean(y) - mean(x) * sd(y) / sd(x),
  sd(y) / sd(x),
  lwd = 2)
points(mean(x), mean(y), cex = 2, pch = 19)
```


child
parent
62
64
66
68
70
72
74

Historical side note, Regression to Mediocrity

Regression to the mean

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A historically famous idea, Regression to the Mean

- Why is it that the children of tall parents tend to be tall, but not as tall as their parents?
- Why do children of short parents tend to be short, but not as short as their parents?
- Why do parents of very short children, tend to be short, but not a short as their child? And the same with parents of very tall children?
- Why do the best performing athletes this year tend to do a little worse the following?

Regression to the mean

- These phenomena are all examples of so-called regression to the mean
- Invented by Francis Galton in the paper "Regression towvards mediocrity in hereditary stature" The Journal of the Anthropological Institute of Great Britain and Ireland , Vol. 15, (1886).
- Think of it this way, imagine if you simulated pairs of random normals
  - The largest first ones would be the largest by chance, and the probability that there are smaller for the second simulation is high.
  - In other words $P(Y < x|X = x)$ gets bigger as x heads into the very large values.
  - Similarly $P(Y > x|X = x)$ gets bigger as x heads to very small values.
- Think of the regression line as the intrisic part.
  - Unless $Cor(Y, X) = 1$ the intrinsic part isn't perfect

Regression to the mean

- Suppose that we normalize X (child's height) and Y (parent's height) so that they both have mean 0 and variance 1.
- Then, recall, our regression line passes through $(0, 0)$ (the mean of the X and Y).
- If the slope of the regression line is $\mathrm{Cor}(\mathrm{Y}, \mathrm{X})$, regardless of which variable is the outcome (recall, both standard deviations are 1).
- Notice if X is the outcome and you create a plot where X is the horizontal axis, the slope of the least squares line that you plot is $1/\mathrm{Cor}(\mathrm{Y}, \mathrm{X})$.

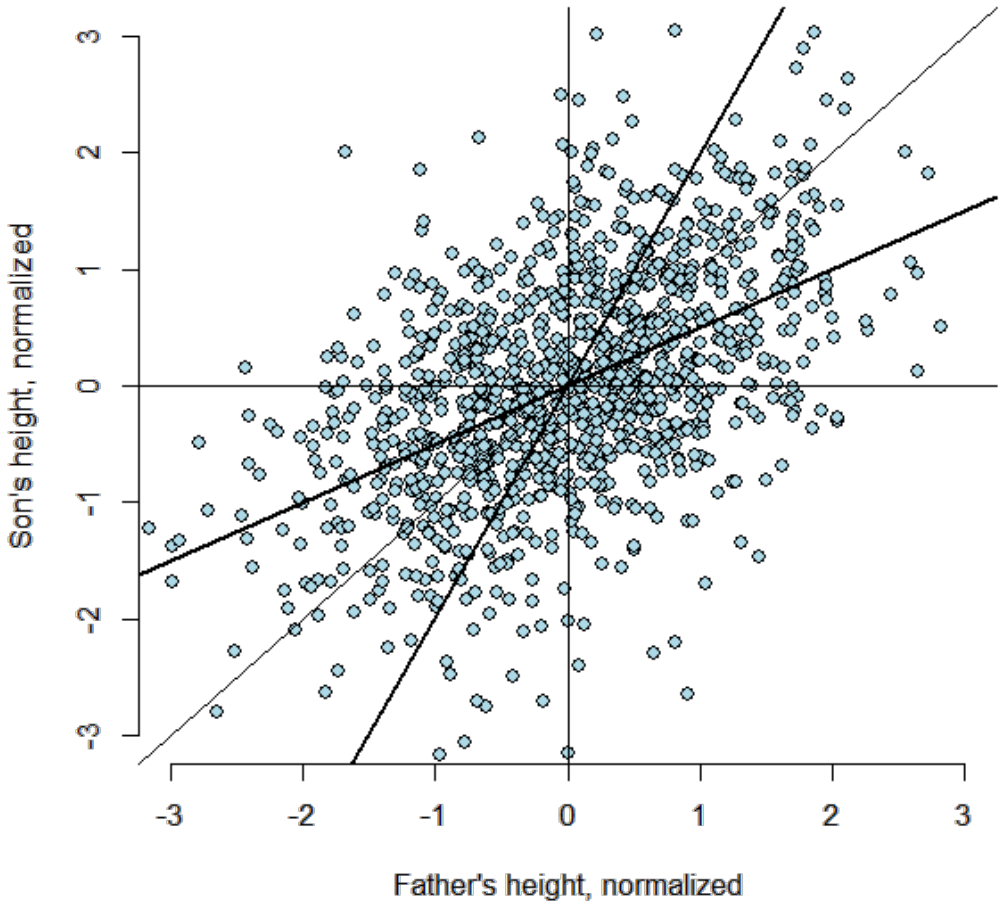
Normalizing the data and setting plotting parameters

```
library(UsingR)
data(father.son)
y <- (father.son$sheight - mean(father.son$sheight)) / sd(father.son$sheight)
x <- (father.son$fheight - mean(father.son$fheight)) / sd(father.son$fheight)
rho <- cor(x, y)
myPlot <- function(x, y) {
  plot(x, y,
       xlab = "Father's height, normalized",
       ylab = "Son's height, normalized",
       xlim = c(-3, 3), ylim = c(-3, 3),
       bg = "lightblue", col = "black", cex = 1.1, pch = 21,
       frame = FALSE)
}
```

Plot the data, code

```
myPlot(x, y)
abline(0, 1) # if there were perfect correlation
abline(0, rho, lwd = 2) # father predicts son
abline(0, 1 / rho, lwd = 2) # son predicts father, son on vertical axis
abline(h = 0); abline(v = 0) # reference lines for no relathionship
```

Plot the data, results



Discussion

- If you had to predict a son's normalized height, it would be $\mathrm{Cor}(Y, X) * X_i$
- If you had to predict a father's normalized height, it would be $\mathrm{Cor}(Y, X) * Y_i$
- Multiplication by this correlation shrinks toward 0 (regression toward the mean)
- If the correlation is 1 there is no regression to the mean (if father's height perfectly determine's child's height and vice versa)
- Note, regression to the mean has been thought about quite a bit and generalized

Statistical linear regression models

Brian Caffo, Jeff Leek, Roger Peng
Johns Hopkins Bloomberg School of Public Health

Basic regression model with additive Gaussian errors.

- Least squares is an estimation tool, how do we do inference?
- Consider developing a probabilistic model for linear regression

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

- Here the ϵ_i are assumed iid $N(0, \sigma^2)$.
- Note, $E[Y_i \mid X_i = x_i] = \mu_i = \beta_0 + \beta_1 x_i$
- Note, $Var(Y_i \mid X_i = x_i) = \sigma^2$.
- Likelihood equivalent model specification is that the Y_i are independent $N(\mu_i, \sigma^2)$.

Likelihood

$$>(\beta, \sigma) = \prod_{i=1}^{n} \left\{ (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{1}{2\sigma^2} (y_i - \mu_i)^2 \right) \right\}$$

so that the twice the negative log (base e) likelihood is

$$-2 \log\{>(\beta, \sigma)\} = \frac{1}{\sigma^2} \sum_{i=1}^{n} (y_i - \mu_i)^2 + n \log(\sigma^2)$$

Discussion

- Maximizing the likelihood is the same as minimizing -2 log likelihood
- The least squares estimate for $\mu_i = \beta_0 + \beta_1 x_i$ is exactly the maximimum likelihood estimate (regardless of σ)

Recap

- Model $Y_i = \mu_i + \epsilon_i = \beta_0 + \beta_1 X_i + \epsilon_i$ where ϵ_i are iid $N(0, \sigma^2)$
- ML estimates of β_0 and β_1 are the least squares estimates

$$\hat{\beta}_1 = \text{Cor}(Y, X) \frac{\text{Sd}(Y)}{\text{Sd}(X)} \quad \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$$

- $E[Y \mid X = x] = \beta_0 + \beta_1 x$
- $\text{Var}(Y \mid X = x) = \sigma^2$

Interpretting regression coefficients, the itc

- β_0 is the expected value of the response when the predictor is 0

$$E[Y|X = 0] = \beta_0 + \beta_1 \times 0 = \beta_0$$

- Note, this isn't always of interest, for example when $X = 0$ is impossible or far outside of the range of data. (X is blood pressure, or height etc.)
- Consider that

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i = \beta_0 + a\beta_1 + \beta_1(X_i - a) + \epsilon_i = \tilde{\beta}_0 + \beta_1(X_i - a) + \epsilon_i$$

  So, shifting you X values by value a changes the intercept, but not the slope.

- Often a is set to $\bar{X}$ so that the intercept is interpretted as the expected response at the average X value.

Interpretting regression coefficients, the slope

- β_1 is the expected change in response for a 1 unit change in the predictor

$$E[Y \mid X = x + 1] - E[Y \mid X = x] = \beta_0 + \beta_1(x + 1) - (\beta_0 + \beta_1 x) = \beta_1$$

- Consider the impact of changing the units of X.

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i = \beta_0 + \frac{\beta_1}{a}(X_i a) + \epsilon_i = \beta_0 + \tilde{\beta}_1(X_i a) + \epsilon_i$$

- Therefore, multiplication of X by a factor a results in dividing the coefficient by a factor of a.
- Example: X is height in m and Y is weight in kg. Then β_1 is kg/m. Converting X to cm implies multiplying X by $100cm/m$. To get β_1 in the right units, we have to divide by $100cm/m$ to get it to have the right units.

$$Xm \times \frac{100cm}{m} = (100X)cm \text{ and } \beta_1 \frac{kg}{m} \times \frac{1m}{100cm} = \left(\frac{\beta_1}{100}\right)\frac{kg}{cm}$$

Using regression coeficients for prediction

- If we would like to guess the outcome at a particular value of the predictor, say X, the regression model guesses

$$\hat{\beta}_0 + \hat{\beta}_1 X$$

- Note that at the observed value of Xs, we obtain the predictions

$$\hat{\mu}_i = \hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$$

- Remember that least squares minimizes

$$\sum_{i=1}^{n} (Y_i - \mu_i)$$

for μ_i expressed as points on a line

Example

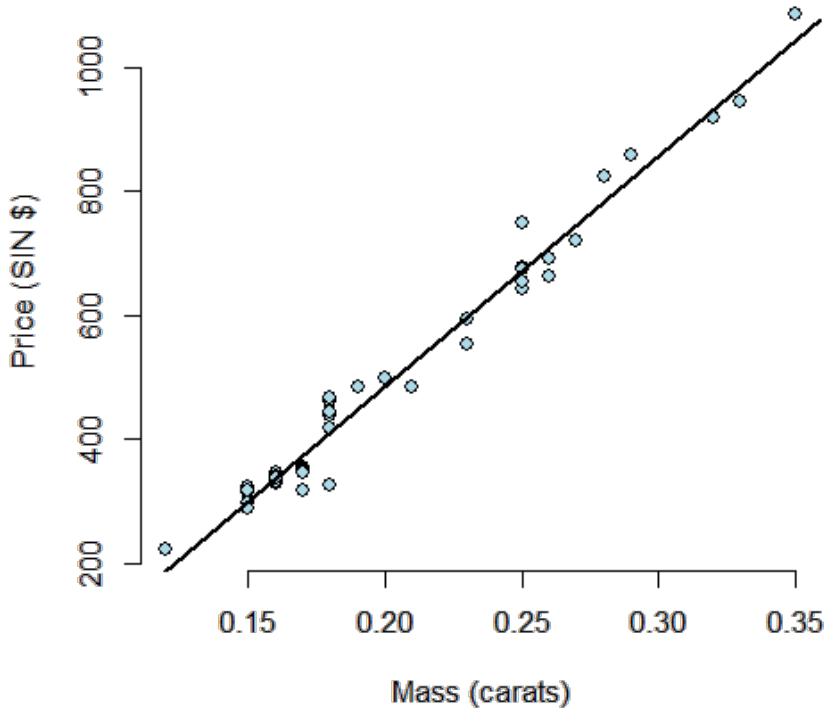
`diamond` data set from `UsingR`

Data is diamond prices (Signapore dollars) and diamond weight in carats (standard measure of diamond mass, 0.2 g). To get the data use `library(UsingR); data(diamond)`

Plotting the fitted regression line and data

```
data(diamond)
plot(diamond$carat, diamond$price,
     xlab = "Mass (carats)",
     ylab = "Price (SIN $)",
     bg = "lightblue",
     col = "black", cex = 1.1, pch = 21,frame = FALSE)
abline(lm(price ~ carat, data = diamond), lwd = 2)
```

The plot



Fitting the linear regression model

```
fit <- lm(price ~ carat, data = diamond)
coef(fit)
```

```
(Intercept)       carat
     -259.6      3721.0
```

- We estimate an expected 3721.02 (SIN) dollar increase in price for every carat increase in mass of diamond.
- The intercept -259.63 is the expected price of a 0 carat diamond.

Getting a more interpretable intercept

```
fit2 <- lm(price ~ I(carat - mean(carat)), data = diamond)
coef(fit2)
```

```
          (Intercept) I(carat - mean(carat))
                500.1                3721.0
```

Thus $500.1 is the expected price for the average sized diamond of the data (0.2042 carats).

Changing scale

- A one carat increase in a diamond is pretty big, what about changing units to 1/10th of a carat?
- We can just do this by just dividing the coeficient by 10.
    - We expect a 372.102 (SIN) dollar change in price for every 1/10th of a carat increase in mass of diamond.
- Showing that it's the same if we rescale the Xs and refit

```
fit3 <- lm(price ~ I(carat * 10), data = diamond)
coef(fit3)
```

```
  (Intercept) I(carat * 10)
       -259.6         372.1
```

Predicting the price of a diamond

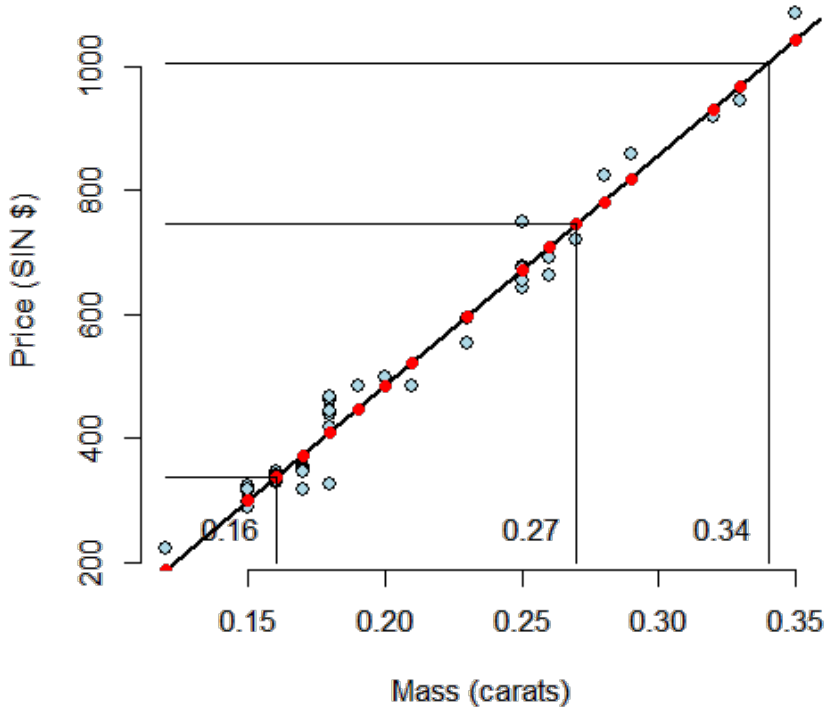
```
newx <- c(0.16, 0.27, 0.34)
coef(fit)[1] + coef(fit)[2] * newx
```

```
[1]  335.7  745.1 1005.5
```

```
predict(fit, newdata = data.frame(carat = newx))
```

```
     1      2      3
 335.7  745.1 1005.5
```

Predicted values at the observed Xs (red) and at the new Xs (lines)



Residuals and residual variation

Brian Caffo, Jeff Leek and Roger Peng
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Residuals

- Model $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$ where $\epsilon_i \sim N(0, \sigma^2)$.
- Observed outcome i is Y_i at predictor value X_i
- Predicted outcome i is $\hat{Y}_i$ at predictor valuve X_i is

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i$$

- Residual, the between the observed and predicted outcome

$$e_i = Y_i - \hat{Y}_i$$

  - The vertical distance between the observed data point and the regression line

- Least squares minimizes $\sum_{i=1}^{n} e_i^2$
- The e_i can be thought of as estimates of the ϵ_i.

Properties of the residuals

- $E[e_i] = 0$.
- If an intercept is included, $\sum_{i=1}^{n} e_i = 0$
- If a regressor variable, X_i, is included in the model $\sum_{i=1}^{n} e_i X_i = 0$.
- Residuals are useful for investigating poor model fit.
- Positive residuals are above the line, negative residuals are below.
- Residuals can be thought of as the outcome (Y) with the linear association of the predictor (X) removed.
- One differentiates residual variation (variation after removing the predictor) from systematic variation (variation explained by the regression model).
- Residual plots highlight poor model fit.

Code

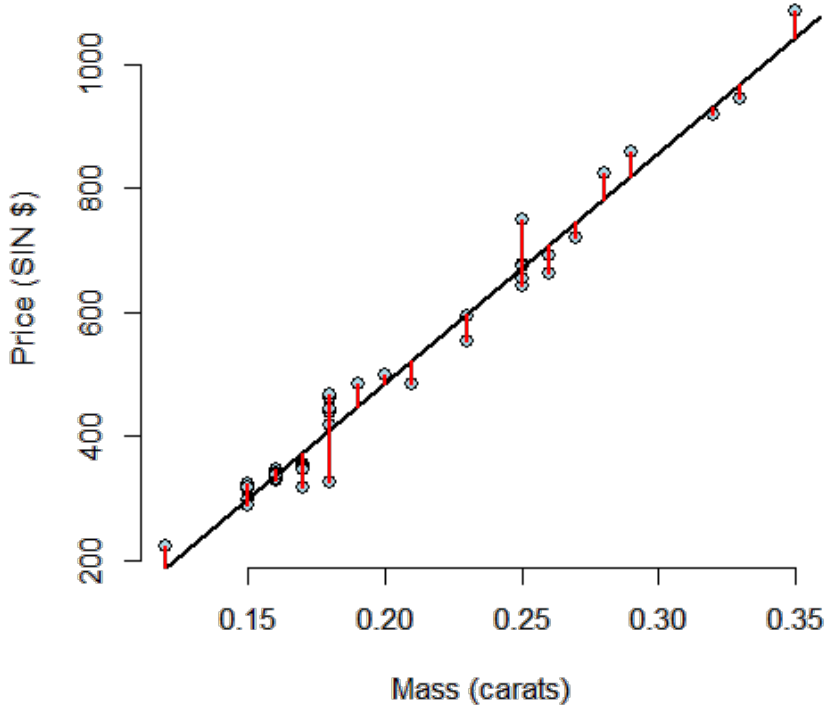
```
data(diamond)
y <- diamond$price; x <- diamond$carat; n <- length(y)
fit <- lm(y ~ x)
e <- resid(fit)
yhat <- predict(fit)
max(abs(e -(y - yhat)))
```

```
[1] 9.486e-13
```

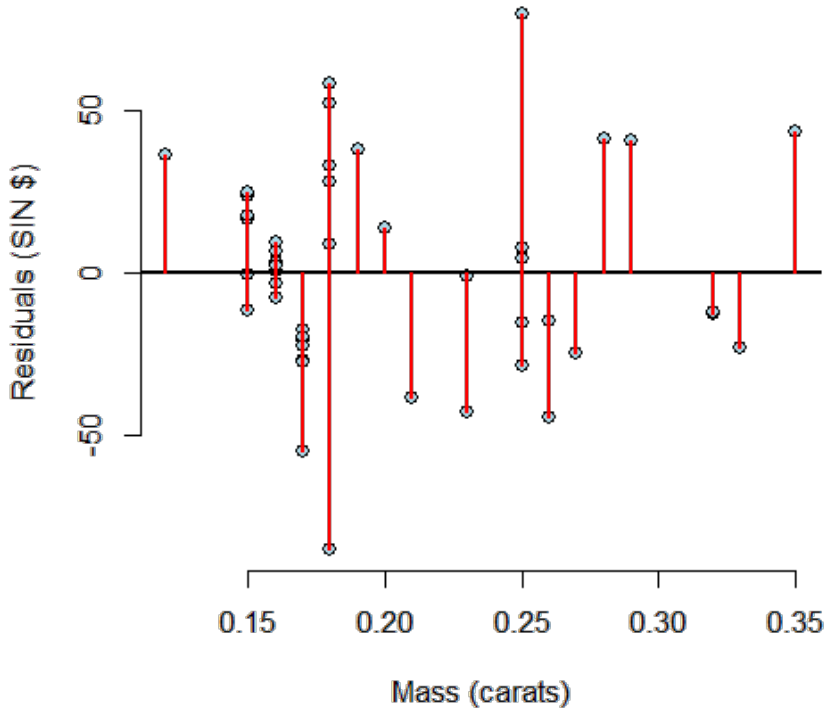
```
max(abs(e - (y - coef(fit)[1] - coef(fit)[2] * x)))
```

```
[1] 9.486e-13
```

Residuals are the signed length of the red lines

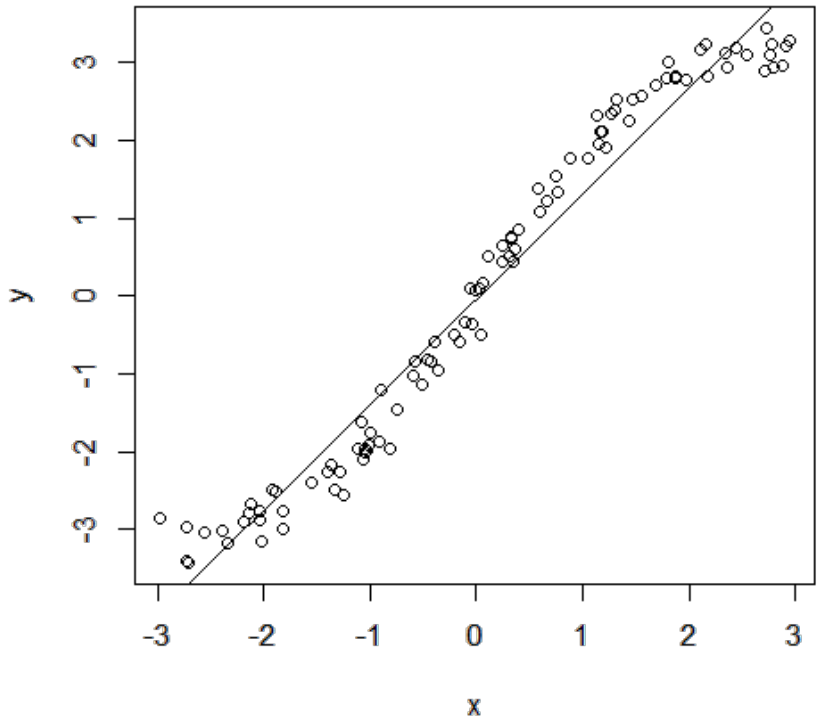


Residuals versus X

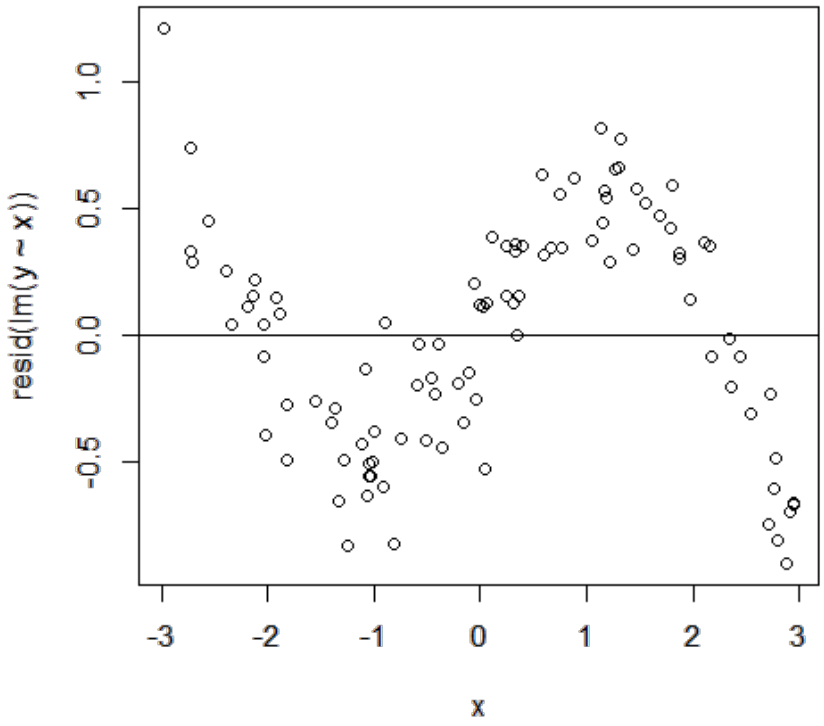


Non-linear data

```
x <- runif(100, -3, 3); y <- x + sin(x) + rnorm(100, sd = .2);
plot(x, y); abline(lm(y ~ x))
```

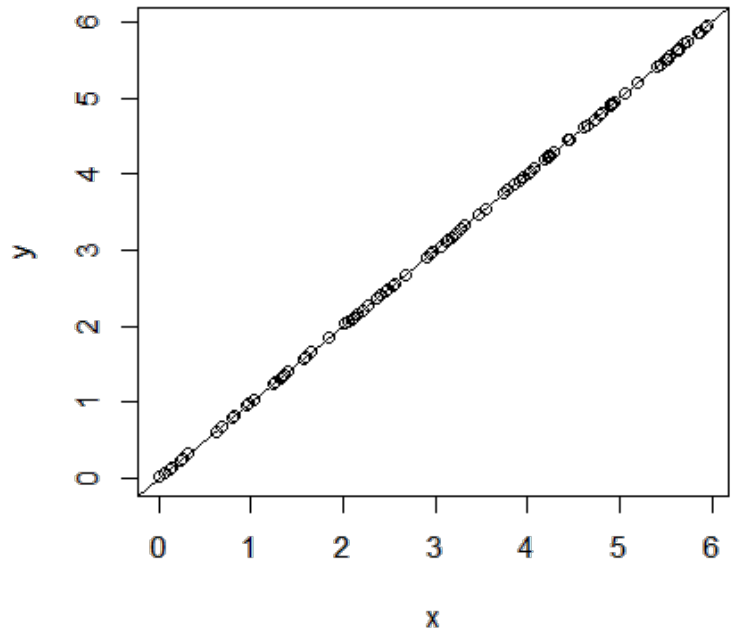


```
plot(x, resid(lm(y ~ x)));
abline(h = 0)
```



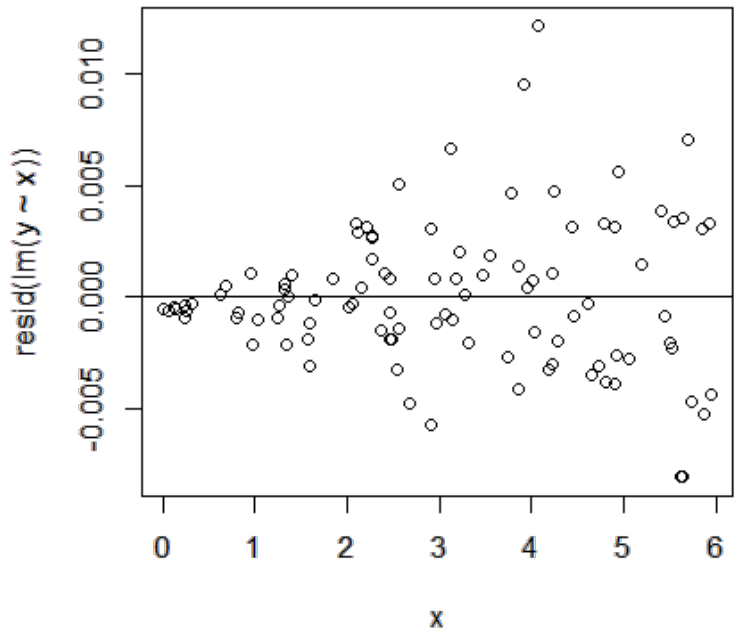
Heteroskedasticity

```
x <- runif(100, 0, 6); y <- x + rnorm(100,  mean = 0, sd = .001 * x);
plot(x, y); abline(lm(y ~ x))
```



Getting rid of the blank space can be helpful

```
plot(x, resid(lm(y ~ x)));
abline(h = 0)
```



Estimating residual variation

- Model $Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$ where $\epsilon_i \sim N(0, \sigma^2)$.
- The ML estimate of σ^2 is $\frac{1}{n}\sum_{i=1}^{n} e_i^2$, the average squared residual.
- Most people use

$$\hat{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n} e_i^2.$$

- The $n-2$ instead of n is so that $E[\hat{\sigma}^2] = \sigma^2$

Diamond example

```
y <- diamond$price; x <- diamond$carat; n <- length(y)
fit <- lm(y ~ x)
summary(fit)$sigma
```

```
[1] 31.84
```

```
sqrt(sum(resid(fit)^2) / (n - 2))
```

```
[1] 31.84
```

Summarizing variation

$$\sum_{i=1}^{n}(Y_i - \bar{Y})^2 = \sum_{i=1}^{n}(Y_i - \hat{Y}_i + \hat{Y}_i - \bar{Y})^2$$

$$= \sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 + 2\sum_{i=1}^{n}(Y_i - \hat{Y}_i)(\hat{Y}_i - \bar{Y}) + \sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2$$

Scratch work

$(Y_i - \hat{Y}_i) = \{Y_i - (\bar{Y} - \hat{\beta}_1\bar{X}) - \hat{\beta}_1 X_i\} = (Y_i - \bar{Y}) - \hat{\beta}_1(X_i - \bar{X})$

$(\hat{Y}_i - \bar{Y}) = (\bar{Y} - \hat{\beta}_1\bar{X} - \hat{\beta}_1 X_i - \bar{Y}) = \hat{\beta}_1(X_i - \bar{X})$

$\sum_{i=1}^{n}(Y_i - \hat{Y}_i)(\hat{Y}_i - \bar{Y}) = \sum_{i=1}^{n}\{(Y_i - \bar{Y}) - \hat{\beta}_1(X_i - \bar{X}))\}\{\hat{\beta}_1(X_i - \bar{X})\}$

$= \hat{\beta}_1 \sum_{i=1}^{n}(Y_i - \bar{Y})(X_i - \bar{X}) - \hat{\beta}_1^2 \sum_{i=1}^{n}(X_i - \bar{X})^2$

$= \hat{\beta}_1^2 \sum_{i=1}^{n}(X_i - \bar{X})^2 - \hat{\beta}_1^2 \sum_{i=1}^{n}(X_i - \bar{X})^2 = 0$

Summarizing variation

$$\sum_{i=1}^{n}(Y_i - \bar{Y})^2 = \sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 + \sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2$$

Or

Total Variation = Residual Variation + Regression Variation

Define the percent of total varation described by the model as

$$R^2 = \frac{\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}$$

Relation between R^2 and r (the correlation)

Recall that $(\hat{Y}_i - \bar{Y}) = \hat{\beta}_1(X_i - \bar{X})$ so that

$$R^2 = \frac{\sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} = \hat{\beta}_1^2 \frac{\sum_{i=1}^{n}(X_i - \bar{X})}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} = \text{Cor}(Y, X)^2$$

Since, recall,

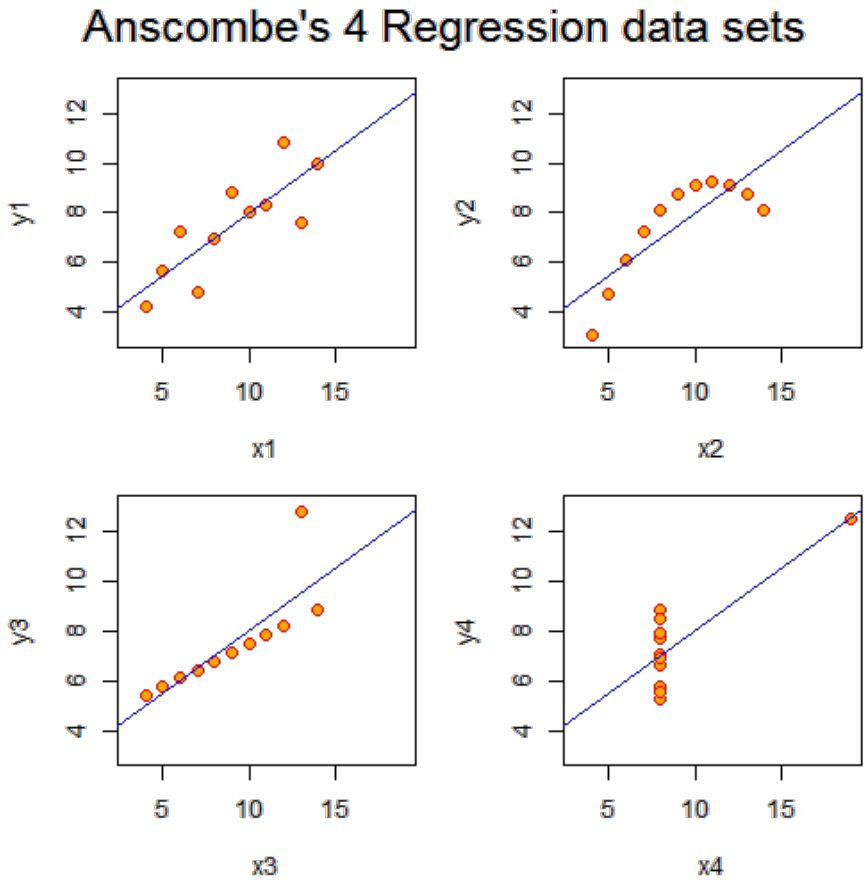
$$\hat{\beta}_1 = \text{Cor}(Y, X) \frac{\text{Sd}(Y)}{\text{Sd}(X)}$$

So, R^2 is literally r squared.

Some facts about R^2

- R^2 is the percentage of variation explained by the regression model.
- $0 \leq R^2 \leq 1$
- R^2 is the sample correlation squared.
- R^2 can be a misleading summary of model fit.
  - Deleting data can inflate R^2.
  - (For later.) Adding terms to a regression model always increases R^2.
- Do `example(anscombe)` to see the following data.
  - Basically same mean and variance of X and Y.
  - Identical correlations (hence same R^2).
  - Same linear regression relationship.

`data(anscombe);example(anscombe)`



Inference in regression

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Recall our model and fitted values

- Consider the model

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

- $\epsilon \sim N(0, \sigma^2)$.
- We assume that the true model is known.
- We assume that you've seen confidence intervals and hypothesis tests before.
- $\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{X}$
- $\hat{\beta}_1 = Cor(Y, X) \frac{Sd(Y)}{Sd(X)}$.

Review

- Statistics like $\frac{\hat{\theta}-\theta}{\hat{\sigma}_{\hat{\theta}}}$ often have the following properties.
  1. Is normally distributed and has a finite sample Student's T distribution if the estimated variance is replaced with a sample estimate (under normality assumptions).
  2. Can be used to test $H_0 : \theta = \theta_0$ versus $H_a : \theta >, <, \neq \theta_0$.
  3. Can be used to create a confidence interval for θ via $\hat{\theta} \pm Q_{1-\alpha/2}\hat{\sigma}_{\hat{\theta}}$ where $Q_{1-\alpha/2}$ is the relevant quantile from either a normal or T distribution.
- In the case of regression with iid sampling assumptions and normal errors, our inferences will follow very similarily to what you saw in your inference class.
- We won't cover asymptotics for regression analysis, but suffice it to say that under assumptions on the ways in which the X values are collected, the iid sampling model, and mean model, the normal results hold to create intervals and confidence intervals

Standard errors (conditioned on X)

$$
\begin{aligned}
\mathrm{Var}(\hat{\beta}_1) &= \mathrm{Var}\left(\frac{\sum_{i=1}^{n} (Y_i - \bar{Y})(X_i - \bar{X})}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right) \\
&= \frac{\mathrm{Var}\left(\sum_{i=1}^{n} Y_i (X_i - \bar{X}) \right)}{\left(\sum_{i=1}^{n} (X_i - \bar{X})^2 \right)^2} \\
&= \frac{\sum_{i=1}^{n} \sigma^2 (X_i - \bar{X})^2}{\left(\sum_{i=1}^{n} (X_i - \bar{X})^2 \right)^2} \\
&= \frac{\sigma^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2}
\end{aligned}
$$

Results

- $\sigma^2_{\hat{\beta}_1} = \mathrm{Var}(\hat{\beta}_1) = \sigma^2 / \sum_{i=1}^{n} (X_i - \bar{X})^2$
- $\sigma^2_{\hat{\beta}_0} = \mathrm{Var}(\hat{\beta}_0) = \left(\frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^{n} (X_i - \bar{X})^2} \right) \sigma^2$
- In practice, σ is replaced by its estimate.
- It's probably not surprising that under iid Gaussian errors

$$\frac{\hat{\beta}_j - \beta_j}{\hat{\sigma}_{\hat{\beta}_j}}$$

  follows a t distribution with $n - 2$ degrees of freedom and a normal distribution for large n.
- This can be used to create confidence intervals and perform hypothesis tests.

Example diamond data set

```
library(UsingR); data(diamond)
y <- diamond$price; x <- diamond$carat; n <- length(y)
beta1 <- cor(y, x) * sd(y) / sd(x)
beta0 <- mean(y) - beta1 * mean(x)
e <- y - beta0 - beta1 * x
sigma <- sqrt(sum(e^2) / (n-2))
ssx <- sum((x - mean(x))^2)
seBeta0 <- (1 / n + mean(x) ^ 2 / ssx) ^ .5 * sigma
seBeta1 <- sigma / sqrt(ssx)
tBeta0 <- beta0 / seBeta0; tBeta1 <- beta1 / seBeta1
pBeta0 <- 2 * pt(abs(tBeta0), df = n - 2, lower.tail = FALSE)
pBeta1 <- 2 * pt(abs(tBeta1), df = n - 2, lower.tail = FALSE)
coefTable <- rbind(c(beta0, seBeta0, tBeta0, pBeta0), c(beta1, seBeta1, tBeta1, pBeta1))
colnames(coefTable) <- c("Estimate", "Std. Error", "t value", "P(>|t|)")
rownames(coefTable) <- c("(Intercept)", "x")
```

Example continued

```
coefTable
```

```
            Estimate Std. Error t value   P(>|t|)
(Intercept)   -259.6      17.32  -14.99 2.523e-19
x             3721.0      81.79   45.50 6.751e-40
```

```
fit <- lm(y ~ x);
summary(fit)$coefficients
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept)   -259.6      17.32  -14.99 2.523e-19
x             3721.0      81.79   45.50 6.751e-40
```

Getting a confidence interval

```
sumCoef <- summary(fit)$coefficients
sumCoef[1,1] + c(-1, 1) * qt(.975, df = fit$df) * sumCoef[1, 2]
```

```
[1] -294.5 -224.8
```

```
sumCoef[2,1] + c(-1, 1) * qt(.975, df = fit$df) * sumCoef[2, 2]
```

```
[1] 3556 3886
```

With 95% confidence, we estimate that a 0.1 carat increase in diamond size results in a 355.6 to 388.6 increase in price in (Singapore) dollars.

Prediction of outcomes

- Consider predicting Y at a value of X
  - Predicting the price of a diamond given the carat
  - Predicting the height of a child given the height of the parents
- The obvious estimate for prediction at point x_0 is

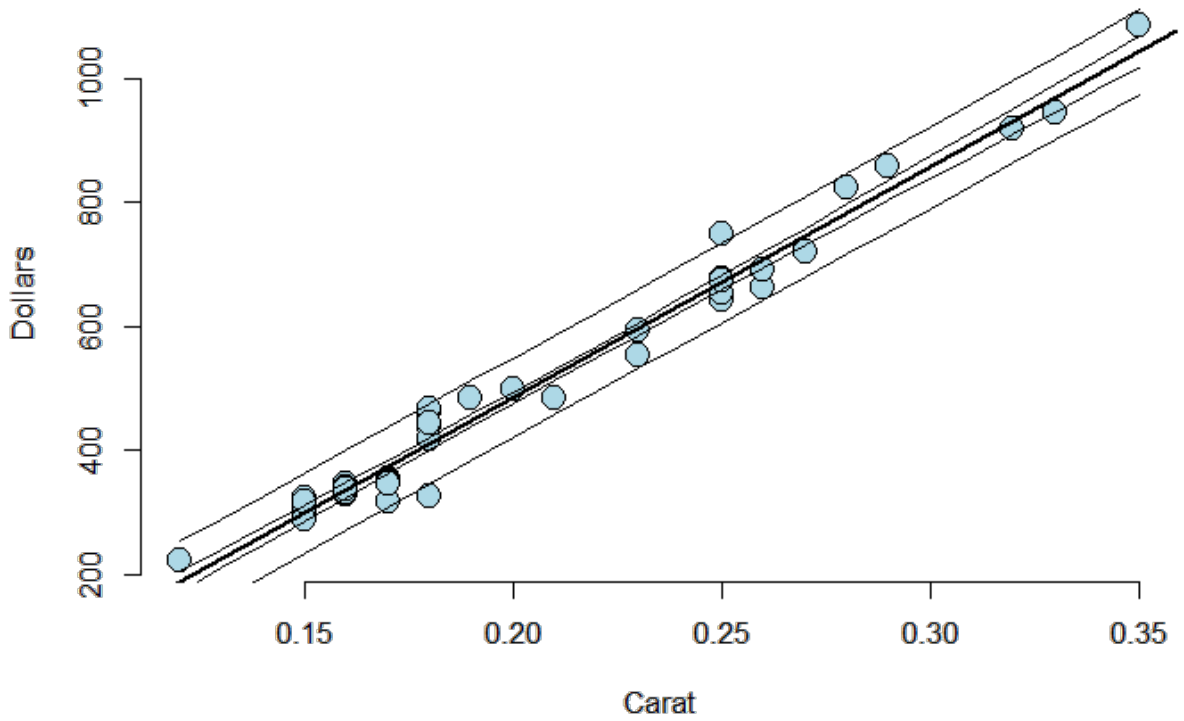
$$\hat{\beta}_0 + \hat{\beta}_1 x_0$$

- A standard error is needed to create a prediction interval.
- There's a distinction between intervals for the regression line at point x_0 and the prediction of what a y would be at point x_0.
- Line at x_0 se, $\hat{\sigma}\sqrt{\frac{1}{n} + \frac{(x_0 - \bar{X})^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}}$
- Prediction interval se at x_0, $\hat{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{X})^2}{\sum_{i=1}^{n}(X_i - \bar{X})^2}}$

Plotting the prediction intervals

```
plot(x, y, frame=FALSE,xlab="Carat",ylab="Dollars",pch=21,col="black", bg="lightblue", cex=2)
abline(fit, lwd = 2)
xVals <- seq(min(x), max(x), by = .01)
yVals <- beta0 + beta1 * xVals
se1 <- sigma * sqrt(1 / n + (xVals - mean(x))^2/ssx)
se2 <- sigma * sqrt(1 + 1 / n + (xVals - mean(x))^2/ssx)
lines(xVals, yVals + 2 * se1)
lines(xVals, yVals - 2 * se1)
lines(xVals, yVals + 2 * se2)
lines(xVals, yVals - 2 * se2)
```

Plotting the prediction intervals



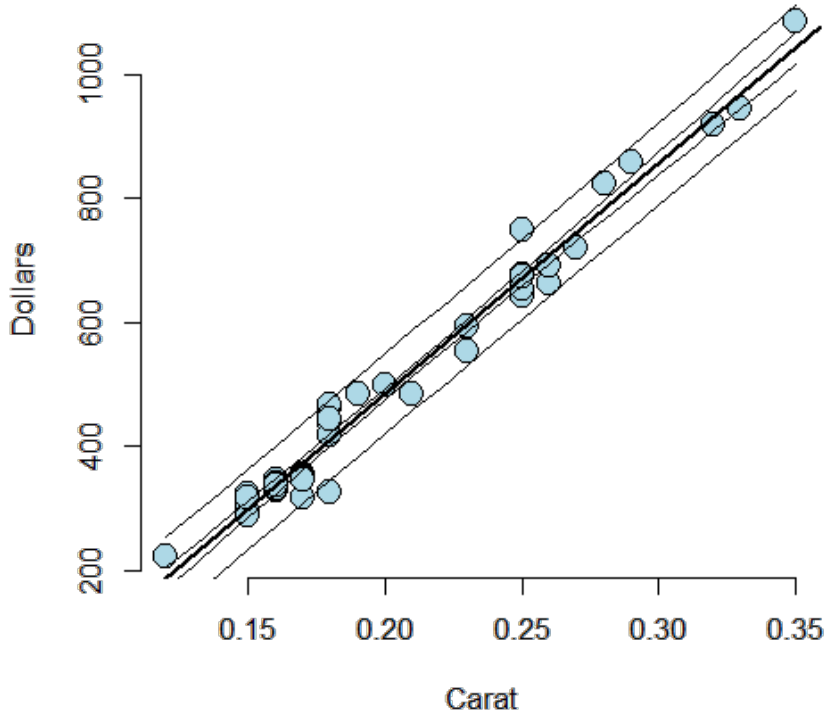
Discussion

- Both intervals have varying widths.
  - Least width at the mean of the Xs.
- We are quite confident in the regression line, so that interval is very narrow.
  - If we knew β_0 and β_1 this interval would have zero width.
- The prediction interval must incorporate the variabilibity in the data around the line.
  - Even if we knew β_0 and β_1 this interval would still have width.

In R

```
newdata <- data.frame(x = xVals)
p1 <- predict(fit, newdata, interval = ("confidence"))
p2 <- predict(fit, newdata, interval = ("prediction"))
plot(x, y, frame=FALSE,xlab="Carat",ylab="Dollars",pch=21,col="black", bg="lightblue", cex=2)
abline(fit, lwd = 2)
lines(xVals, p1[,2]); lines(xVals, p1[,3])
lines(xVals, p2[,2]); lines(xVals, p2[,3])
```

In R



Multivariable regression

Brian Caffo, Roger Peng and Jeff Leek
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Multivariable regression analyses

- If I were to present evidence of a relationship between breath mint useage (mints per day, X) and pulmonary function (measured in FEV), you would be skeptical.
  - Likely, you would say, 'smokers tend to use more breath mints than non smokers, smoking is related to a loss in pulmonary function. That's probably the culprit.'
  - If asked what would convince you, you would likely say, 'If non-smoking breath mint users had lower lung function than non-smoking non-breath mint users and, similarly, if smoking breath mint users had lower lung function than smoking non-breath mint users, I'd be more inclined to believe you'.
- In other words, to even consider my results, I would have to demonstrate that they hold while holding smoking status fixed.

Multivariable regression analyses

- An insurance company is interested in how last year's claims can predict a person's time in the hospital this year.
  - They want to use an enormous amount of data contained in claims to predict a single number. Simple linear regression is not equipped to handle more than one predictor.
- How can one generalize SLR to incoporate lots of regressors for the purpose of prediction?
- What are the consequences of adding lots of regressors?
  - Surely there must be consequences to throwing variables in that aren't related to Y?
  - Surely there must be consequences to omitting variables that are?

The linear model

- The general linear model extends simple linear regression (SLR) by adding terms linearly into the model.

$$Y_i = \beta_1 X_{1i} + \beta_2 X_{2i} + \ldots + \beta_p X_{pi} + \epsilon_i = \sum_{k=1}^{p} X_{ik}\beta_j + \epsilon_i$$

- Here $X_{1i} = 1$ typically, so that an intercept is included.
- Least squares (and hence ML estimates under iid Gaussianity of the errors) minimizes

$$\sum_{i=1}^{n} \left(Y_i - \sum_{k=1}^{p} X_{ki}\beta_j \right)^2$$

- Note, the important linearity is linearity in the coefficients. Thus

$$Y_i = \beta_1 X_{1i}^2 + \beta_2 X_{2i}^2 + \ldots + \beta_p X_{pi}^2 + \epsilon_i$$

  is still a linear model. (We've just squared the elements of the predictor variables.)

How to get estimates

- The real way requires linear algebra. We'll go over an intuitive development instead.
- Recall that the LS estimate for regression through the origin, $E[Y_i] = X_{1i}\beta_1$, was $\sum X_i Y_i / \sum X_i^2$.
- Let's consider two regressors, $E[Y_i] = X_{1i}\beta_1 + X_{2i}\beta_2 = \mu_i$.
- Also, recall, that if $\hat{\mu}_i$ satisfies

$$\sum_{i=1}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = 0$$

for all possible values of μ_i, then we've found the LS estimates.

$$\sum_{i=1}^{n}(Y_i - \hat{\mu}_i)(\hat{\mu}_i - \mu_i) = \sum_{i=1}^{n}(Y_i - \hat{\beta}_1 X_{1i} - \hat{\beta}_2 X_{2i})\Big\{X_{1i}(\hat{\beta}_1 - \beta_1) + X_{2i}(\hat{\beta}_2 - \beta_2)\Big\}$$

- Thus we need
  1. $\sum_{i=1}^{n}(Y_i - \hat{\beta}_1 X_{1i} - \hat{\beta}_2 X_{2i})X_{1i} = 0$
  2. $\sum_{i=1}^{n}(Y_i - \hat{\beta}_1 X_{1i} - \hat{\beta}_2 X_{2i})X_{2i} = 0$
- Hold $\hat{\beta}_1$ fixed in 2. and solve and we get that

$$\hat{\beta}_2 = \frac{\sum_{i=1}(Y_i - X_{1i}\hat{\beta}_1)X_{2i}}{\sum_{i=1}^{n} X_{2i}^2}$$

- Plugging this into 1. we get that

$$0 = \sum_{i=1}^{n}\left\{Y_i - \frac{\sum_j X_{2j}Y_j}{\sum_j X_{2j}^2}\,X_{2i} + \beta_1\left(X_{1i} - \frac{\sum_j X_{2j}X_{1j}}{\sum_j X_{2j}^2}\,X_{2i}\right)\right\}X_{1i}$$

Continued

- Re writing this we get

$$0 = \sum_{i=1}^{n} \left\{ e_{i,Y|X_2} - \hat{\beta}_1 e_{i,X_1|X_2} \right\} X_{1i}$$

  where $e_{i,a|b} = a_i - \frac{\sum_{j=1}^{n} a_j b_j}{\sum_{i=1}^{n} b_j^2} b_i$ is the residual when regressing b from a without an intercept.

- We get the solution

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} e_{i,Y|X_2} e_{i,X_1|X_2}}{\sum_{i=1}^{n} e_{i,X_1|X_2} X_1}$$

- But note that

$$\sum_{i=1}^{n} e_{i,X_1|X_2}^2 = \sum_{i=1}^{n} e_{i,X_1|X_2} \left(X_{1i} - \frac{\sum_j X_{2j} X_{1j}}{\sum_j X_{2j}^2} X_{2i} \right)$$

$$= \sum_{i=1}^{n} e_{i,X_1|X_2} X_{1i} - \frac{\sum_j X_{2j} X_{1j}}{\sum_j X_{2j}^2} \sum_{i=1}^{n} e_{i,X_1|X_2} X_{2i}$$

But $\sum_{i=1}^{n} e_{i,X_1|X_2} X_{2i} = 0$. So we get that

$$\sum_{i=1}^{n} e_{i,X_1|X_2}^2 = \sum_{i=1}^{n} e_{i,X_1|X_2} X_{1i}$$

Thus we get that

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} e_{i,Y|X_2} e_{i,X_1|X_2}}{\sum_{i=1}^{n} e_{i,X_1|X_2}^2}$$

Summing up fitting with two regressors

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} e_{i,Y|X_2} e_{i,X_1|X_2}}{\sum_{i=1}^{n} e_{i,X_1|X_2}^2}$$

- That is, the regression estimate for β_1 is the regression through the origin estimate having regressed X_2 out of both the response and the predictor.
- (Similarly, the regression estimate for β_2 is the regression through the origin estimate having regressed X_1 out of both the response and the predictor.)
- More generally, multivariate regression estimates are exactly those having removed the linear relationship of the other variables from both the regressor and response.

Example with two variables, simple linear regression

- $Y_i = \beta_1 X_{1i} + \beta_2 X_{2i}$ where $X_{2i} = 1$ is an intercept term.
- Then $\frac{\sum_j X_{2j} X_{1j}}{\sum_j X_{2j}^2} X_{2i} = \frac{\sum_j X_{1j}}{n} = \bar{X}_1$.
- $e_{i,X_1|X_2} = X_{1i} - \bar{X}_1$.
- Simiarly $e_{i,Y|X_2} = Y_i - \bar{Y}$.
- Thus

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n e_{i,Y|X_2} e_{i,X_1|X_2}}{\sum_{i=1}^n e_{i,X_1|X_2}^2} = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sum_{i=1}^n (X_i - \bar{X})^2} = Cor(X,Y) \frac{Sd(Y)}{Sd(X)}$$

The general case

- The equations

$$\sum_{i=1}^{n}(Y_i - X_{1i}\hat{\beta}_1 - \ldots - X_{ip}\hat{\beta}_p)X_k = 0$$

  for $k = 1, \ldots, p$ yields p equations with p unknowns.

- Solving them yields the least squares estimates. (With obtaining a good, fast, general solution requiring some knowledge of linear algebra.)
- The least squares estimate for the coefficient of a multivariate regression model is exactly regression through the origin with the linear relationships with the other regressors removed from both the regressor and outcome by taking residuals.
- In this sense, multivariate regression "adjusts" a coefficient for the linear impact of the other variables.

Fitting LS equations

Just so I don't leave you hanging, let's show a way to get estimates. Recall the equations:

$$\sum_{i=1}^{n}(Y_i - X_{1i}\hat{\beta}_1 - \ldots - X_{ip}\hat{\beta}_p)X_k = 0$$

If I hold $\hat{\beta}_1, \ldots, \hat{\beta}_{p-1}$ fixed then we get that

$$\hat{\beta}_p = \frac{\sum_{i=1}^{n}(Y_i - X_{1i}\hat{\beta}_1 - \ldots - X_{i,p-1}\hat{\beta}_{p-1})X_{ip}}{\sum_{i=1}^{n} X_{ip}^2}$$

Plugging this back into the equations, we wind up with

$$\sum_{i=1}^{n}(e_{i,Y|X_p} - e_{i,X_1|X_p}\hat{\beta}_1 - \ldots - e_{i,X_{p-1}|X_p}\hat{\beta}_{p-1})X_k = 0$$

We can tidy it up a bit more, though

Note that

$$X_k = e_{i,X_k|X_p} + \frac{\sum_{i=1}^n X_{ik}X_{ip}}{\sum_{i=1}^n X_{ip^2}} X_p$$

and $\sum_{i=1}^n e_{i,X_j|X_p} X_{ip} = 0$. Thus

$$\sum_{i=1}^n (e_{i,Y|X_p} - e_{i,X_1|X_p}\hat{\beta}_1 - \ldots - e_{i,X_{p-1}|X_p}\hat{\beta}_{p-1})X_k = 0$$

is equal to

$$\sum_{i=1}^n (e_{i,Y|X_p} - e_{i,X_1|X_p}\hat{\beta}_1 - \ldots - e_{i,X_{p-1}|X_p}\hat{\beta}_{p-1})e_{i,X_k|X_p} = 0$$

To sum up

- We've reduced p LS equations and p unknowns to $p-1$ LS equations and $p-1$ unknowns.
  - Every variable has been replaced by its residual with X_p.
  - This process can then be iterated until only Y and one variable remains.
- Think of it as follows. If we want an adjusted relationship between y and x, keep taking residuals over confounders and do regression through the origin.
  - The order that you do the confounders doesn't matter.
  - (It can't because our choice of doing p first was arbitrary.)
- This isn't a terribly efficient way to get estimates. But, it's nice conceputally, as it shows how regression estimates are adjusted for the linear relationship with other variables.

Demonstration that it works using an example

Linear model with two variables and an intercept

```
n <- 100; x <- rnorm(n); x2 <- rnorm(n); x3 <- rnorm(n)
y <- x + x2 + x3 + rnorm(n, sd = .1)
e <- function(a, b) a -  sum( a * b ) / sum( b ^ 2) * b
ey <- e(e(y, x2), e(x3, x2))
ex <- e(e(x, x2), e(x3, x2))
sum(ey * ex) / sum(ex ^ 2)
```

```
[1] 1.004
```

```
coef(lm(y ~ x + x2 + x3 - 1)) #the -1 removes the intercept term
```

```
     x     x2     x3
1.0040 0.9899 1.0078
```

Showing that order doesn't matter

```
ey <- e(e(y, x3), e(x2, x3))
ex <- e(e(x, x3), e(x2, x3))
sum(ey * ex) / sum(ex ^ 2)
```

```
[1] 1.004
```

```
coef(lm(y ~ x + x2 + x3 - 1)) #the -1 removes the intercept term
```

```
     x     x2     x3
1.0040 0.9899 1.0078
```

Residuals again

```
ey <- resid(lm(y ~ x2 + x3 - 1))
ex <- resid(lm(x ~ x2 + x3 - 1))
sum(ey * ex) / sum(ex ^ 2)
```

```
[1] 1.004
```

```
coef(lm(y ~ x + x2 + x3 - 1)) #the -1 removes the intercept term
```

```
     x     x2     x3
1.0040 0.9899 1.0078
```

Interpretation of the coeficient

$$E[Y|X_1 = x_1, \ldots, X_p = x_p] = \sum_{k=1}^{p} x_k \beta_k$$

So that

$$E[Y|X_1 = x_1 + 1, \ldots, X_p = x_p] - E[Y|X_1 = x_1, \ldots, X_p = x_p]$$

$$= (x_1 + 1)\beta_1 + \sum_{k=2}^{p} x_k + \sum_{k=1}^{p} x_k \beta_k = \beta_1$$

So that the interpretation of a multivariate regression coefficient is the expected change in the response per unit change in the regressor, holding all of the other regressors fixed.

In the next lecture, we'll do examples and go over context-specific interpretations.

Fitted values, residuals and residual variation

All of our SLR quantities can be extended to linear models

- Model $Y_i = \sum_{k=1}^{p} X_{ik}\beta_k + \epsilon_i$ where $\epsilon_i \sim N(0, \sigma^2)$
- Fitted responses $\hat{Y}_i = \sum_{k=1}^{p} X_{ik}\hat{\beta}_k$
- Residuals $e_i = Y_i - \hat{Y}_i$
- Variance estimate $\hat{\sigma}^2 = \frac{1}{n-p}\sum_{i=1}^{n} e_i^2$
- To get predicted responses at new values, $x_1, \ldots, x_p$, simply plug them into the linear model $\sum_{k=1}^{p} x_k\hat{\beta}_k$
- Coefficients have standard errors, $\hat{\sigma}_{\hat{\beta}_k}$, and $\frac{\hat{\beta}_k - \beta_k}{\hat{\sigma}_{\hat{\beta}_k}}$ follows a T distribution with $n-p$ degrees of freedom.
- Predicted responses have standard errors and we can calculate predicted and expected response intervals.

Linear models

- Linear models are the single most important applied statistical and machine learning techniqe, *by far*.
- Some amazing things that you can accomplish with linear models
  - Decompose a signal into its harmonics.
  - Flexibly fit complicated functions.
  - Fit factor variables as predictors.
  - Uncover complex multivariate relationships with the response.
  - Build accurate prediction models.

Multivariable regression examples

Regression Models

Brian Caffo, Jeff Leek and Roger Peng
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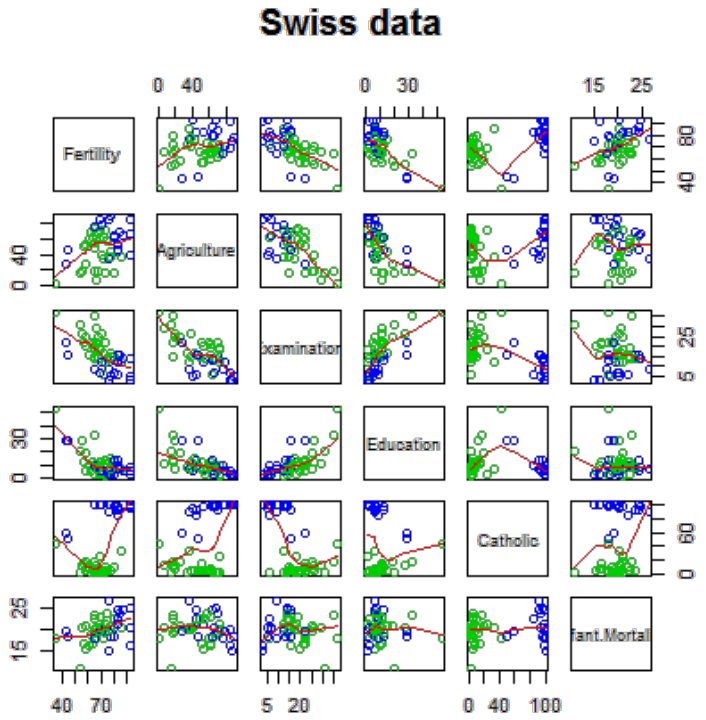
Swiss fertility data

```
library(datasets); data(swiss); require(stats); require(graphics)
pairs(swiss, panel = panel.smooth, main = "Swiss data", col = 3 + (swiss$Catholic > 50))
```



?swiss

Description

Standardized fertility measure and socio-economic indicators for each of 47 French-speaking provinces of Switzerland at about 1888.

A data frame with 47 observations on 6 variables, each of which is in percent, i.e., in [0, 100].

- [,1] Fertility Ig, ‘ common standardized fertility measure’
- [,2] Agriculture % of males involved in agriculture as occupation
- [,3] Examination % draftees receiving highest mark on army examination
- [,4] Education % education beyond primary school for draftees.
- [,5] Catholic % ‘catholic’ (as opposed to ‘protestant’).
- [,6] Infant.Mortality live births who live less than 1 year.

All variables but ‘Fertility’ give proportions of the population.

Calling `lm`

```
summary(lm(Fertility ~ . , data = swiss))
```

```
                 Estimate Std. Error t value  Pr(>|t|)
(Intercept)       66.9152   10.70604   6.250 1.906e-07
Agriculture       -0.1721    0.07030  -2.448 1.873e-02
Examination       -0.2580    0.25388  -1.016 3.155e-01
Education         -0.8709    0.18303  -4.758 2.431e-05
Catholic           0.1041    0.03526   2.953 5.190e-03
Infant.Mortality   1.0770    0.38172   2.822 7.336e-03
```

Example interpretation

- Agriculture is expressed in percentages (0 - 100)
- Estimate is -0.1721.
- We estimate an expected 0.17 decrease in standardized fertility for every 1\% increase in percentage of males involved in agriculture in holding the remaining variables constant.
- The t-test for $H_0 : \beta_{Agri} = 0$ versus $H_a : \beta_{Agri} \neq 0$ is significant.
- Interestingly, the unadjusted estimate is

```
summary(lm(Fertility ~ Agriculture, data = swiss))$coefficients
```

```
             Estimate Std. Error t value  Pr(>|t|)
(Intercept)  60.3044    4.25126  14.185 3.216e-18
Agriculture   0.1942    0.07671   2.532 1.492e-02
```

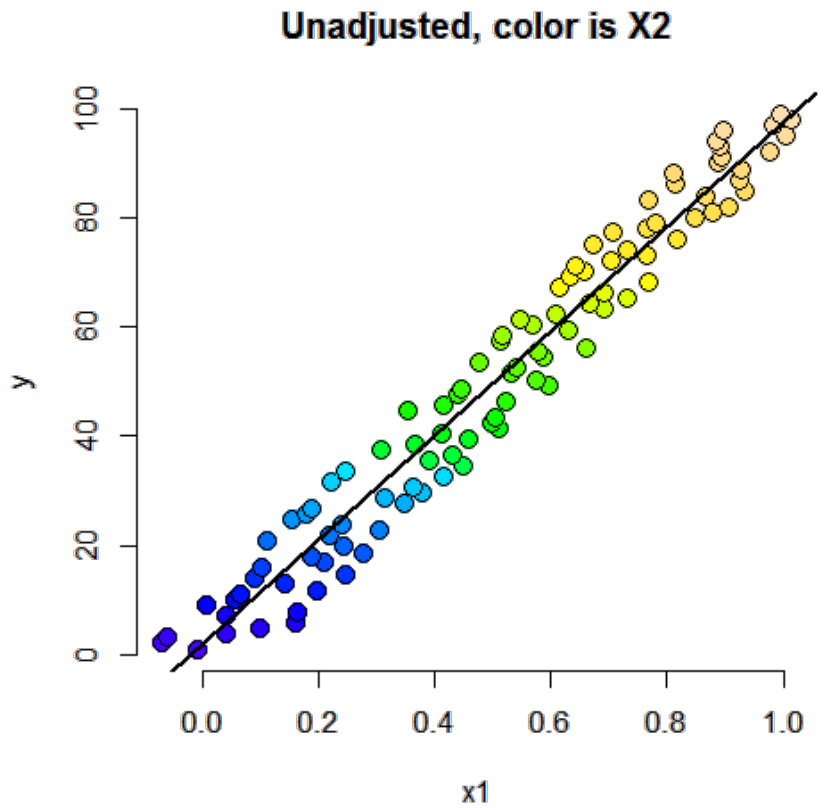
How can adjustment reverse the sign of an effect? Let's try a simulation.

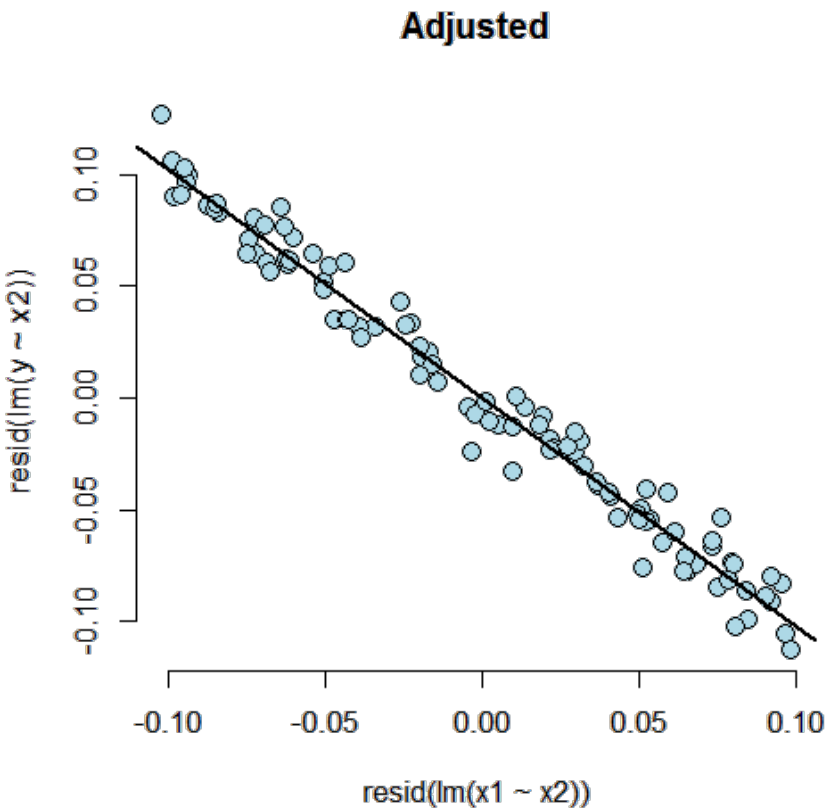
```
n <- 100; x2 <- 1 : n; x1 <- .01 * x2 + runif(n, -.1, .1); y = -x1 + x2 + rnorm(n, sd = .01)
summary(lm(y ~ x1))$coef
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept)    1.618      1.200   1.349 1.806e-01
x1            95.854      2.058  46.579 1.153e-68
```

```
summary(lm(y ~ x1 + x2))$coef
```

```
              Estimate Std. Error   t value   Pr(>|t|)
(Intercept)  0.0003683  0.0020141    0.1829  8.553e-01
x1          -1.0215256  0.0166372  -61.4001  1.922e-79
x2           1.0001909  0.0001681 5950.1818 1.369e-271
```


Unadjusted, color is X2
y
x1
0
20
40
60
80
100
0.0
0.2
0.4
0.6
0.8
1.0


Adjusted
resid(lm(y ~ x2))
resid(lm(x1 ~ x2))
-0.10
-0.05
0.00
0.05
0.10

Back to this data set

- The sign reverses itself with the inclusion of Examination and Education, but of which are negatively correlated with Agriculture.
- The percent of males in the province working in agriculture is negatively related to educational attainment (correlation of -0.6395) and Education and Examination (correlation of 0.6984) are obviously measuring similar things.
    - Is the positive marginal an artifact for not having accounted for, say, Education level? (Education does have a stronger effect, by the way.)
- At the minimum, anyone claiming that provinces that are more agricultural have higher fertility rates would immediately be open to criticism.

What if we include an unnecessary variable?

z adds no new linear information, since it's a linear combination of variables already included. R just drops terms that are linear combinations of other terms.

```
z <- swiss$Agriculture + swiss$Education
lm(Fertility ~ . + z, data = swiss)
```

```

Call:
lm(formula = Fertility ~ . + z, data = swiss)

Coefficients:
     (Intercept)       Agriculture       Examination         Education          Catholic
          66.915            -0.172            -0.258            -0.871             0.104
Infant.Mortality                 z
           1.077                NA
```

Dummy variables are smart

- Consider the linear model

$$Y_i = \beta_0 + X_{i1}\beta_1 + \epsilon_i$$

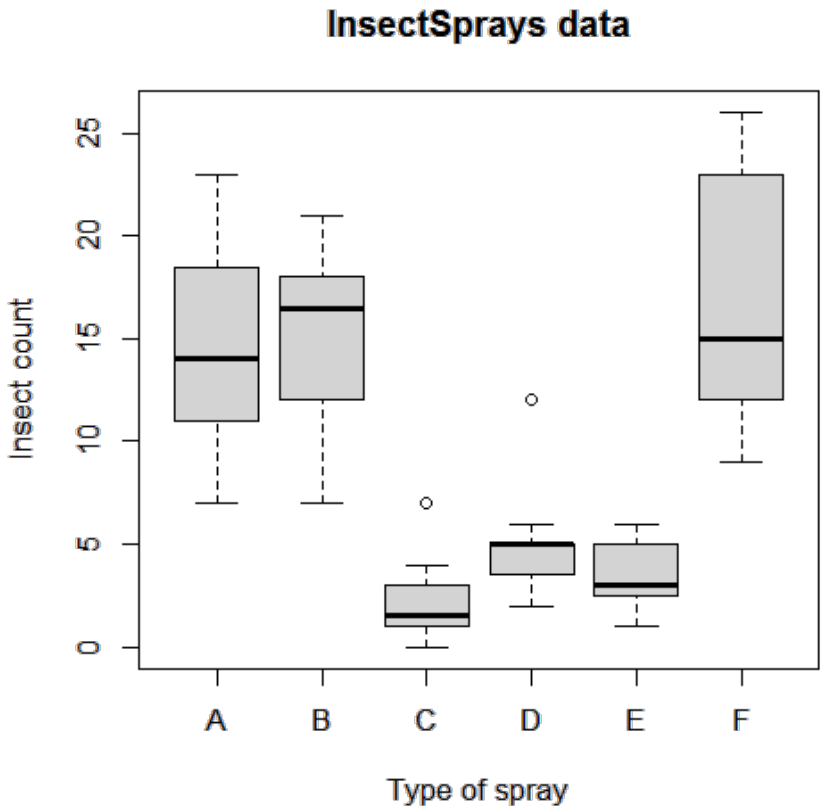
  where each X_{i1} is binary so that it is a 1 if measurement i is in a group and 0 otherwise. (Treated versus not in a clinical trial, for example.)

- Then for people in the group $E[Y_i] = \beta_0 + \beta_1$
- And for people not in the group $E[Y_i] = \beta_0$
- The LS fits work out to be $\hat{\beta}_0 + \hat{\beta}_1$ is the mean for those in the group and $\hat{\beta}_0$ is the mean for those not in the group.
- β_1 is interpretted as the increase or decrease in the mean comparing those in the group to those not.
- Note including a binary variable that is 1 for those not in the group would be redundant. It would create three parameters to describe two means.

More than 2 levels

- Consider a multilevel factor level. For didactic reasons, let's say a three level factor (example, US political party affiliation: Republican, Democrat, Independent)
- $Y_i = \beta_0 + X_{i1}\beta_1 + X_{i2}\beta_2 + \epsilon_i$.
- X_{i1} is 1 for Republicans and 0 otherwise.
- X_{i2} is 1 for Democrats and 0 otherwise.
- If i is Republican $E[Y_i] = \beta_0 + \beta_1$
- If i is Democrat $E[Y_i] = \beta_0 + \beta_2$.
- If i is Independent $E[Y_i] = \beta_0$.
- β_1 compares Republicans to Independents.
- β_2 compares Democrats to Independents.
- $\beta_1 - \beta_2$ compares Republicans to Democrats.
- (Choice of reference category changes the interpretation.)

Insect Sprays



Linear model fit, group A is the reference

```
summary(lm(count ~ spray, data = InsectSprays))$coef
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept)  14.5000      1.132 12.8074 1.471e-19
sprayB        0.8333      1.601  0.5205 6.045e-01
sprayC      -12.4167      1.601 -7.7550 7.267e-11
sprayD       -9.5833      1.601 -5.9854 9.817e-08
sprayE      -11.0000      1.601 -6.8702 2.754e-09
sprayF        2.1667      1.601  1.3532 1.806e-01
```

Hard coding the dummy variables

```
summary(lm(count ~
            I(1 * (spray == 'B')) + I(1 * (spray == 'C')) +
            I(1 * (spray == 'D')) + I(1 * (spray == 'E')) +
            I(1 * (spray == 'F'))
          , data = InsectSprays))$coef
```

```
                    Estimate Std. Error t value  Pr(>|t|)
(Intercept)          14.5000      1.132 12.8074 1.471e-19
I(1 * (spray == "B"))  0.8333      1.601  0.5205 6.045e-01
I(1 * (spray == "C")) -12.4167      1.601 -7.7550 7.267e-11
I(1 * (spray == "D"))  -9.5833      1.601 -5.9854 9.817e-08
I(1 * (spray == "E")) -11.0000      1.601 -6.8702 2.754e-09
I(1 * (spray == "F"))   2.1667      1.601  1.3532 1.806e-01
```

What if we include all 6?

```
lm(count ~
   I(1 * (spray == 'B')) + I(1 * (spray == 'C')) +
   I(1 * (spray == 'D')) + I(1 * (spray == 'E')) +
   I(1 * (spray == 'F')) + I(1 * (spray == 'A')), data = InsectSprays)
```

```
Call:
lm(formula = count ~ I(1 * (spray == "B")) + I(1 * (spray ==
    "C")) + I(1 * (spray == "D")) + I(1 * (spray == "E")) + I(1 *
    (spray == "F")) + I(1 * (spray == "A")), data = InsectSprays)

Coefficients:
          (Intercept)  I(1 * (spray == "B"))  I(1 * (spray == "C"))  I(1 * (spray == "D"))
               14.500                 0.833                -12.417                -9.583
I(1 * (spray == "E"))  I(1 * (spray == "F"))  I(1 * (spray == "A"))
              -11.000                 2.167                     NA
```

What if we omit the intercept?

```
summary(lm(count ~ spray - 1, data = InsectSprays))$coef
```

```
       Estimate Std. Error t value  Pr(>|t|)
sprayA   14.500      1.132  12.807 1.471e-19
sprayB   15.333      1.132  13.543 1.002e-20
sprayC    2.083      1.132   1.840 7.024e-02
sprayD    4.917      1.132   4.343 4.953e-05
sprayE    3.500      1.132   3.091 2.917e-03
sprayF   16.667      1.132  14.721 1.573e-22
```

```
unique(ave(InsectSprays$count, InsectSprays$spray))
```

```
[1] 14.500 15.333  2.083  4.917  3.500 16.667
```

Summary

- If we treat Spray as a factor, R includes an intercept and omits the alphabetically first level of the factor.
  - All t-tests are for comparisons of Sprays versus Spray A.
  - Emprirical mean for A is the intercept.
  - Other group means are the itc plus their coefficient.
- If we omit an intercept, then it includes terms for all levels of the factor.
  - Group means are the coefficients.
  - Tests are tests of whether the groups are different than zero. (Are the expected counts zero for that spray.)
- If we want comparisons between, Spray B and C, say we could refit the model with C (or B) as the reference level.

Reordering the levels

```
spray2 <- relevel(InsectSprays$spray, "C")
summary(lm(count ~ spray2, data = InsectSprays))$coef
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept)    2.083      1.132  1.8401 7.024e-02
spray2A       12.417      1.601  7.7550 7.267e-11
spray2B       13.250      1.601  8.2755 8.510e-12
spray2D        2.833      1.601  1.7696 8.141e-02
spray2E        1.417      1.601  0.8848 3.795e-01
spray2F       14.583      1.601  9.1083 2.794e-13
```

Doing it manually

Equivalently

$$\text{Var}(\hat{\beta}_B - \hat{\beta}_C) = \text{Var}(\hat{\beta}_B) + \text{Var}(\hat{\beta}_C) - 2\text{Cov}(\hat{\beta}_B, \hat{\beta}_C)$$

```
fit <- lm(count ~ spray, data = InsectSprays) #A is ref
bbmbc <- coef(fit)[2] - coef(fit)[3] #B - C
temp <- summary(fit)
se <- temp$sigma * sqrt(temp$cov.unscaled[2, 2] + temp$cov.unscaled[3,3] - 2 *temp$cov.unscaled[2,3])
t <- (bbmbc) / se
p <- pt(-abs(t), df = fit$df)
out <- c(bbmbc, se, t, p)
names(out) <- c("B - C", "SE", "T", "P")
round(out, 3)
```

```
 B - C     SE      T      P
13.250  1.601  8.276  0.000
```

Other thoughts on this data

- Counts are bounded from below by 0, violates the assumption of normality of the errors.
    - Also there are counts near zero, so both the actual assumption and the intent of the assumption are violated.
- Variance does not appear to be constant.
- Perhaps taking logs of the counts would help.
    - There are 0 counts, so maybe log(Count + 1)
- Also, we'll cover Poisson GLMs for fitting count data.

Example - Millenium Development Goal 1

http://www.un.org/millenniumgoals/pdf/MDG_FS_1_EN.pdf

http://apps.who.int/gho/athena/data/GHO/WHOSIS_000008.csv?profile=text&filter=COUNTRY:;*SEX:*

WHO childhood hunger data

```
#download.file("http://apps.who.int/gho/athena/data/GHO/WHOSIS_000008.csv?profile=text&filter=COUNTRY:*
hunger <- read.csv("hunger.csv")
hunger <- hunger[hunger$Sex!="Both sexes",]
head(hunger)
```

```
                              Indicator Data.Source PUBLISH.STATES Year           WHO.region
1 Children aged <5 years underweight (%) NLIS_310044      Published 1986               Africa
2 Children aged <5 years underweight (%) NLIS_310233      Published 1990             Americas
3 Children aged <5 years underweight (%) NLIS_312902      Published 2005             Americas
5 Children aged <5 years underweight (%) NLIS_312522      Published 2002 Eastern Mediterranean
6 Children aged <5 years underweight (%) NLIS_312955      Published 2008               Africa
8 Children aged <5 years underweight (%) NLIS_312963      Published 2008               Africa
        Country    Sex Display.Value Numeric Low High Comments
1       Senegal   Male          19.3    19.3  NA   NA       NA
2      Paraguay   Male           2.2     2.2  NA   NA       NA
3     Nicaragua   Male           5.3     5.3  NA   NA       NA
5        Jordan Female           3.2     3.2  NA   NA       NA
6 Guinea-Bissau Female          17.0    17.0  NA   NA       NA
8         Ghana   Male          15.7    15.7  NA   NA       NA
```

Plot percent hungry versus time

```
lm1 <- lm(hunger$Numeric ~ hunger$Year)
plot(hunger$Year,hunger$Numeric,pch=19,col="blue")
```

Remember the linear model

$$Hu_i = b_0 + b_1 Y_i + e_i$$

b_0 = percent hungry at Year 0

b_1 = decrease in percent hungry per year

e_i = everything we didn't measure

Add the linear model

```
lm1 <- lm(hunger$Numeric ~ hunger$Year)
plot(hunger$Year,hunger$Numeric,pch=19,col="blue")
lines(hunger$Year,lm1$fitted,lwd=3,col="darkgrey")
```

Color by male/female

```
plot(hunger$Year,hunger$Numeric,pch=19)
points(hunger$Year,hunger$Numeric,pch=19,col=((hunger$Sex=="Male")*1+1))
```

Now two lines

$$HuF_i = bf_0 + bf_1 YF_i + ef_i$$

bf_0 = percent of girls hungry at Year 0

bf_1 = decrease in percent of girls hungry per year

ef_i = everything we didn't measure

$$HuM_i = bm_0 + bm_1 YM_i + em_i$$

bm_0 = percent of boys hungry at Year 0

bm_1 = decrease in percent of boys hungry per year

em_i = everything we didn't measure

Color by male/female

```
lmM <- lm(hunger$Numeric[hunger$Sex=="Male"] ~ hunger$Year[hunger$Sex=="Male"])
lmF <- lm(hunger$Numeric[hunger$Sex=="Female"] ~ hunger$Year[hunger$Sex=="Female"])
plot(hunger$Year,hunger$Numeric,pch=19)
points(hunger$Year,hunger$Numeric,pch=19,col=((hunger$Sex=="Male")*1+1))
lines(hunger$Year[hunger$Sex=="Male"],lmM$fitted,col="black",lwd=3)
lines(hunger$Year[hunger$Sex=="Female"],lmF$fitted,col="red",lwd=3)
```

Two lines, same slope

$$Hu_i = b_0 + b_1 \mathbb{1}(Sex_i = \text{" Male "}) + b_2 Y_i + e_i^*$$

b_0 - percent hungry at year zero for females

$b_0 + b_1$ - percent hungry at year zero for males

b_2 - change in percent hungry (for either males or females) in one year

e_i^* - everything we didn't measure

Two lines, same slope in R

```
lmBoth <- lm(hunger$Numeric ~ hunger$Year + hunger$Sex)
plot(hunger$Year,hunger$Numeric,pch=19)
points(hunger$Year,hunger$Numeric,pch=19,col=((hunger$Sex=="Male")*1+1))
abline(c(lmBoth$coeff[1],lmBoth$coeff[2]),col="red",lwd=3)
abline(c(lmBoth$coeff[1] + lmBoth$coeff[3],lmBoth$coeff[2] ),col="black",lwd=3)
```

Two lines, different slopes (interactions)

$$Hu_i = b_0 + b_1 \mathbb{1}(Sex_i = \text{" Male "}) + b_2 Y_i + b_3 \mathbb{1}(Sex_i = \text{" Male "}) \times Y_i + e_i^+$$

b_0 - percent hungry at year zero for females

$b_0 + b_1$ - percent hungry at year zero for males

b_2 - change in percent hungry (females) in one year

$b_2 + b_3$ - change in percent hungry (males) in one year

e_i^+ - everything we didn't measure

Two lines, different slopes in R

```
lmBoth <- lm(hunger$Numeric ~ hunger$Year + hunger$Sex + hunger$Sex*hunger$Year)
plot(hunger$Year,hunger$Numeric,pch=19)
points(hunger$Year,hunger$Numeric,pch=19,col=((hunger$Sex=="Male")*1+1))
abline(c(lmBoth$coeff[1],lmBoth$coeff[2]),col="red",lwd=3)
abline(c(lmBoth$coeff[1] + lmBoth$coeff[3],lmBoth$coeff[2] +lmBoth$coeff[4]),col="black",lwd=3)
```

Two lines, different slopes in R

```
summary(lmBoth)
```

```

Call:
lm(formula = hunger$Numeric ~ hunger$Year + hunger$Sex + hunger$Sex *
    hunger$Year)

Residuals:
   Min     1Q Median     3Q    Max
-25.91 -11.25  -1.85   7.09  46.15

Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
(Intercept)               603.5058   171.0552    3.53  0.00044 ***
hunger$Year                -0.2934     0.0855   -3.43  0.00062 ***
hunger$SexMale             61.9477   241.9086    0.26  0.79795
hunger$Year:hunger$SexMale -0.0300     0.1209   -0.25  0.80402
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 13.2 on 944 degrees of freedom
Multiple R-squared:  0.0318,    Adjusted R-squared:  0.0287
```

Interpretting a continuous interaction

$$E[Y_i|X_{1i} = x_1, X_{2i} = x_2] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

Holding X_2 constant we have

$$E[Y_i|X_{1i} = x_1 + 1, X_{2i} = x_2] - E[Y_i|X_{1i} = x_1, X_{2i} = x_2] = \beta_1 + \beta_3 x_2$$

And thus the expected change in Y per unit change in X_1 holding all else constant is not constant. β_1 is the slope when $x_2 = 0$. Note further that:

$$E[Y_i|X_{1i} = x_1 + 1, X_{2i} = x_2 + 1] - E[Y_i|X_{1i} = x_1, X_{2i} = x_2 + 1]$$

$$-E[Y_i|X_{1i} = x_1 + 1, X_{2i} = x_2] - E[Y_i|X_{1i} = x_1, X_{2i} = x_2]$$

$$= \beta_3$$

Thus, β_3 is the change in the expected change in Y per unit change in X_1, per unit change in X_2.

Or, the change in the slope relating X_1 and Y per unit change in X_2.

Example

$$Hu_i = b_0 + b_1 In_i + b_2 Y_i + b_3 In_i \times Y_i + e_i^+$$

b_0 - percent hungry at year zero for children with whose parents have no income

b_1 - change in percent hungry for each dollar of income in year zero

b_2 - change in percent hungry in one year for children whose parents have no income

b_3 - increased change in percent hungry by year for each dollar of income - e.g. if income is $10,000, then change in percent hungry in one year will be

$$b_2 + 1e4 \times b_3$$

e_i^+ - everything we didn't measure

Lot's of care/caution needed!

Multivariable regression

Regression

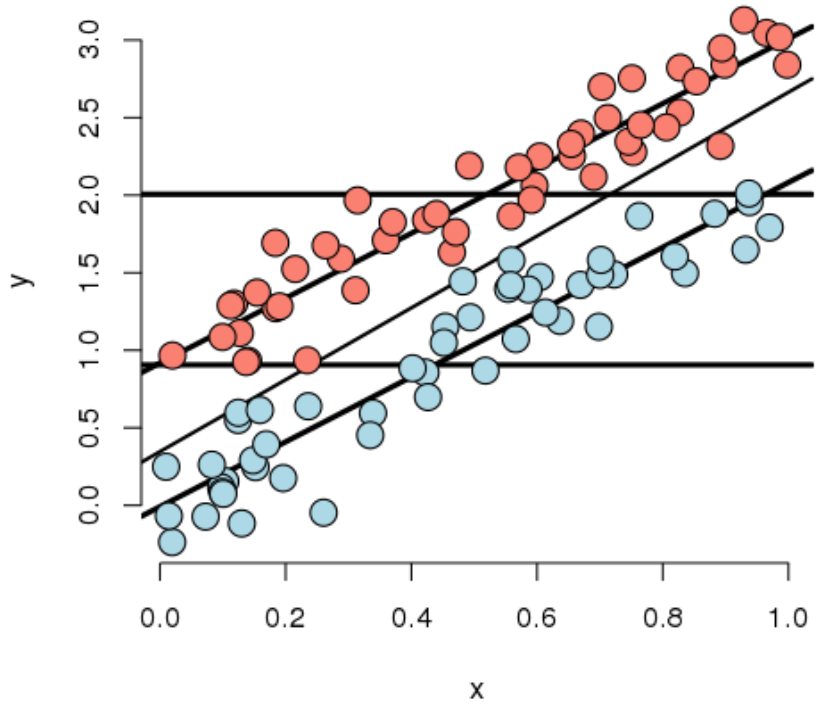
Brian Caffo, Jeff Leek, Roger Peng
Johns Hopkins Bloomberg School of Public Health

Consider the following simulated data

Code for the first plot, rest omitted (See the git repo for the rest of the code.)

```
n <- 100; t <- rep(c(0, 1), c(n/2, n/2)); x <- c(runif(n/2), runif(n/2));
beta0 <- 0; beta1 <- 2; tau <- 1; sigma <- .2
y <- beta0 + x * beta1 + t * tau + rnorm(n, sd = sigma)
plot(x, y, type = "n", frame = FALSE)
abline(lm(y ~ x), lwd = 2)
abline(h = mean(y[1 : (n/2)]), lwd = 3)
abline(h = mean(y[(n/2 + 1) : n]), lwd = 3)
fit <- lm(y ~ x + t)
abline(coef(fit)[1], coef(fit)[2], lwd = 3)
abline(coef(fit)[1] + coef(fit)[3], coef(fit)[2], lwd = 3)
points(x[1 : (n/2)], y[1 : (n/2)], pch = 21, col = "black", bg = "lightblue", cex = 2)
points(x[(n/2 + 1) : n], y[(n/2 + 1) : n], pch = 21, col = "black", bg = "salmon", cex = 2)
```

Simulation 1

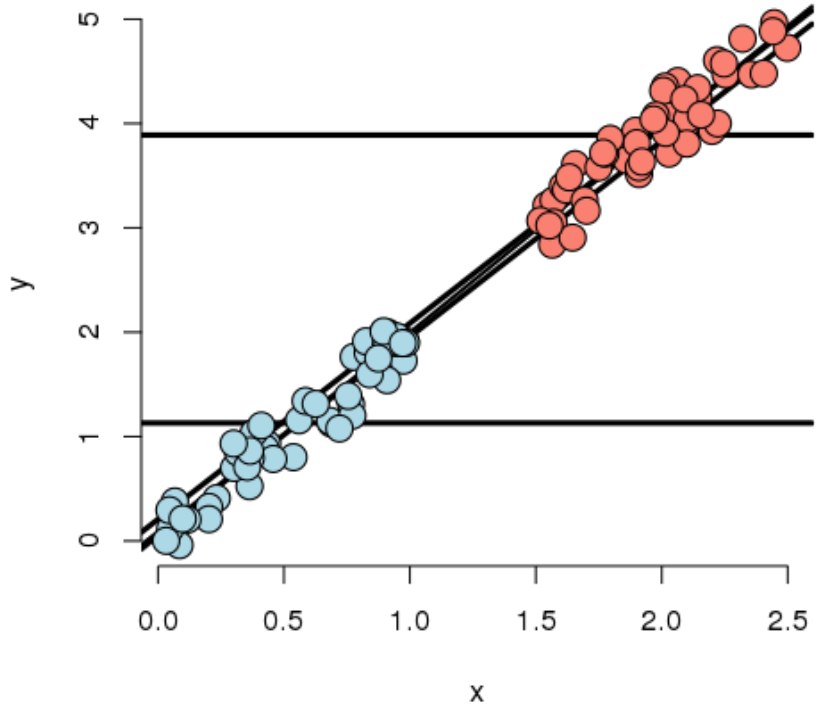


Discussion

Some things to note in this simulation

- The X variable is unrelated to group status
- The X variable is related to Y, but the intercept depends on group status.
- The group variable is related to Y.
    - The relationship between group status and Y is constant depending on X.
    - The relationship between group and Y disregarding X is about the same as holding X constant

Simulation 2

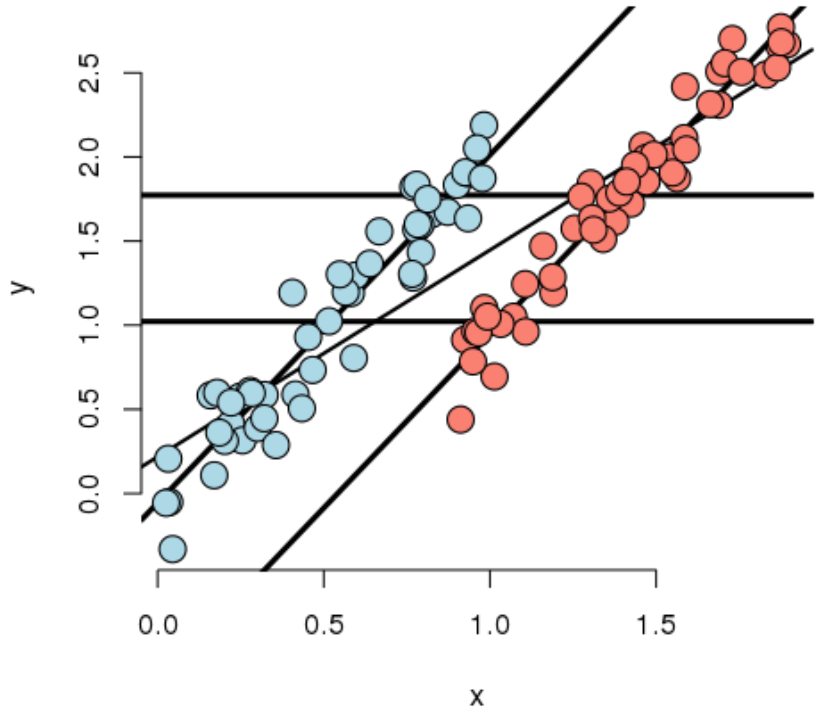


Discussion

Some things to note in this simulation

- The X variable is highly related to group status
- The X variable is related to Y, the intercept doesn't depend on the group variable.
    - The X variable remains related to Y holding group status constant
- The group variable is marginally related to Y disregarding X.
- The model would estimate no adjusted effect due to group.
    - There isn't any data to inform the relationship between group and Y.
    - This conclusion is entirely based on the model.

Simulation 3

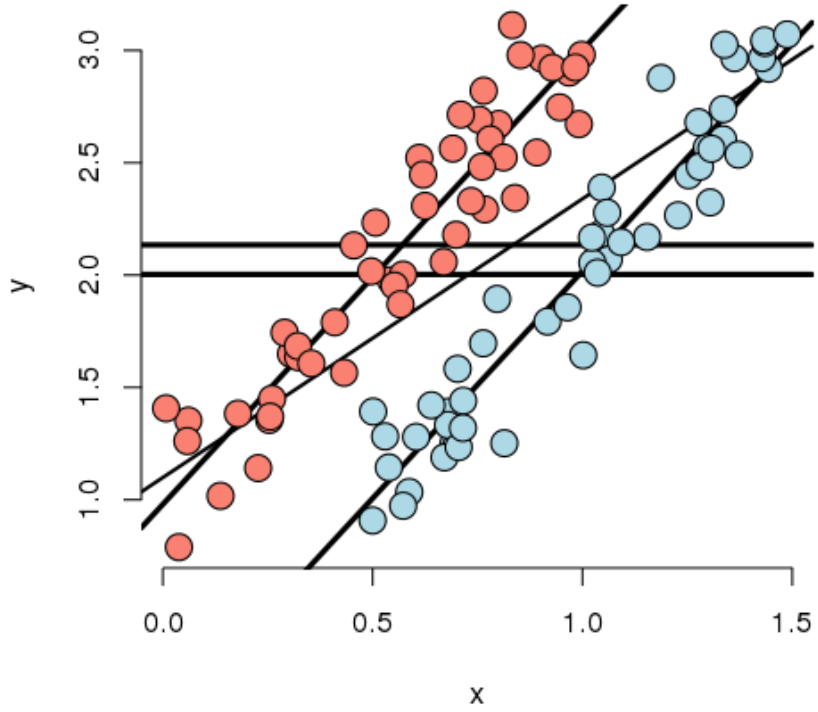


Discussion

Some things to note in this simulation

- Marginal association has red group higher than blue.
- Adjusted relationship has blue group higher than red.
- Group status related to X.
- There is some direct evidence for comparing red and blue holding X fixed.

Simulation 4

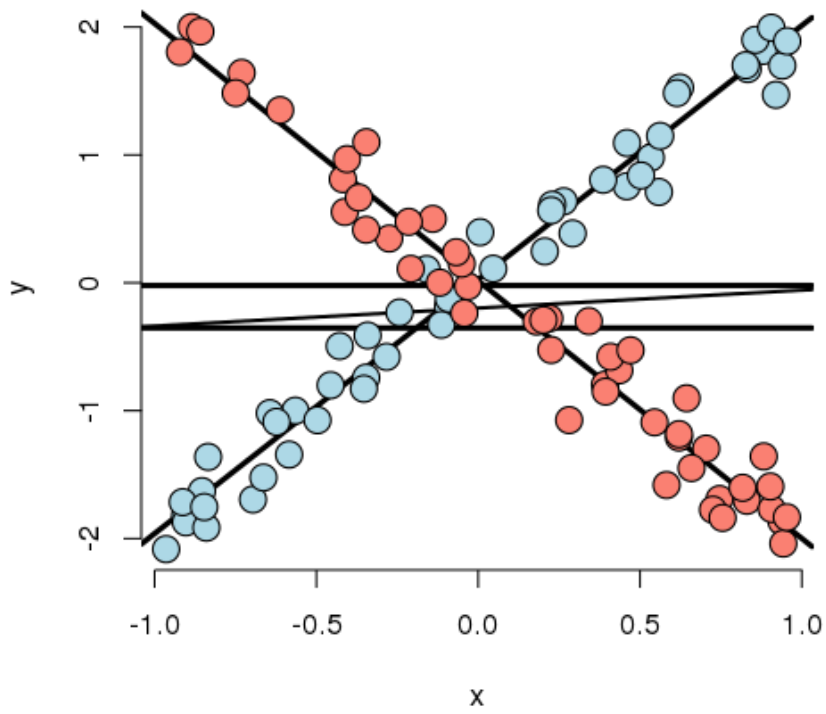


Discussion

Some things to note in this simulation

- No marginal association between group status and Y.
- Strong adjusted relationship.
- Group status not related to X.
- There is lots of direct evidence for comparing red and blue holding X fixed.

Simulation 5

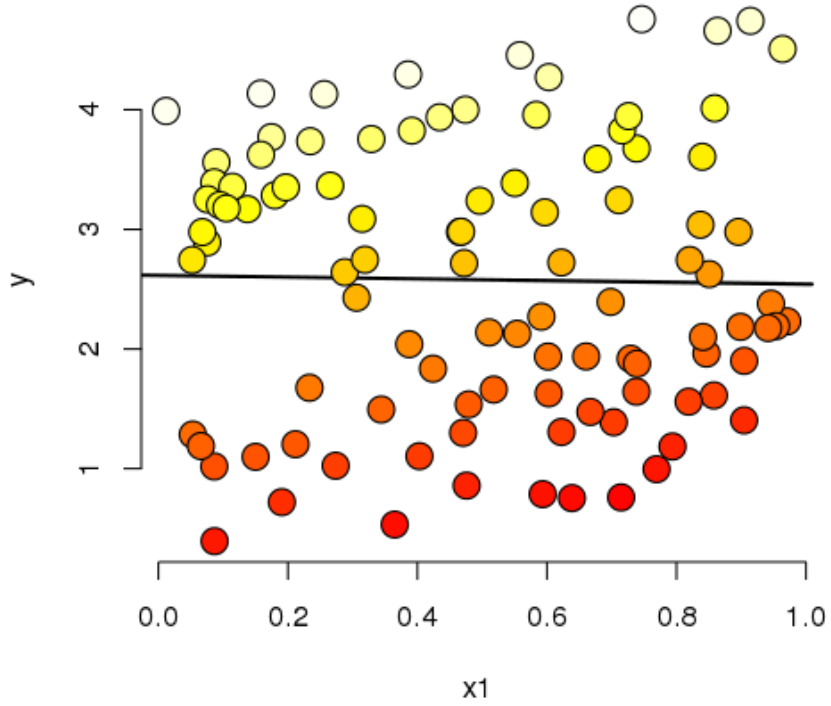


Discussion

Some things to note from this simulation

- There is no such thing as a group effect here.
  - The impact of group reverses itself depending on X.
  - Both intercept and slope depends on group.
- Group status and X unrelated.
  - There's lots of information about group effects holding X fixed.

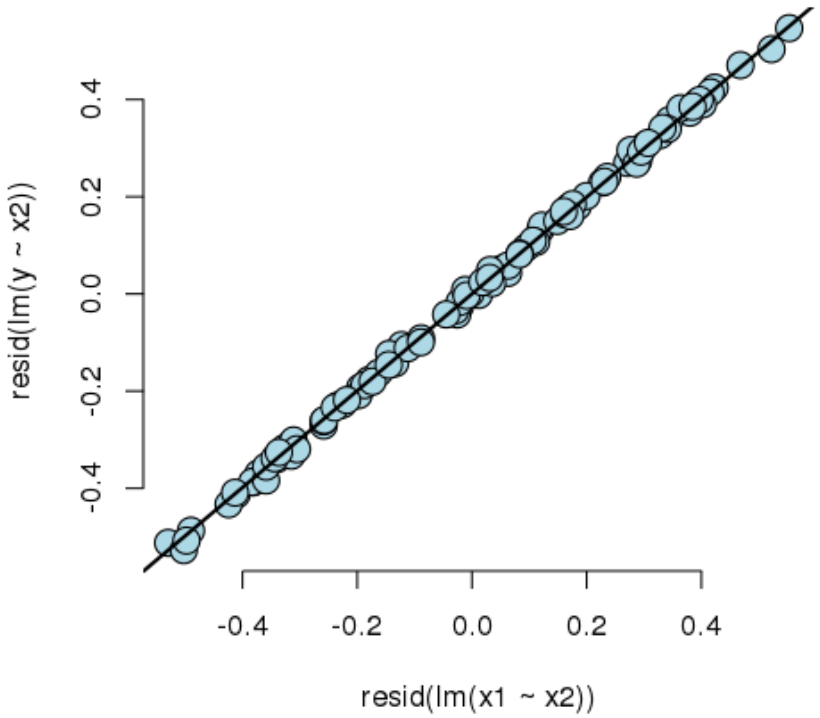
Simulation 6



Do this to investigate the bivariate relationship

```
library(rgl)
plot3d(x1, x2, y)
```

Residual relationship



Discussion

Some things to note from this simulation

- X1 unrelated to X2
- X2 strongly related to Y
- Adjusted relationship between X1 and Y largely unchanged by considering X2.
    - Almost no residual variability after accounting for X2.

Some final thoughts

- Modeling multivariate relationships is difficult.
- Play around with simulations to see how the inclusion or exclustion of another variable can change analyses.
- The results of these analyses deal with the impact of variables on associations.
    - Ascertaining mechanisms or cause are difficult subjects to be added on top of difficulty in understanding multivariate associations.

Residuals, diagnostics, variation

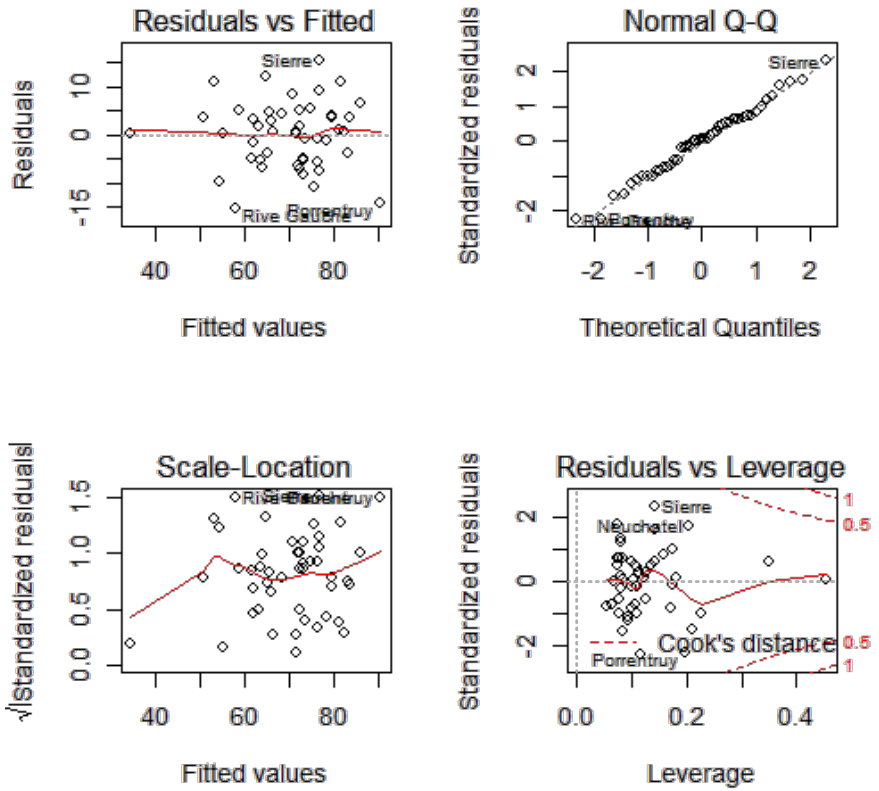
Regression

Brian Caffo, Jeff Leek, Roger Peng
Johns Hopkins Bloomberg School of Public Health

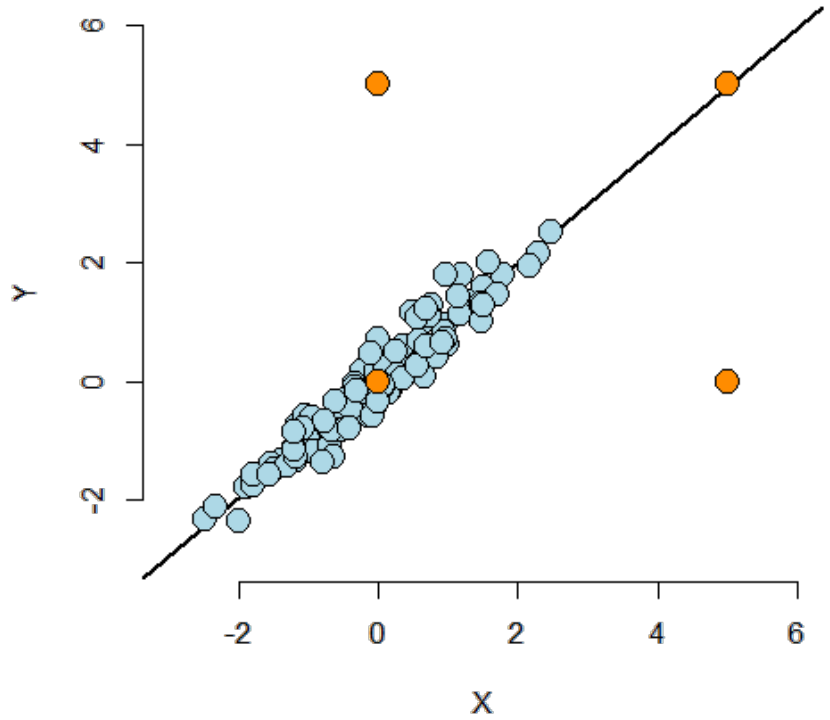
The linear model

- Specified as $Y_i = \sum_{k=1}^{p} X_{ik} \beta_j + \epsilon_i$
- We'll also assume here that $\epsilon_i \overset{iid}{\sim} N(0, \sigma^2)$
- Define the residuals as $e_i = Y_i - \hat{Y}_i = Y_i - \sum_{k=1}^{p} X_{ik} \hat{\beta}_j$
- Our estimate of residual variation is $\hat{\sigma}^2 = \frac{\sum_{i=1}^{n} e_i^2}{n-p}$, the $n - p$ so that $E[\hat{\sigma}^2] = \sigma^2$

```
data(swiss); par(mfrow = c(2, 2))
fit <- lm(Fertility ~ . , data = swiss); plot(fit)
```



Influential, high leverage and outlying points



Summary of the plot

Calling a point an outlier is vague.

- Outliers can be the result of spurious or real processes.
- Outliers can have varying degrees of influence.
- Outliers can conform to the regression relationship (i.e being marginally outlying in X or Y, but not outlying given the regression relationship).
    - Upper left hand point has low leverage, low influence, outlies in a way not conforming to the regression relationship.
    - Lower left hand point has low leverage, low influence and is not to be an outlier in any sense.
    - Upper right hand point has high leverage, but chooses not to extert it and thus would have low actual influence by conforming to the regresison relationship of the other points.
    - Lower right hand point has high leverage and would exert it if it were included in the fit.

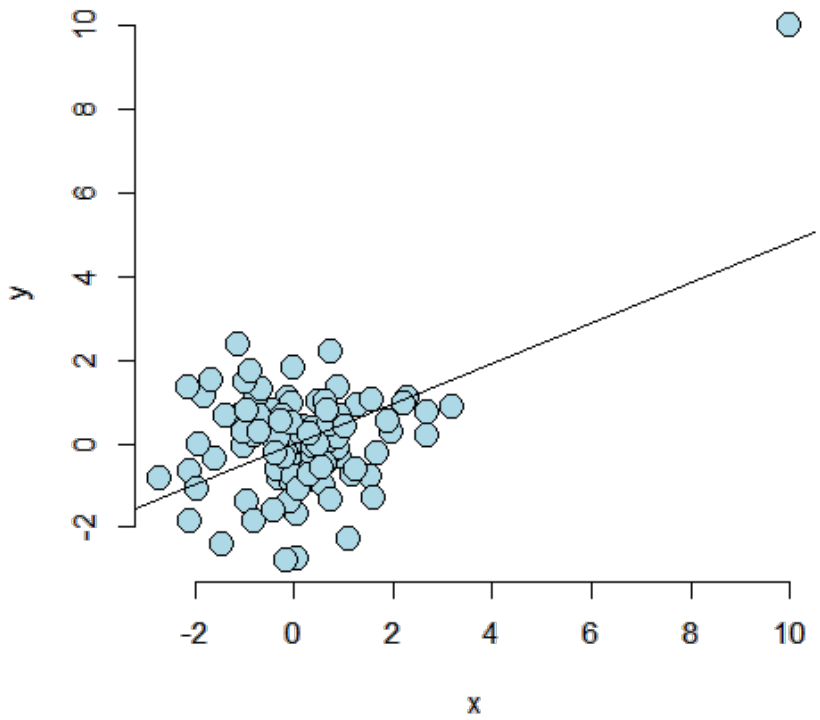
Influence measures

- Do `?influence.measures` to see the full suite of influence measures in stats. The measures include
  - `rstandard` - standardized residuals, residuals divided by their standard deviations)
  - `rstudent` - standardized residuals, residuals divided by their standard deviations, where the ith data point was deleted in the calculation of the standard deviation for the residual to follow a t distribution
  - `hatvalues` - measures of leverage
  - `dffits` - change in the predicted response when the i^{th} point is deleted in fitting the model.
  - `dfbetas` - change in individual coefficients when the i^{th} point is deleted in fitting the model.
  - `cooks.distance` - overall change in teh coefficients when the i^{th} point is deleted.
  - `resid` - returns the ordinary residuals
  - `resid(fit) / (1 - hatvalues(fit))` where `fit` is the linear model fit returns the PRESS residuals, i.e. the leave one out cross validation residuals - the difference in the response and the predicted response at data point i, where it was not included in the model fitting.

How do I use all of these things?

- Be wary of simplistic rules for diagnostic plots and measures. The use of these tools is context specific. It's better to understand what they are trying to accomplish and use them judiciously.
- Not all of the measures have meaningful absolute scales. You can look at them relative to the values across the data.
- They probe your data in different ways to diagnose different problems.
- Patterns in your residual plots generally indicate some poor aspect of model fit. These can include:
    - Heteroskedasticity (non constant variance).
    - Missing model terms.
    - Temporal patterns (plot residuals versus collection order).
- Residual QQ plots investigate normality of the errors.
- Leverage measures (hat values) can be useful for diagnosing data entry errors.
- Influence measures get to the bottom line, 'how does deleting or including this point impact a particular aspect of the model'.

Case 1



The code

```
n <- 100; x <- c(10, rnorm(n)); y <- c(10, c(rnorm(n)))
plot(x, y, frame = FALSE, cex = 2, pch = 21, bg = "lightblue", col = "black")
abline(lm(y ~ x))
```

- The point `c(10, 10)` has created a strong regression relationship where there shouldn't be one.

Showing a couple of the diagnostic values

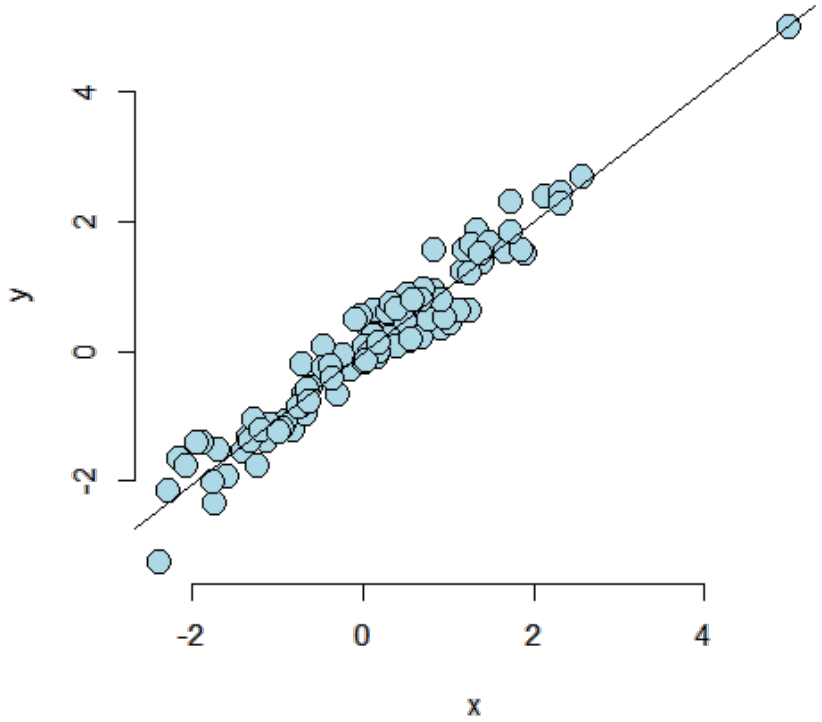
```
fit <- lm(y ~ x)
round(dfbetas(fit)[1 : 10, 2], 3)
```

```
     1      2      3      4      5      6      7      8      9     10
 6.007 -0.019 -0.007  0.014 -0.002 -0.083 -0.034 -0.045 -0.112 -0.008
```

```
round(hatvalues(fit)[1 : 10], 3)
```

```
    1     2     3     4     5     6     7     8     9    10
0.445 0.010 0.011 0.011 0.030 0.017 0.012 0.033 0.021 0.010
```

Case 2



Looking at some of the diagnostics

```
round(dfbetas(fit2)[1 : 10, 2], 3)
```

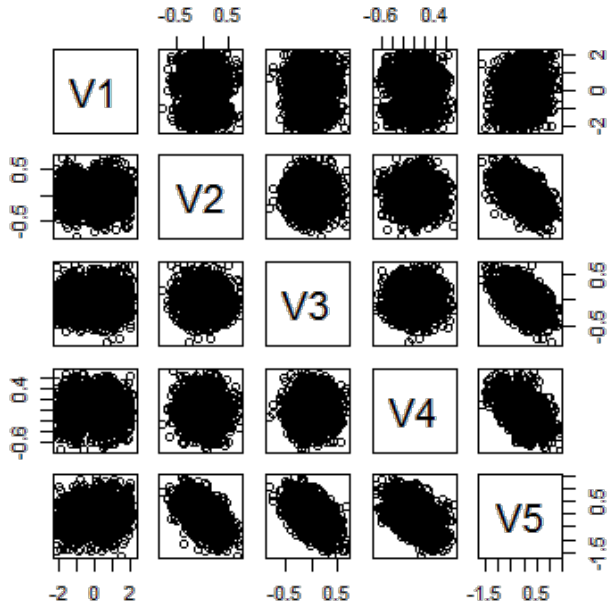
```
     1      2      3      4      5      6      7      8      9     10
-0.072 -0.041 -0.007  0.012  0.008 -0.187  0.017  0.100 -0.059  0.035
```

```
round(hatvalues(fit2)[1 : 10], 3)
```

```
    1     2     3     4     5     6     7     8     9    10
0.164 0.011 0.014 0.012 0.010 0.030 0.017 0.017 0.013 0.021
```

Example described by Stefanski TAS 2007 Vol 61.

```
## Don't everyone hit this server at once.  Read the paper first.
dat <- read.table('http://www4.stat.ncsu.edu/~stefanski/NSF_Supported/Hidden_Images/orly_owl_files/orly
pairs(dat)
```



Got our P-values, should we bother to do a residual plot?

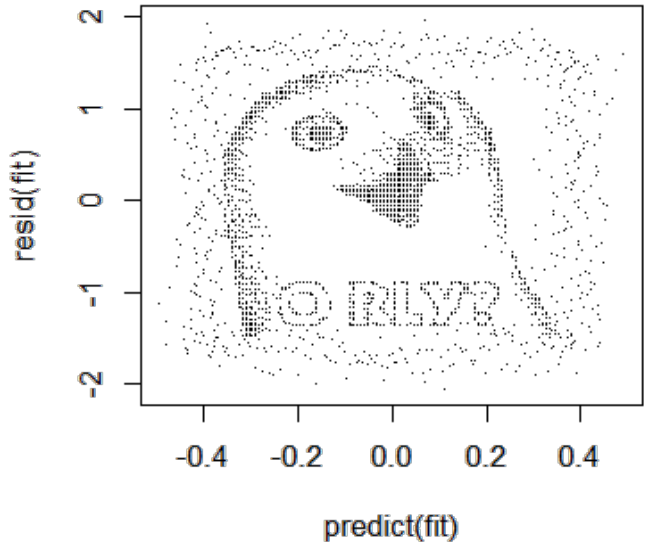
```
summary(lm(V1 ~ . -1, data = dat))$coef
```

```
   Estimate Std. Error t value  Pr(>|t|)
V2   0.9856    0.12798   7.701 1.989e-14
V3   0.9715    0.12664   7.671 2.500e-14
V4   0.8606    0.11958   7.197 8.301e-13
V5   0.9267    0.08328  11.127 4.778e-28
```

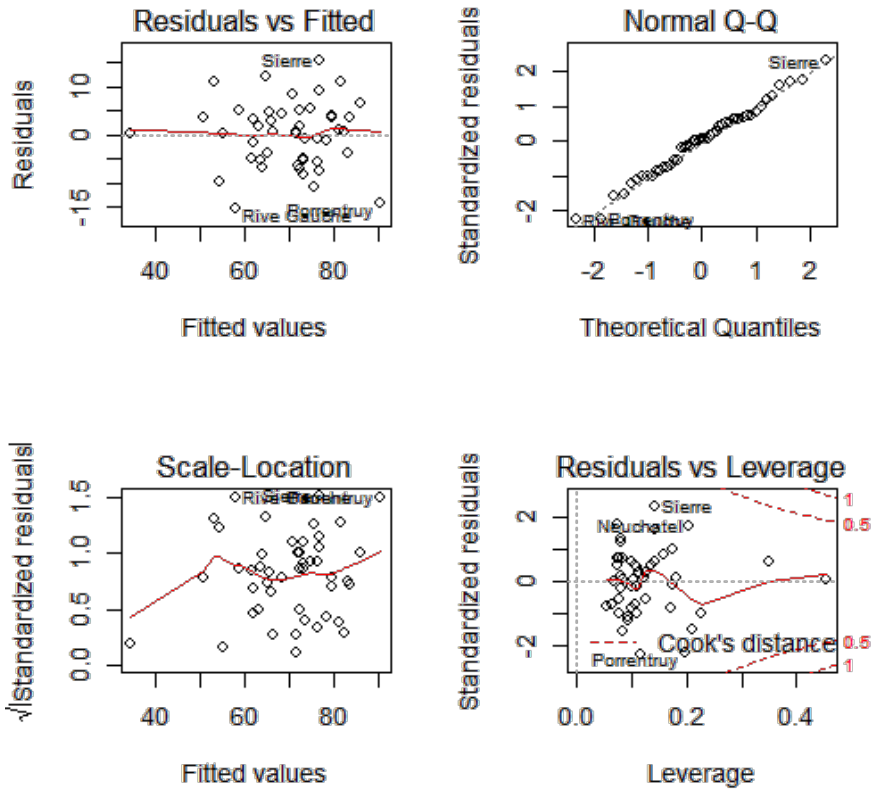
Residual plot

P-values significant, O RLY?

```
fit <- lm(V1 ~ . - 1, data = dat); plot(predict(fit), resid(fit), pch = '.')
```



Back to the Swiss data



Multiple variables

Regression

Brian Caffo, Jeff Leek, Roger Peng
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Multivariable regression

- We have an entire class on prediction and machine learning, so we'll focus on modeling.
  - Prediction has a different set of criteria, needs for interpretability and standards for generalizability.
  - In modeling, our interest lies in parsimonious, interpretable representations of the data that enhance our understanding of the phenomena under study.
  - A model is a lense through which to look at your data. (I attribute this quote to Scott Zeger)
  - Under this philosophy, what's the right model? Whatever model connects the data to a true, parsimonious statement about what you're studying.
- There are nearly uncontable ways that a model can be wrong, in this lecture, we'll focus on variable inclusion and exclusion.
- Like nearly all aspects of statistics, good modeling decisions are context dependent.
  - A good model for prediction versus one for studying mechanisms versus one for trying to establish causal effects may not be the same.

The Rumsfeldian triplet

There are known knowns. These are things we know that we know. There are known unknowns. That is to say, there are things that we know we don't know. But there are also unknown unknowns. There are things we don't know we don't know. Donald Rumsfeld

In our context

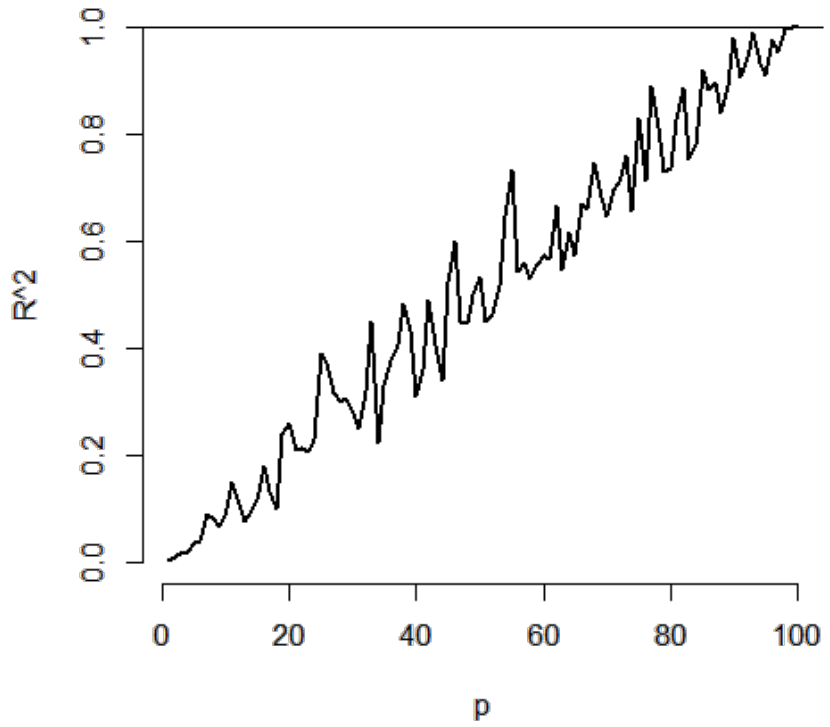
- (Known knowns) Regressors that we know we should check to include in the model and have.
- (Known Unknowns) Regressors that we would like to include in the model, but don't have.
- (Unknown Unknowns) Regressors that we don't even know about that we should have included in the model.

General rules

- Omitting variables results in bias in the coeficients of interest - unless their regressors are uncorrelated with the omitted ones.
  - This is why we randomize treatments, it attempts to uncorrelate our treatment indicator with variables that we don't have to put in the model.
  - (If there's too many unobserved confounding variables, even randomization won't help you.)
- Including variables that we shouldn't have increases standard errors of the regression variables.
  - Actually, including any new variables increasese (actual, not estimated) standard errors of other regressors. So we don't want to idly throw variables into the model.
- The model must tend toward perfect fit as the number of non-redundant regressors approaches n.
- R^2 increases monotonically as more regressors are included.
- The SSE decreases monotonically as more regressors are included.

Plot of R^2 versus n

For simulations as the number of variables included equals increases to $n = 100$. No actual regression relationship exist in any simulation



Variance inflation

```
n <- 100; nosim <- 1000
x1 <- rnorm(n); x2 <- rnorm(n); x3 <- rnorm(n);
betas <- sapply(1 : nosim, function(i){
  y <- x1 + rnorm(n, sd = .3)
  c(coef(lm(y ~ x1))[2],
    coef(lm(y ~ x1 + x2))[2],
    coef(lm(y ~ x1 + x2 + x3))[2])
})
round(apply(betas, 1, sd), 5)
```

```
     x1      x1      x1
0.02839 0.02872 0.02884
```

Variance inflation

```
n <- 100; nosim <- 1000
x1 <- rnorm(n); x2 <- x1/sqrt(2) + rnorm(n) /sqrt(2)
x3 <- x1 * 0.95 + rnorm(n) * sqrt(1 - 0.95^2);
betas <- sapply(1 : nosim, function(i){
  y <- x1 + rnorm(n, sd = .3)
  c(coef(lm(y ~ x1))[2],
    coef(lm(y ~ x1 + x2))[2],
    coef(lm(y ~ x1 + x2 + x3))[2])
})
round(apply(betas, 1, sd), 5)
```

```
     x1      x1      x1
0.03131 0.04270 0.09653
```

Variance inflation factors

- Notice variance inflation was much worse when we included a variable that was highly related to `x1`.
- We don't know σ, so we can only estimate the increase in the actual standard error of the coefficients for including a regressor.
- However, σ drops out of the relative standard errors. If one sequentially adds variables, one can check the variance (or sd) inflation for including each one.
- When the other regressors are actually orthogonal to the regressor of interest, then there is no variance inflation.
- The variance inflation factor (VIF) is the increase in the variance for the ith regressor compared to the ideal setting where it is orthogonal to the other regressors.
  - (The square root of the VIF is the increase in the sd ...)
- Remember, variance inflation is only part of the picture. We want to include certain variables, even if they dramatically inflate our variance.

Revisting our previous simulation

```
##doesn't depend on which y you use,
y <- x1 + rnorm(n, sd = .3)
a <- summary(lm(y ~ x1))$cov.unscaled[2,2]
c(summary(lm(y ~ x1 + x2))$cov.unscaled[2,2],
  summary(lm(y~ x1 + x2 + x3))$cov.unscaled[2,2]) / a
```

```
[1] 1.895 9.948
```

```
temp <- apply(betas, 1, var); temp[2 : 3] / temp[1]
```

```
   x1    x1
1.860 9.506
```

Swiss data

```
data(swiss);
fit1 <- lm(Fertility ~ Agriculture, data = swiss)
a <- summary(fit1)$cov.unscaled[2,2]
fit2 <- update(fit, Fertility ~ Agriculture + Examination)
fit3 <- update(fit, Fertility ~ Agriculture + Examination + Education)
  c(summary(fit2)$cov.unscaled[2,2],
    summary(fit3)$cov.unscaled[2,2]) / a
```

```
[1] 1.892 2.089
```

Swiss data VIFs,

```
library(car)
fit <- lm(Fertility ~ . , data = swiss)
vif(fit)
```

```
     Agriculture      Examination        Education         Catholic Infant.Mortality 
           2.284            3.675            2.775            1.937            1.108 
```

```
sqrt(vif(fit)) #I prefer sd
```

```
     Agriculture      Examination        Education         Catholic Infant.Mortality 
           1.511            1.917            1.666            1.392            1.052 
```

What about residual variance estimation?

- Assuming that the model is linear with additive iid errors (with finite variance), we can mathematically describe the impact of omitting necessary variables or including unnecessary ones.
  - If we underfit the model, the variance estimate is biased.
  - If we correctly or overfit the model, including all necessary covariates and/or unnecessary covariates, the variance estimate is unbiased.
  - However, the variance of the variance is larger if we include unnecessary variables.

Covariate model selection

- Automated covariate selection is a difficult topic. It depends heavily on how rich of a covariate space one wants to explore.
    - The space of models explodes quickly as you add interactions and polynomial terms.
- In the prediction class, we'll cover many modern methods for traversing large model spaces for the purposes of prediction.
- Principal components or factor analytic models on covariates are often useful for reducing complex covariate spaces.
- Good design can often eliminate the need for complex model searches at analyses; though often control over the design is limited.
- If the models of interest are nested and without lots of parameters differentiating them, it's fairly uncontroversial to use nested likelihood ratio tests. (Example to follow.)
- My favoriate approach is as follows. Given a coefficient that I'm interested in, I like to use covariate adjustment and multiple models to probe that effect to evaluate it for robustness and to see what other covariates knock it out. This isn't a terribly systematic approach, but it tends to teach you a lot about the the data as you get your hands dirty.

How to do nested model testing in R

```
fit1 <- lm(Fertility ~ Agriculture, data = swiss)
fit3 <- update(fit, Fertility ~ Agriculture + Examination + Education)
fit5 <- update(fit, Fertility ~ Agriculture + Examination + Education + Catholic + Infant.Mortality)
anova(fit1, fit3, fit5)
```

```
Analysis of Variance Table

Model 1: Fertility ~ Agriculture
Model 2: Fertility ~ Agriculture + Examination + Education
Model 3: Fertility ~ Agriculture + Examination + Education + Catholic +
    Infant.Mortality
  Res.Df  RSS Df Sum of Sq    F  Pr(>F)
1     45 6283
2     43 3181  2      3102 30.2 8.6e-09 ***
3     41 2105  2      1076 10.5 0.00021 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Generalized linear models

Regression Models

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Linear models

- Linear models are the most useful applied statistical technique. However, they are not without their limitations.
  - Additive response models don't make much sense if the response is discrete, or stricly positive.
  - Additive error models often don't make sense, for example if the outcome has to be positive.
  - Transformations are often hard to interpret.
  - There's value in modeling the data on the scale that it was collected.
  - Particularly interpetable transformations, natural logarithms in specific, aren't applicable for negative or zero values.

Generalized linear models

- Introduced in a 1972 RSSB paper by Nelder and Wedderburn.
- Involves three components
  - An *exponential family* model for the response.
  - A systematic component via a linear predictor.
  - A link function that connects the means of the response to the linear predictor.

Example, linear models

- Assume that $Y_i \sim N(\mu_i, \sigma^2)$ (the Gaussian distribution is an exponential family distribution.)
- Define the linear predictor to be $\eta_i = \sum_{k=1}^{p} X_{ik} \beta_k$.
- The link function as g so that $g(\mu) = \eta$.
  - For linear models $g(\mu) = \mu$ so that $\mu_i = \eta_i$
- This yields the same likelihood model as our additive error Gaussian linear model

$$Y_i = \sum_{k=1}^{p} X_{ik} \beta_k + \epsilon_i$$

where $\epsilon_i \overset{iid}{\sim} N(0, \sigma^2)$

Example, logistic regression

- Assume that $Y_i \sim \text{Bernoulli}(\mu_i)$ so that $E[Y_i] = \mu_i$ where $0 \leq \mu_i \leq 1$.
- Linear predictor $\eta_i = \sum_{k=1}^{p} X_{ik} \beta_k$
- Link function $g(\mu) = \eta = \log\left(\frac{\mu}{1-\mu}\right)$ g is the (natural) log odds, referred to as the **logit**.
- Note then we can invert the logit function as

$$\mu_i = \frac{\exp(\eta_i)}{1 + \exp(\eta_i)} \quad \text{and} \quad 1 - \mu_i = \frac{1}{1 + \exp(\eta_i)}$$

Thus the likelihood is

$$\prod_{i=1}^{n} \mu_i^{y_i} (1 - \mu_i)^{1-y_i} = \exp\left(\sum_{i=1}^{n} y_i \eta_i\right) \prod_{i=1}^{n} (1 + \eta_i)^{-1}$$

Example, Poisson regression

- Assume that $Y_i \sim \text{Poisson}(\mu_i)$ so that $E[Y_i] = \mu_i$ where $0 \leq \mu_i$
- Linear predictor $\eta_i = \sum_{k=1}^{p} X_{ik} \beta_k$
- Link function $g(\mu) = \eta = \log(\mu)$
- Recall that e^x is the inverse of $\log(x)$ so that

$$\mu_i = e^{\eta_i}$$

Thus, the likelihood is

$$\prod_{i=1}^{n} (y_i!)^{-1} \mu_i^{y_i} e^{-\mu_i} \propto \exp\left(\sum_{i=1}^{n} y_i \eta_i - \sum_{i=1}^{n} \mu_i \right)$$

Some things to note

- In each case, the only way in which the likelihood depends on the data is through

$$\sum_{i=1}^{n} y_i \eta_i = \sum_{i=1}^{n} y_i \sum_{k=1}^{p} X_{ik} \beta_k = \sum_{k=1}^{p} \beta_k \sum_{i=1}^{n} X_{ik} y_i$$

  Thus if we don't need the full data, only $\sum_{i=1}^{n} X_{ik} y_i$. This simplification is a consequence of chosing so-called 'canonical' link functions.

- (This has to be derived). All models acheive their maximum at the root of the so called normal equations

$$0 = \sum_{i=1}^{n} \frac{(Y_i - \mu_i)}{\mathrm{Var}(Y_i)} W_i$$

  where W_i are the derivative of the inverse of the link function.

About variances

$$0 = \sum_{i=1}^{n} \frac{(Y_i - \mu_i)}{\mathrm{Var}(Y_i)} W_i$$

- For the linear model $\mathrm{Var}(Y_i) = \sigma^2$ is constant.
- For Bernoulli case $\mathrm{Var}(Y_i) = \mu_i(1 - \mu_i)$
- For the Poisson case $\mathrm{Var}(Y_i) = \mu_i$.
- In the latter cases, it is often relevant to have a more flexible variance model, even if it doesn't correspond to an actual likelihood

$$0 = \sum_{i=1}^{n} \frac{(Y_i - \mu_i)}{\phi\mu_i(1 - \mu_i)} W_i \quad \text{and} \quad 0 = \sum_{i=1}^{n} \frac{(Y_i - \mu_i)}{\phi\mu_i} W_i$$

- These are called 'quasi-likelihood' normal equations

Odds and ends

- The normal equations have to be solved iteratively. Resulting in $\hat{\beta}_k$ and, if included, $\hat{\phi}$.
- Predicted linear predictor responses can be obtained as $\hat{\eta} = \sum_{k=1}^{p} X_k \hat{\beta}_k$
- Predicted mean responses as $\hat{\mu} = g^{-1}(\hat{\eta})$
- Coefficients are interpretted as

$$g(E[Y|X_k = x_k + 1, X_{\sim k} = x_{\sim k}]) - g(E[Y|X_k = x_k, X_{\sim k} = x_{\sim k}]) = \beta_k$$

  or the change in the link function of the expected response per unit change in X_k holding other regressors constant.
- Variations on Newon/Raphson's algorithm are used to do it.
- Asymptotics are used for inference usually.
- Many of the ideas from linear models can be brought over to GLMs.

Generalized linear models, binary data

Regression models

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Key ideas

- Frequently we care about outcomes that have two values
  - Alive/dead
  - Win/loss
  - Success/Failure
  - etc
- Called binary, Bernoulli or 0/1 outcomes
- Collection of exchangeable binary outcomes for the same covariate data are called binomial outcomes.

Example Baltimore Ravens win/loss

Ravens Data

```
download.file("https://dl.dropboxusercontent.com/u/7710864/data/ravensData.rda"
              , destfile="./data/ravensData.rda",method="curl")
load("./data/ravensData.rda")
head(ravensData)
```

```
  ravenWinNum ravenWin ravenScore opponentScore
1           1        W         24             9
2           1        W         38            35
3           1        W         28            13
4           1        W         34            31
5           1        W         44            13
6           0        L         23            24
```

Linear regression

$$RW_i = b_0 + b_1 RS_i + e_i$$

RW_i - 1 if a Ravens win, 0 if not

RS_i - Number of points Ravens scored

b_0 - probability of a Ravens win if they score 0 points

b_1 - increase in probability of a Ravens win for each additional point

e_i - residual variation due

Linear regression in R

```
lmRavens <- lm(ravensData$ravenWinNum ~ ravensData$ravenScore)
summary(lmRavens)$coef
```

```
                    Estimate Std. Error t value Pr(>|t|)
(Intercept)           0.2850   0.256643   1.111  0.28135
ravensData$ravenScore 0.0159   0.009059   1.755  0.09625
```

Odds

Binary Outcome 0/1

$$RW_i$$

Probability (0,1)

$$\Pr(RW_i|RS_i, b_0, b_1)$$

Odds $(0, \infty)$

$$\frac{\Pr(RW_i|RS_i, b_0, b_1)}{1 - \Pr(RW_i|RS_i, b_0, b_1)}$$

Log odds $(-\infty, \infty)$

$$\log\left(\frac{\Pr(RW_i|RS_i, b_0, b_1)}{1 - \Pr(RW_i|RS_i, b_0, b_1)}\right)$$

Linear vs. logistic regression

Linear

$$RW_i = b_0 + b_1 RS_i + e_i$$

or

$$E[RW_i | RS_i, b_0, b_1] = b_0 + b_1 RS_i$$

Logistic

$$Pr(RW_i | RS_i, b_0, b_1) = \frac{\exp(b_0 + b_1 RS_i)}{1 + \exp(b_0 + b_1 RS_i)}$$

or

$$\log\left(\frac{Pr(RW_i | RS_i, b_0, b_1)}{1 - Pr(RW_i | RS_i, b_0, b_1)} \right) = b_0 + b_1 RS_i$$

Interpreting Logistic Regression

$$\log\left(\frac{\Pr(RW_i|RS_i, b_0, b_1)}{1-\Pr(RW_i|RS_i, b_0, b_1)}\right) = b_0 + b_1 RS_i$$

b_0 - Log odds of a Ravens win if they score zero points

b_1 - Log odds ratio of win probability for each point scored (compared to zero points)

$\exp(b_1)$ - Odds ratio of win probability for each point scored (compared to zero points)

Odds

- Imagine that you are playing a game where you flip a coin with success probability p.
- If it comes up heads, you win X. If it comes up tails, you lose Y.
- What should we set X and Y for the game to be fair?

$$E[\text{earnings}] = Xp - Y(1-p) = 0$$

- Implies

$$\frac{Y}{X} = \frac{p}{1-p}$$

- The odds can be said as "How much should you be willing to pay for a p probability of winning a dollar?"
  - (If $p > 0.5$ you have to pay more if you lose than you get if you win.)
  - (If $p < 0.5$ you have to pay less if you lose than you get if you win.)

Visualizing fitting logistic regression curves

```
x <- seq(-10, 10, length = 1000)
manipulate(
    plot(x, exp(beta0 + beta1 * x) / (1 + exp(beta0 + beta1 * x)),
         type = "l", lwd = 3, frame = FALSE),
    beta1 = slider(-2, 2, step = .1, initial = 2),
    beta0 = slider(-2, 2, step = .1, initial = 0)
    )
```

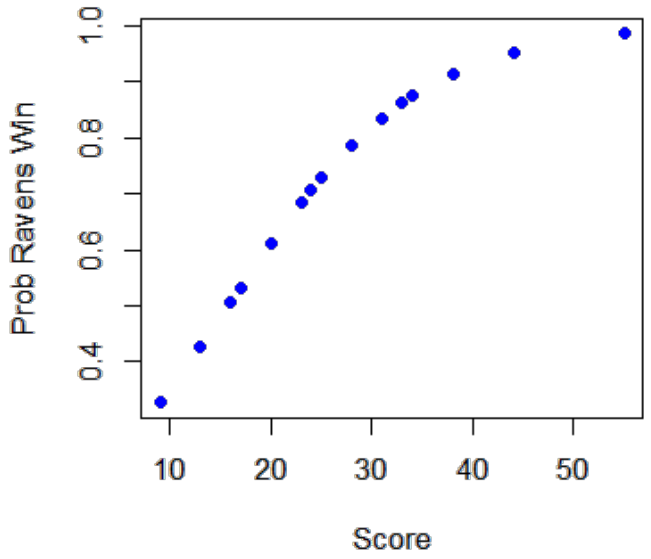
Ravens logistic regression

```
logRegRavens <- glm(ravensData$ravenWinNum ~ ravensData$ravenScore,family="binomial")
summary(logRegRavens)
```

```

Call:
glm(formula = ravensData$ravenWinNum ~ ravensData$ravenScore,
    family = "binomial")

Deviance Residuals:
   Min      1Q  Median      3Q     Max
-1.758  -1.100   0.530   0.806   1.495

Coefficients:
                     Estimate Std. Error z value Pr(>|z|)
(Intercept)           -1.6800     1.5541   -1.08     0.28
ravensData$ravenScore  0.1066     0.0667    1.60     0.11

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 24.435  on 19  degrees of freedom
Residual deviance: 20.895  on 18  degrees of freedom
AIC: 24.89
```

Ravens fitted values

```
plot(ravensData$ravenScore,logRegRavens$fitted,pch=19,col="blue",xlab="Score",ylab="Prob Ravens Win")
```



Odds ratios and confidence intervals

```
exp(logRegRavens$coeff)
```

```
          (Intercept) ravensData$ravenScore
               0.1864                1.1125
```

```
exp(confint(logRegRavens))
```

```
                        2.5 % 97.5 %
(Intercept)           0.005675  3.106
ravensData$ravenScore 0.996230  1.303
```

ANOVA for logistic regression

```
anova(logRegRavens,test="Chisq")
```

```
Analysis of Deviance Table

Model: binomial, link: logit

Response: ravensData$ravenWinNum

Terms added sequentially (first to last)

                     Df Deviance Resid. Df Resid. Dev Pr(>Chi)
NULL                                    19       24.4
ravensData$ravenScore  1     3.54        18       20.9     0.06 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Interpreting Odds Ratios

- Not probabilities
- Odds ratio of 1 = no difference in odds
- Log odds ratio of 0 = no difference in odds
- Odds ratio < 0.5 or > 2 commonly a "moderate effect"
- Relative risk $\frac{\Pr(RW_i|RS_i=10)}{\Pr(RW_i|RS_i=0)}$ often easier to interpret, harder to estimate
- For small probabilities RR ≈ OR but **they are not the same**!

Wikipedia on Odds Ratio

Further resources

- Wikipedia on Logistic Regression
- Logistic regression and glms in R
- Brian Caffo's lecture notes on: Simpson's paradox, Case-control studies
- Open Intro Chapter on Logistic Regression

Count outcomes, Poisson GLMs

Regression Models

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Key ideas

- Many data take the form of counts
  - Calls to a call center
  - Number of flu cases in an area
  - Number of cars that cross a bridge
- Data may also be in the form of rates
  - Percent of children passing a test
  - Percent of hits to a website from a country
- Linear regression with transformation is an option

Poisson distribution

- The Poisson distribution is a useful model for counts and rates
- Here a rate is count per some monitoring time
- Some examples uses of the Poisson distribution
  - Modeling web traffic hits
  - Incidence rates
  - Approximating binomial probabilities with small p and large n
  - Analyzing contigency table data

The Poisson mass function

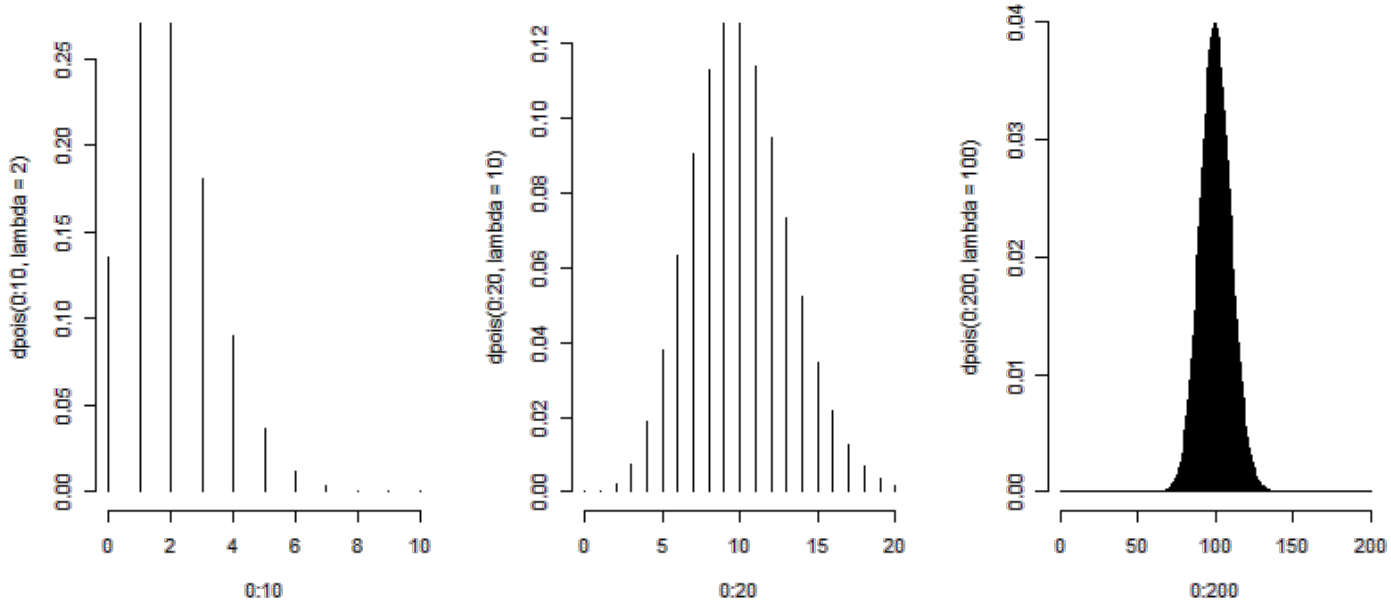
- $X \sim \text{Poisson}(t\lambda)$ if

$$P(X = x) = \frac{(t\lambda)^x e^{-t\lambda}}{x!}$$

  For $x = 0, 1, \ldots$.

- The mean of the Poisson is $E[X] = t\lambda$, thus $E[X/t] = \lambda$
- The variance of the Poisson is $\text{Var}(X) = t\lambda$.
- The Poisson tends to a normal as $t\lambda$ gets large.

```r
par(mfrow = c(1, 3))
plot(0 : 10, dpois(0 : 10, lambda = 2), type = "h", frame = FALSE)
plot(0 : 20, dpois(0 : 20, lambda = 10), type = "h", frame = FALSE)
plot(0 : 200, dpois(0 : 200, lambda = 100), type = "h", frame = FALSE)
```



Poisson distribution

Sort of, showing that the mean and variance are equal

```
x <- 0 : 10000; lambda = 3
mu <- sum(x * dpois(x, lambda = lambda))
sigmasq <- sum((x - mu)^2 * dpois(x, lambda = lambda))
c(mu, sigmasq)
```

```
[1] 3 3
```

Example: Leek Group Website Traffic

- Consider the daily counts to Jeff Leek's web site

http://biostat.jhsph.edu/~jleek/

- Since the unit of time is always one day, set $t = 1$ and then the Poisson mean is interpretted as web hits per day. (If we set $t = 24$, it would be web hits per hour).

Website data

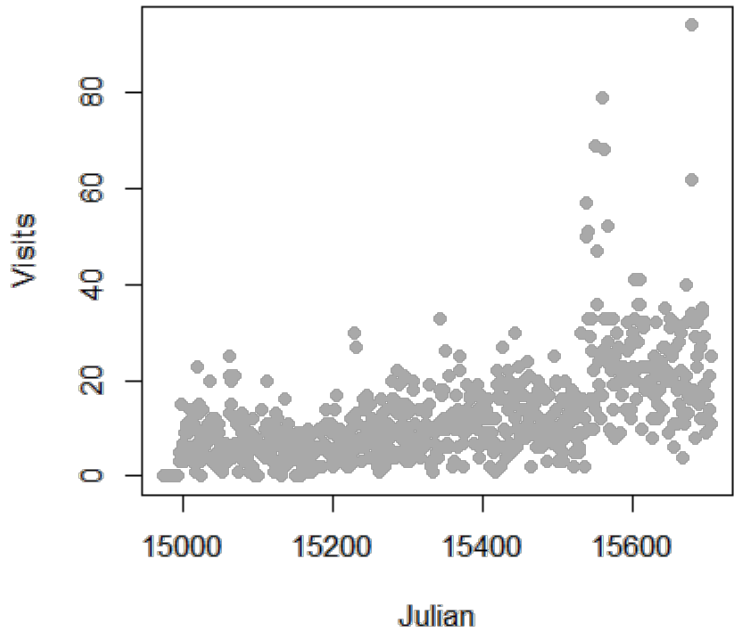
```
download.file("https://dl.dropboxusercontent.com/u/7710864/data/gaData.rda",destfile="./data/gaData.rda
load("./data/gaData.rda")
gaData$julian <- julian(gaData$date)
head(gaData)
```

```
        date visits simplystats julian
1 2011-01-01      0           0  14975
2 2011-01-02      0           0  14976
3 2011-01-03      0           0  14977
4 2011-01-04      0           0  14978
5 2011-01-05      0           0  14979
6 2011-01-06      0           0  14980
```

http://skardhamar.github.com/rga/

Plot data

```
plot(gaData$julian,gaData$visits,pch=19,col="darkgrey",xlab="Julian",ylab="Visits")
```



Linear regression

$$NH_i = b_0 + b_1 JD_i + e_i$$

NH_i - number of hits to the website

JD_i - day of the year (Julian day)

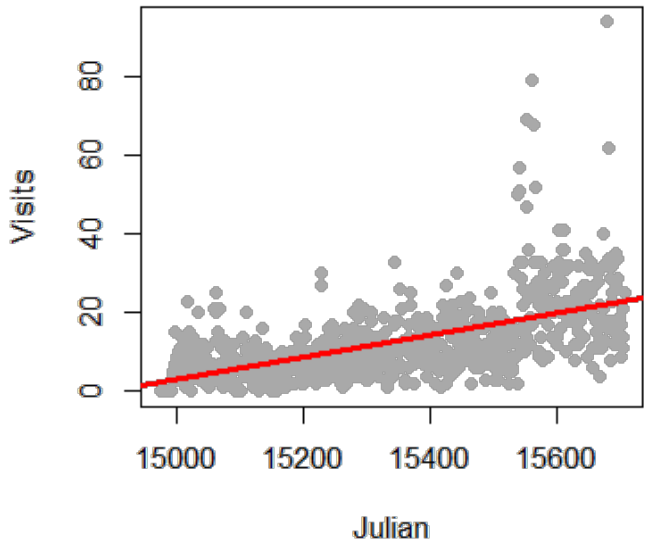
b_0 - number of hits on Julian day 0 (1970-01-01)

b_1 - increase in number of hits per unit day

e_i - variation due to everything we didn't measure

Linear regression line

```
plot(gaData$julian,gaData$visits,pch=19,col="darkgrey",xlab="Julian",ylab="Visits")
lm1 <- lm(gaData$visits ~ gaData$julian)
abline(lm1,col="red",lwd=3)
```



Aside, taking the log of the outcome

- Taking the natural log of the outcome has a specific interpretation.
- Consider the model

$$\log(NH_i) = b_0 + b_1 JD_i + e_i$$

NH_i - number of hits to the website

JD_i - day of the year (Julian day)

b_0 - log number of hits on Julian day 0 (1970-01-01)

b_1 - increase in log number of hits per unit day

e_i - variation due to everything we didn't measure

Exponentiating coefficients

- $e^{E[\log(Y)]}$ geometric mean of Y.
  - With no covariates, this is estimated by $e^{\frac{1}{n}\sum_{i=1}^{n}\log(y_i)} = (\prod_{i=1}^{n} y_i)^{1/n}$
- When you take the natural log of outcomes and fit a regression model, your exponentiated coefficients estimate things about geometric means.
- e^{β_0} estimated geometric mean hits on day 0
- e^{β_1} estimated relative increase or decrease in geometric mean hits per day
- There's a problem with logs with you have zero counts, adding a constant works

```
round(exp(coef(lm(I(log(gaData$visits + 1)) ~ gaData$julian))), 5)
```

```
  (Intercept) gaData$julian
        0.000         1.002
```

Linear vs. Poisson regression

Linear

$$NH_i = b_0 + b_1 JD_i + e_i$$

or

$$E[NH_i | JD_i, b_0, b_1] = b_0 + b_1 JD_i$$

Poisson/log-linear

$$\log\left(E[NH_i | JD_i, b_0, b_1]\right) = b_0 + b_1 JD_i$$

or

$$E[NH_i | JD_i, b_0, b_1] = \exp\left(b_0 + b_1 JD_i\right)$$

Multiplicative differences

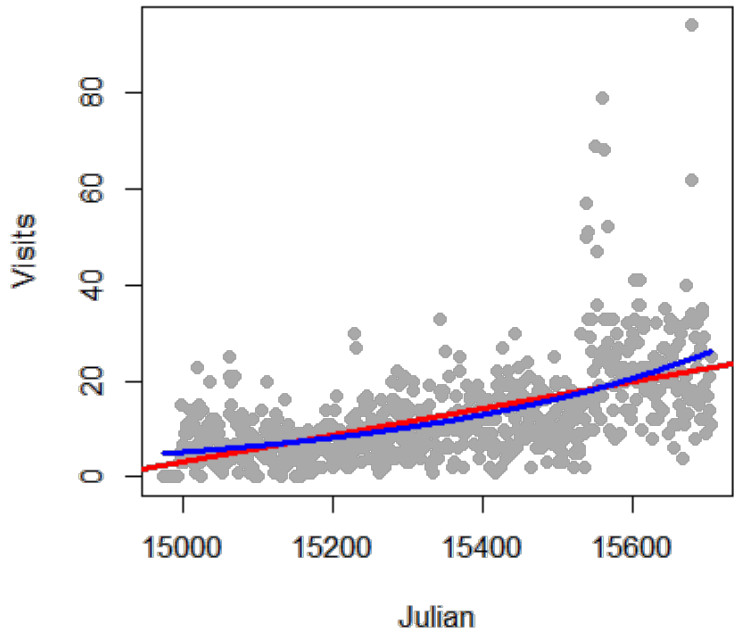
$$E[NH_i|JD_i, b_0, b_1] = \exp\left(b_0 + b_1 JD_i\right)$$

$$E[NH_i|JD_i, b_0, b_1] = \exp\left(b_0\right) \exp\left(b_1 JD_i\right)$$

If JD_i is increased by one unit, $E[NH_i|JD_i, b_0, b_1]$ is multiplied by $\exp\left(b_1\right)$

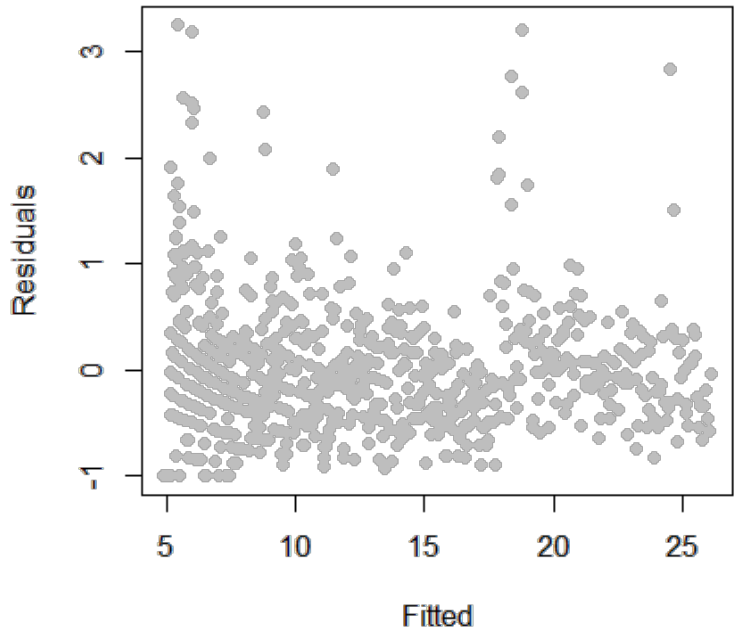
Poisson regression in R

```
plot(gaData$julian,gaData$visits,pch=19,col="darkgrey",xlab="Julian",ylab="Visits")
glm1 <- glm(gaData$visits ~ gaData$julian,family="poisson")
abline(lm1,col="red",lwd=3); lines(gaData$julian,glm1$fitted,col="blue",lwd=3)
```



Mean-variance relationship?

```
plot(glm1$fitted,glm1$residuals,pch=19,col="grey",ylab="Residuals",xlab="Fitted")
```



Model agnostic standard errors

```
library(sandwich)
confint.agnostic <- function (object, parm, level = 0.95, ...)
{
    cf <- coef(object); pnames <- names(cf)
    if (missing(parm))
        parm <- pnames
    else if (is.numeric(parm))
        parm <- pnames[parm]
    a <- (1 - level)/2; a <- c(a, 1 - a)
    pct <- stats:::format.perc(a, 3)
    fac <- qnorm(a)
    ci <- array(NA, dim = c(length(parm), 2L), dimnames = list(parm,
                                                               pct))
    ses <- sqrt(diag(sandwich::vcovHC(object)))[parm]
    ci[] <- cf[parm] + ses %o% fac
    ci
}
```

http://stackoverflow.com/questions/3817182/vcovhc-and-confidence-interval

Estimating confidence intervals

```
confint(glm1)
```

```
                  2.5 %     97.5 %
(Intercept)   -34.34658 -31.159716
gaData$julian   0.00219   0.002396
```

```
confint.agnostic(glm1)
```

```
                  2.5 %     97.5 %
(Intercept)   -36.362675 -29.136997
gaData$julian   0.002058   0.002528
```

Rates

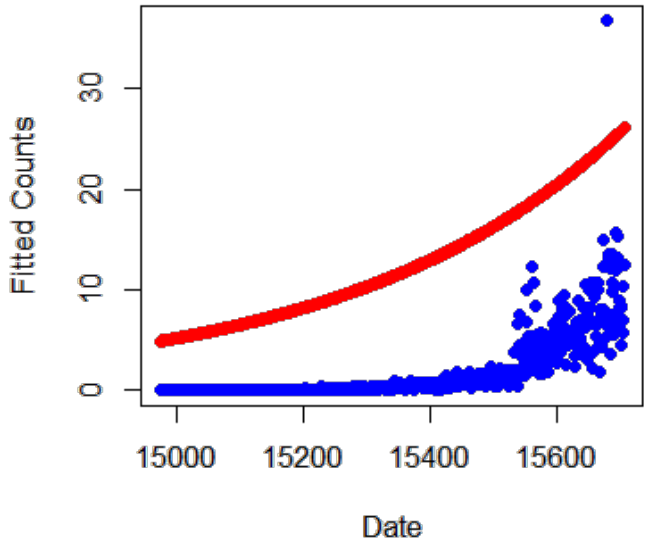
$$E[NHSS_i|JD_i, b_0, b_1]/NH_i = \exp\left(b_0 + b_1 JD_i\right)$$

$$\log\left(E[NHSS_i|JD_i, b_0, b_1]\right) - \log(NH_i) = b_0 + b_1 JD_i$$

$$\log\left(E[NHSS_i|JD_i, b_0, b_1]\right) = \log(NH_i) + b_0 + b_1 JD_i$$

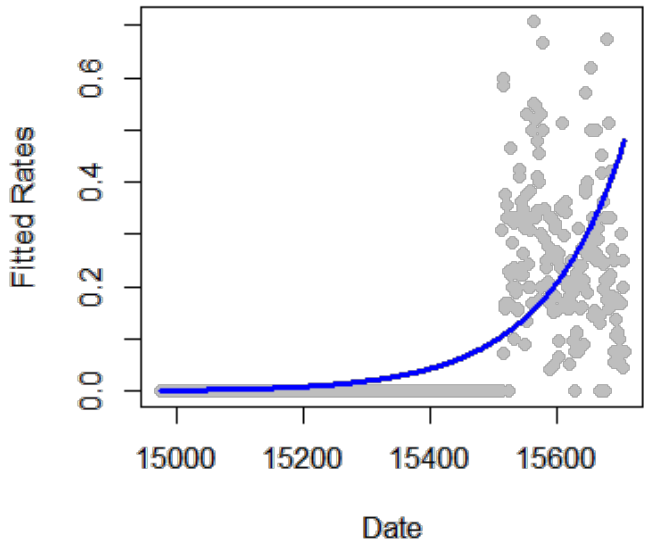
Fitting rates in R

```
glm2 <- glm(gaData$simplystats ~ julian(gaData$date),offset=log(visits+1),
            family="poisson",data=gaData)
plot(julian(gaData$date),glm2$fitted,col="blue",pch=19,xlab="Date",ylab="Fitted Counts")
points(julian(gaData$date),glm1$fitted,col="red",pch=19)
```



Fitting rates in R

```
glm2 <- glm(gaData$simplystats ~ julian(gaData$date),offset=log(visits+1),
            family="poisson",data=gaData)
plot(julian(gaData$date),gaData$simplystats/(gaData$visits+1),col="grey",xlab="Date",
     ylab="Fitted Rates",pch=19)
lines(julian(gaData$date),glm2$fitted/(gaData$visits+1),col="blue",lwd=3)
```



More information

- Log-linear models and multiway tables
- Wikipedia on Poisson regression, Wikipedia on overdispersion
- Regression models for count data in R
- pscl package - the function *zeroinfl* fits zero inflated models.

Hodgepodge

Regression models

Brian Caffo, Jeff Leek, Roger Peng
Johns Hopkins Bloomberg School of Public Health

How to fit functions using linear models

- Consider a model $Y_i = f(X_i) + \epsilon$.
- How can we fit such a model using linear models (called scatterplot smoothing)
- Consider the model

$$Y_i = \beta_0 + \beta_1 X_i + \sum_{k=1}^{d} (x_i - \xi_k)_+ \gamma_k + \epsilon_i$$

where $(a)_+ = a$ if $a > 0$ and 0 otherwise and $\xi_1 \leq \ldots \leq \xi_d$ are known knot points.

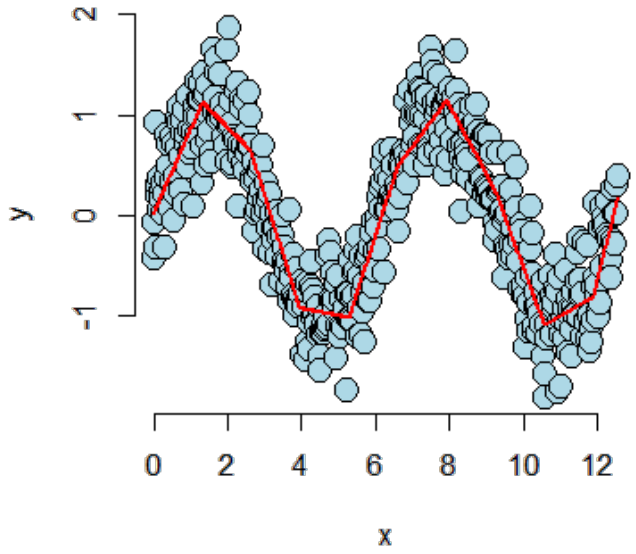
- Prove to yourelf that the mean function

$$\beta_0 + \beta_1 X_i + \sum_{k=1}^{d} (x_i - \xi_k)_+ \gamma_k$$

is continuous at the knot points.

Simulated example

```
n <- 500; x <- seq(0, 4 * pi, length = n); y <- sin(x) + rnorm(n, sd = .3)
knots <- seq(0, 8 * pi, length = 20);
splineTerms <- sapply(knots, function(knot) (x > knot) * (x - knot))
xMat <- cbind(1, x, splineTerms)
yhat <- predict(lm(y ~ xMat - 1))
plot(x, y, frame = FALSE, pch = 21, bg = "lightblue", cex = 2)
lines(x, yhat, col = "red", lwd = 2)
```

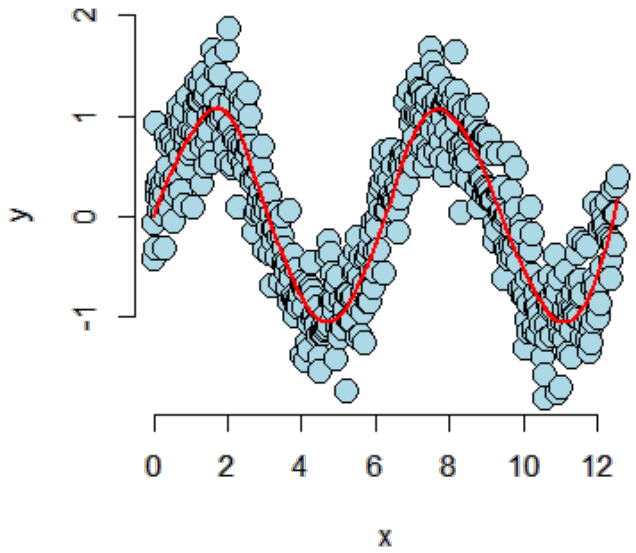


Adding squared terms

- Adding squared terms makes it continuously differentiable at the knot points.
- Adding cubic terms makes it twice continuously differentiable at the knot points; etcetera.

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \sum_{k=1}^{d} (x_i - \xi_k)_+^2 \gamma_k + \epsilon_i$$

```r
splineTerms <- sapply(knots, function(knot) (x > knot) * (x - knot)^2)
xMat <- cbind(1, x, x^2, splineTerms)
yhat <- predict(lm(y ~ xMat - 1))
plot(x, y, frame = FALSE, pch = 21, bg = "lightblue", cex = 2)
lines(x, yhat, col = "red", lwd = 2)
```

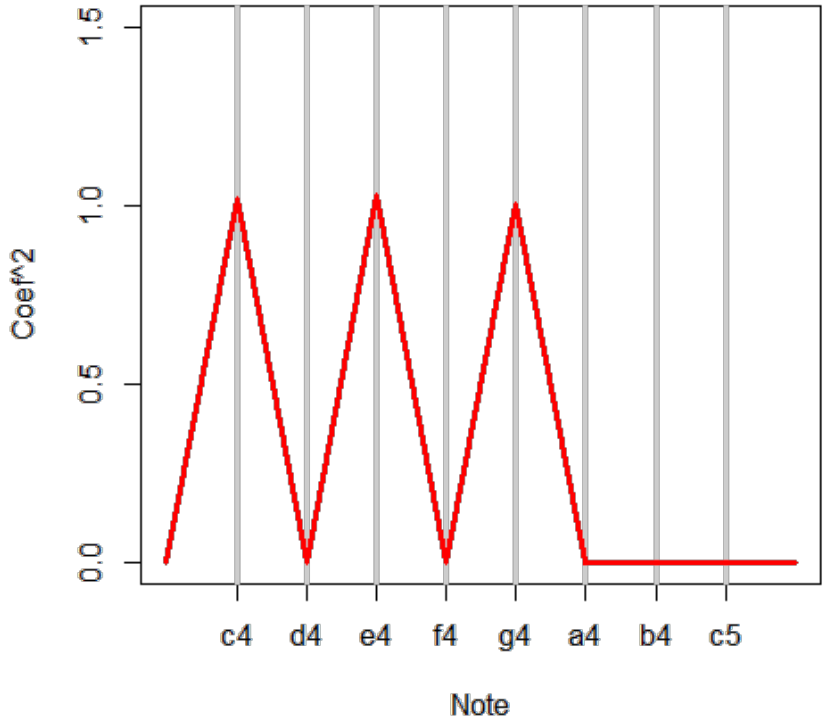


Notes

- The collection of regressors is called a basis.
  - People have spent **a lot** of time thinking about bases for this kind of problem. So, consider this as just a teaser.
- Single knot point terms can fit hockey stick like processes.
- These bases can be used in GLMs as well.
- An issue with these approaches is the large number of parameters introduced.
  - Requires some method of so called regularization.

Harmonics using linear models

```
##Chord finder, playing the white keys on a piano from octave c4 - c5
notes4 <- c(261.63, 293.66, 329.63, 349.23, 392.00, 440.00, 493.88, 523.25)
t <- seq(0, 2, by = .001); n <- length(t)
c4 <- sin(2 * pi * notes4[1] * t); e4 <- sin(2 * pi * notes4[3] * t);
g4 <- sin(2 * pi * notes4[5] * t)
chord <- c4 + e4 + g4 + rnorm(n, 0, 0.3)
x <- sapply(notes4, function(freq) sin(2 * pi * freq * t))
fit <- lm(chord ~ x - 1)
```


Coef^2
0.0
0.5
1.0
1.5
c4
d4
e4
f4
g4
a4
b4
c5
Note

```
##(How you would really do it)
a <- fft(chord); plot(Re(a)^2, type = "l")
```