Topics in Regression

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- 1. Understanding Multiple Regression
- 2. Regression Model Assumptions
- 3. Residual Plots
- 4. Non Linearity
- 5. Variable Interaction
- 6. The Log, Outliers and Standardized Residuals
- 7. Trees

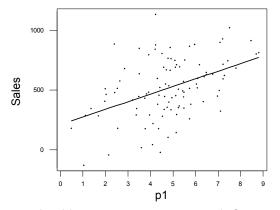
1. Understanding Multiple Regression

- ► There are two, very important things we need to understand about the MLR model:
 - 1. How dependencies between the X's affect our interpretation of a multiple regression;
 - 2. How dependencies between the X's inflate standard errors (aka multicolinearity)
- We will look at a few examples to illustrate the ideas...

The Sales Data:

- ► Sales: units sold in excess of a baseline
- ▶ P1: our price in \$ (in excess of a baseline price)
- ▶ *P2*: competitors price (again, over a baseline)

If we regress Sales on our own price, we obtain a somewhat surprising conclusion... the higher the price the more we sell!!



It looks like we should just raise our prices, right?

The regression equation for Sales on own price (P1) is:

$$Sales = 211 + 63.7P1$$

If now we add the competitors price to the regression we get

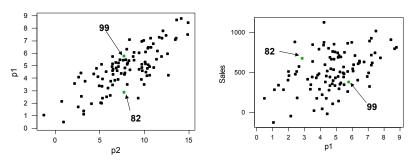
$$Sales = 116 - 97.7P1 + 109P2$$

Does this look better? How did it happen?

Remember: -97.7 is the affect on sales of a change in P1 with P2 held fixed!!

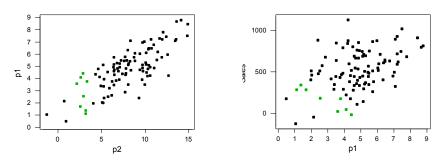
How can we see what is going on? Let's compare Sales in two different observations: weeks 82 and 99.

We see that an increase in P1, holding P2 constant, corresponds to a drop in Sales!



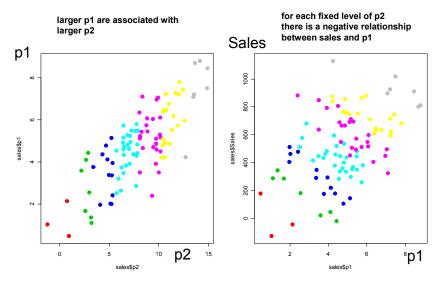
Note the strong relationship (dependence) between P1 and P2!!

Let's look at a subset of points where P1 varies and P2 is held approximately constant...



For a fixed level of P2, variation in P1 is negatively correlated with Sales!!

Below, different colors indicate different ranges for P2...

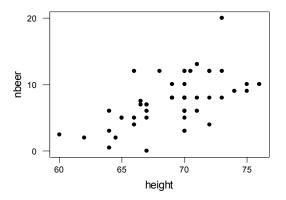


Summary:

- 1. A larger P1 is associated with larger P2 and the overall effect leads to bigger sales
- 2. With P2 held fixed, a larger P1 leads to lower sales
- 3. MLR does the trick and unveils the "correct" economic relationship between Sales and prices!

The Beer Data

- nbeer number of beers before getting drunk
- height and weight



Is number of beers related to height?

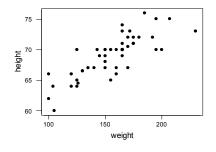
```
nbeers = \beta_0 + \beta_1 height + \epsilon
Call:
lm(formula = nbeer ~ height, data = beerd)
Residuals:
  Min
         10 Median
                              Max
-6.164 -2.005 -0.093 1.738 9.978
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) -36.9200
                        8.9560 -4.122 0.000148 ***
             0.6430
                        0.1296
                                 4.960 9.23e-06 ***
height
---
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 3.109 on 48 degrees of freedom
Multiple R-squared: 0.3389, Adjusted R-squared: 0.3251
F-statistic: 24.6 on 1 and 48 DF, p-value: 9.23e-06
```

Yes! Beers and height are related...

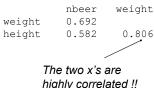
$$nbeers = \beta_0 + \beta_1 weight + \beta_2 height + \epsilon$$

```
Call:
lm(formula = nbeer ~ weight + height, data = beerd)
Residuals:
   Min
            10 Median
                                   Max
-8.5080 -2.0269 0.0652 1.5576 5.9087
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -11.18709 10.76821 -1.039 0.304167
weight
            0.08530
                      0.02381 3.582 0.000806 ***
height
            0.07751 0.19598 0.396 0.694254
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 2.784 on 47 degrees of freedom
Multiple R-squared: 0.4807, Adjusted R-squared: 0.4586
F-statistic: 21.75 on 2 and 47 DF, p-value: 2.056e-07
```

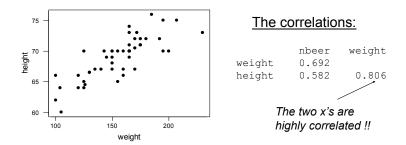
What about now?? Height is not necessarily a factor...



The correlations:



- highly correlated !!
- ▶ If we regress "beers" only on height we see an effect. Bigger heights go with more beers.
- However, when height goes up weight tends to go up as well... in the first regression, height was a proxy for the real cause of drinking ability. Bigger people can drink more and weight is a more accurate measure of "bigness".



In the multiple regression, when we consider only the variation in height that is not associated with variation in weight, we see no relationship between height and beers.

$nbeers = \beta_0 + \beta_1 weight + \epsilon$

```
Call:
lm(formula = nbeer ~ weight, data = beerd)
Residuals:
   Min
            10 Median
                                   Max
-8.7709 -2.0304 -0.0742 1.6580 5.6556
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) -7.02070 2.21329 -3.172 0.00264 **
weight
            0.09289 0.01399 6.642 2.6e-08 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 2.76 on 48 degrees of freedom
Multiple R-squared: 0.4789, Adjusted R-squared: 0.4681
F-statistic: 44.12 on 1 and 48 DF, p-value: 2.602e-08
```

Why is this a better model than the one with weight and height??

In general, when we see a relationship between y and x (or x's), that relationship may be driven by variables "lurking" in the background which are related to your current x's.

This makes it hard to reliably find "causal" relationships. Any correlation (association) you find could be caused by other variables in the background... correlation is NOT causation

Any time a report says two variables are related and there's a suggestion of a "causal" relationship, ask yourself whether or not other variables might be the real reason for the effect. Multiple regression allows us to control for all important variables by including them into the regression. "Once we control for weight, height and beers are NOT related"!!

It is *very* common to see a "correlation" reported in the press and then immediately discussed as if it were causation.

Example

"Kids have better grades in school when families eat dinner together"

Does this mean if you randomly pick a family and make them eat dinner together the grades will go up??

Could there be another variable related to both "grades" and "dinners" which is the real "cause"??

Note:

The *gold standard* for establishing a causal link between y and x is to do an experiment where you randomly move x around.

Why is this good?

If you move x around randomly, it can't be correlated with other factors.

If you move x around randomly, it is more the like an arbitrary intervention in the system where you apply the "treatment" of changing x.

Wall Street Journal, August 3, 2023, 'Random Acts of Medicine' Review: Paging Dr. Chance

Most correlation isn't causation, but true wisdom comes from knowing that some correlation is causation. Take the correlation between losing weight and being given Ozempic or Wegovy in a randomized controlled trial.

That correlation is causal, that's the value of a randomized controlled trial, and it explains why the new weight-loss drugs are in high demand.

Such trials are powerful but often not possible. Enter

"Random Acts of Medicine: The Hidden Forces That Sway Doctors, Impact Patients, and Shape Our Health," written by the absurdly overachieving economist and physician Anupam Jena and his only slightly less overachieving co-author,

Christopher Worsham, both of them practicing physicians, researchers and professors at Harvard. Messrs. Jena and Worsham are the Freakonomicists of the medical realm|they specialize in uncovering unique "natural experiments" that shed light on medicine and medical practice.

Correlation, Causation, and the Joint

w: weight, h:height, b:beer.

$$p(h,w,b) = p(w) p(h|w) p(b|h,w)$$

$$could be: p(b|h,w) = p(b|w)$$

$$= p(w) p(h|w) p(b|w)$$

$$Nice Pidure$$

$$(b)$$

h and b are correlated because they are both related to the same underlying cause w.

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Conditional Independence

$$p(h, b \mid w) = p(h \mid w) p(b \mid w)$$

Given W, H and B are independent.

In General:

When x_1 and x_2 are related but only x_2 really matters for y, we can see dependence between x_1 and y but not *conditional* on x_2 .

If I regress y on x_1 , x_1 will seem important. If I regress y on x_1 and x_2 , x_1 will not seem important.

Wall Street Journal, August 30 2023

https://www.wsj.com/us-news/education/female-professors-sue-vassar-college-alleging-gender-based-salary-discrimination-8c3024a5

Female Professors Sue Vassar College, Alleging Gender-Based Salary Discrimination Vassar, founded as one the country's first women's colleges, pays women 10% less, lawsuit says

During the 2021-2022 school year, male professors earned an average salary of \$153,238 while female professors earned \$139,332|or 10% less, according to the suit. The pay gap has ranged between 7.6% and 14.6% since 2003.

"Vassar believes it pays its faculty fairly and equitably and has complied with the law,"" Friscia wrote. "Faculty salaries are set by a faculty-led, peer-review process, per Vassar's governance structure."

Andrew Luna, executive director of institutional research at Austin Peay State University, who has researched faculty pay and gender gaps, said the difference could be explained by the distribution of men and women across disciplines. Business, science and technology faculty positions tend to pay more than faculty positions in the humanities...

..the difference could be explained by the distribution of men and women across disciplines. Business, science and technology faculty positions tend to pay more than faculty positions in the humanities...

G: gender, D:department, P: pay

$$G \Rightarrow D \Rightarrow P$$

G is not independent of P, but given D, G is independent of P.

Kelly Dermody, attorney for the plaintiffs, said that while the data in the lawsuit doesn't take into account pay variation between disciplines, the plaintiffs, which include professors who teach African-American history, physics and psychological science, allege the pay gap is also present within departments.

The suit alleges women are paid less when they are hired and then promoted at a slower pace based on an biased and subjective evaluation process for compensation and promotion. The process includes peer reviews and student reviews.

The average merit rating for female professors is 2.24; for men it is 2.41.

Tricky:

To interpret an estimated effect as causal you have to control for the right variables.

If you put in too many variables, this can inflate the standard errors (see next section !!).

Correlation between x's and Standard Errors

In the regression:

$$nbeers = \beta_0 + \beta_1 height + \epsilon$$

the standard error associated with the height coefficient $\hat{\beta}_1$ is .13.

In the regression:

$$nbeers = \beta_0 + \beta_1 weight + \beta_2 height + \epsilon$$

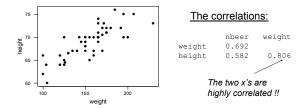
the standard error associated with the height coefficient $\hat{\beta}_2$ is .2.

Why is the se bigger in the multiple regression ???

In this regression

$$nbeers = \beta_0 + \beta_1 height + \epsilon$$

we use all the variation of height to estimate β_1 .



In the regression:

$$nbeers = \beta_0 + \beta_1 weight + \beta_2 height + \epsilon$$

we can only use the variation in height unrelated to variation in weight.

With more than $2 \times x$'s we have the same ideas.

Estimation of the coefficient for x_j depends on variation in x_j unrelated to all the other x's.

2. Regression Model Assumptions

Regression Model Assumptions

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

Recall the key assumptions of our linear regression model:

- (i) The mean of Y is linear in x's.
- (ii) The additive errors (deviations from line)
 - are normally distributed
 - independent from each other
 - identically distributed (i.e., they have constant variance)

$$Y_i|x_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$$

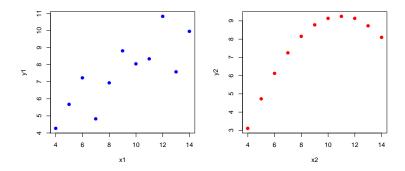
Inference and prediction relies on this model being "true"!

If the model assumptions do not hold, then all bets are off:

- prediction can be systematically biased
- standard errors, intervals, and t-tests are wrong

We will focus on using graphical methods (plots!) to detect violations of the model assumptions.

Example:



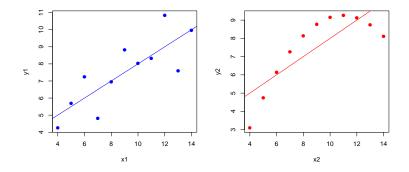
Here we have two datasets... Which one looks compatible with our modeling assumptions?

```
Call:
                      lm(formula = v1 ~ x1, data = ad)
                      Residuals:
                           Min
                                     10 Median
                                                      30
                                                              Max
                      -1.92127 -0.45577 -0.04136 0.70941 1.83882
Regression of
                      Coefficients:
                                  Estimate Std. Error t value Pr(>|t|)
                       (Intercept)
                                    3.0001
                                              1.1247
                                                       2.667 0.02573 *
                                              0.1179
                                                       4.241 0.00217 **
                       v1
                                    0.5001
                      Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
                      Residual standard error: 1.237 on 9 degrees of freedom
                      Multiple R-squared: 0.6665, Adjusted R-squared: 0.6295
                      F-statistic: 17.99 on 1 and 9 DF, p-value: 0.00217
                      Call:
                      lm(formula = y2 ~ x2, data = ad)
                      Residuals:
                          Min
                                   10 Median
                                                   30
                                                         Max
                      -1.9009 -0.7609 0.1291 0.9491 1.2691
Regression of
                      Coefficients:
                                  Estimate Std. Error t value Pr(>|t|)
                                                       2.667 0.02576 *
                      (Intercept)
                                     3.001
                                                1.125
                       x2
                                     0.500
                                                0.118 4.239 0.00218 **
                      Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
                      Residual standard error: 1.237 on 9 degrees of freedom
                      Multiple R-squared: 0.6662, Adjusted R-squared: 0.6292
                      F-statistic: 17.97 on 1 and 9 DF, p-value: 0.002179
```

y1 on x1.

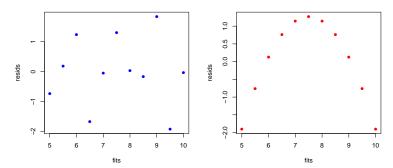
y2 on x2.

The regression output values are exactly the same...



Thus, whatever decision or action we might take based on the output would be the same in both cases!

...the residuals (plotted against \hat{Y}) look totally different!!



Plotting e vs \hat{Y} is your #1 tool for finding fit problems.

If the modelling assumptions are "right", how should the plot of e_i vs. \hat{y}_i look?

3. Residual Plots

We use residual plots to "diagnose" potential problems with the model.

Fits:

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + \hat{\beta}_2 x_{2i} + \dots + \hat{\beta}_k x_{ki}.$$

From the model assumptions, the error term (ϵ) should have a few properties... we use the residuals (e) as a proxy for the errors as:

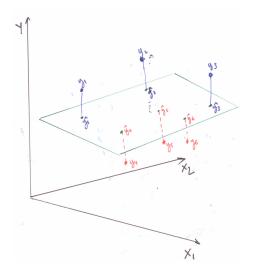
$$\epsilon_{i} = y_{i} - (\beta_{0} + \beta_{1}x_{1i} + \beta_{2}x_{2i} + \dots + \beta_{k}x_{ki})$$

$$\approx y_{i} - (\hat{\beta}_{0} + \hat{\beta}_{1}x_{1i} + \hat{\beta}_{2}x_{2i} + \dots + \hat{\beta}_{k}x_{ki})$$

$$= y_{i} - \hat{y}_{i}$$

$$= e_{i}$$

Fits and Resids with 2 x's



What kind of properties should the residuals have??

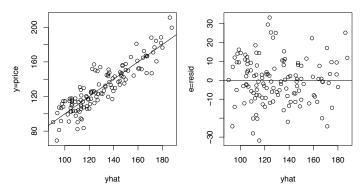
$$e_i \approx N(0, \sigma^2)$$
 iid and independent from the x's

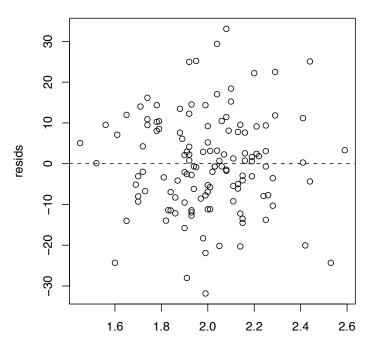
- We should see no pattern between e and each of the x's
- This can be summarized by looking at the plot between \hat{Y} and e, there should be no relationship.
- Remember that \hat{Y} is "pure x", i.e., a linear function of the x's.

If the model is good, the regression should have pulled out of Y all of its "x ness" ... what is left over (the residuals) should have nothing to do with x.

Example - Mid City (Housing)

Left: \hat{y} vs. yRight: \hat{y} vs e





In the Mid City housing example, the residuals plots (both x vs. e and \hat{Y} vs. e) showed no obvious problem...

this is what we want!!

Although these plots don't guarantee that all is well, it is a very good sign that the model is doing a good job.

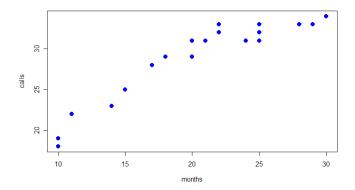
4. Non Linearity

Example: Telemarketing

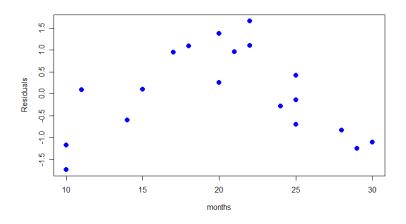
x: time on job in months.

y: number of calls made per day.

How does length of employment affect productivity (number of calls per day)?



Residual plot (x vs. e) highlights the non-linearity!



What can we do to fix this??

We can use multiple regression and transform our \boldsymbol{x} to create a non linear model...

Let's try

$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

The data...

months	months2	calls		
10	100	18		
10	100	19		
11	121	22		
14	196	23		

The Linear fit and resids:

Calls =
$$\beta_0 + \beta_1 months + \epsilon$$

```
Call:
lm(formula = calls ~ months, data = td)
Residuals:
    Min
               10
                   Median
-3.10592 -1.31628 -0.05404 1.69596
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 13.67077
                        1.42697
                                   9.58 1.72e-08 ***
                                  11.15 1.62e-09 ***
months
             0.74351
                        0.06666
               0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1
Signif. codes:
Residual standard error: 1.787 on 18 degrees of freedom
Multiple R-squared: 0.8736, Adjusted R-squared: 0.8666
F-statistic: 124.4 on 1 and 18 DF, p-value: 1.622e-09
```

The Quadratic fit and resids:

Calls =
$$\beta_0 + \beta_1 months + \beta_2 months^2 + \epsilon$$

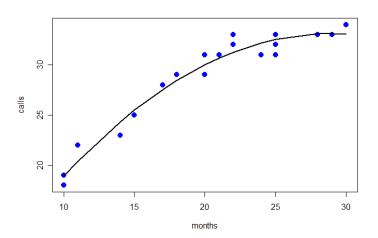
```
Call:
lm(formula = calls ~ ., data = td2)
Residuals:
    Min
               10
                   Median
-1.54068 -0.64294 -0.02111 0.59967
                                    1.73325
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.140471
                       2.322630
                                  -0.060
                                   9.236 4.90e-08 ***
months
             2.310202
                       0.250122
            -0.040118
                       0.006333 -6.335 7.47e-06 ***
months2
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1
Residual standard error: 1.003 on 17 degrees of freedom
Multiple R-squared: 0.9624.Adjusted R-squared: 0.958
F-statistic: 217.5 on 2 and 17 DF, p-value: 7.764e-13
```

Calls =
$$-.14 + 2.231$$
 months $-.04$ months² ± 2

Much smaller s with x^2 . Much bigger R^2 with x^2 . Much better residual plot.

Calls = $-.14 + 2.231 \text{ months} - .04 \text{ months}^2 \pm 2$

$$\hat{Y}_i = b_0 + b_1 X_i + b_2 X_i^2$$



Polynomial Regression

Even though we are limited to a linear mean, it is possible to get nonlinear regression by transforming the x variable.

In general, we can add powers of x to get polynomial regression:

$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 \dots + \beta_m x^m + \epsilon$$

You can fit any mean function if m is big enough.

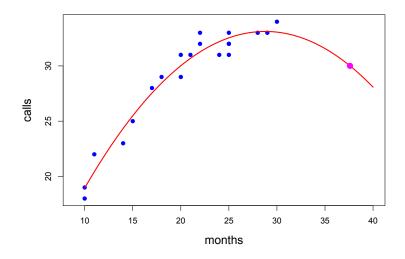
Usually, m = 2 does the trick.

We can always add higher powers (cubic, etc) if necessary.

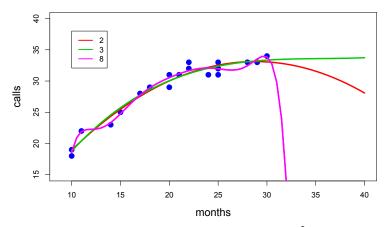
Be very careful about predicting outside the data range. The curve may do unintended things beyond the observed data.

Watch out for over-fitting... remember, simple models are "better".

Be careful when extrapolating...



...and, be careful when adding more polynomial terms!



The 8th order polynomial will have the highest R^2 . Is it the best regression model?

5. Variable Interaction

Imagine you are a trial lawyer and you want to file a suit against a company for salary discrimination... you gather the following data...

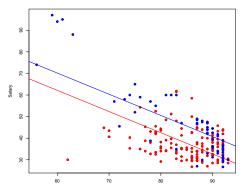
```
YH Gender Salary Sex
1 92 Male 32.00 1
2 81 Female 39.10 0
3 83 Female 33.20 0
4 87 Female 30.60 0
5 92 Male 29.00 1
... ... ...
208 62 Female 30.00 0
```

Every observation corresponds to an employee.

```
y=salary
Gender (=Sex as a binary dummy)
YH is year hired, we'll call it "experience".
```

$$Salary_i = \beta_0 + \beta_1 Exp_i + \beta_2 Sex_i + \epsilon_i$$

Blue:men Red: women.



Does it look like the effect of experience on salary is the same for males and females?

Could we try to expand our analysis by allowing a different slope for each group?

Consider the following model:

$$Salary_i = \beta_0 + \beta_1 Exp_i + \beta_2 Sex_i + \beta_3 Exp_i \times Sex_i + \epsilon_i$$

For Females:

$$Salary_i = \beta_0 + \beta_1 Exp_i + \epsilon_i$$

For Males:

$$Salary_i = (\beta_0 + \beta_2) + (\beta_1 + \beta_3)Exp_i + \epsilon_i$$

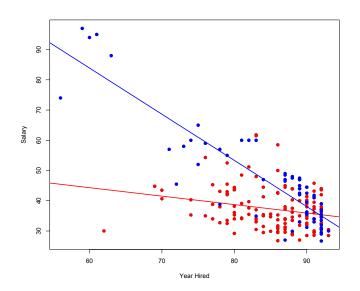
What does the data look like?

	YrHired	Gender	Salary	Sex	SexExp
1	92	Male	32.00	1	92
2	81	${\tt Female}$	39.10	0	0
3	83	${\tt Female}$	33.20	0	0
4	87	${\tt Female}$	30.60	0	0
5	92	Male	29.00	1	92
2	08 62	Female	30.00	0	0

$Salary_i = \beta_0 + \beta_1 Sex_i + \beta_2 Exp + \beta_3 Exp * Sex + \epsilon_i$

```
Call:
lm(formula = Salary ~ ., data = sd1)
Residuals:
              10 Median
    Min
                                30
                                       Max
-20 0685 -4 6506 -0 7679 4 4034 23 9122
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 61.1248
                        8.7709 6.969 4.32e-11 ***
                    11.7012 9.780 < 2e-16 ***
           114.4426
sex
           -0.2800
                      0.1025 -2.733 0.00684 **
exp
            -1.2478
                       0.1367 -9.130 < 2e-16 ***
expsex
---
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 6.816 on 204 degrees of freedom
Multiple R-squared: 0.6386, Adjusted R-squared: 0.6333
F-statistic: 120.2 on 3 and 204 DF, p-value: < 2.2e-16
```

$$Salary_i = 61 + 114 Sex_i + -0.28 Exp + -1.25 Exp * Sex + \epsilon_i$$

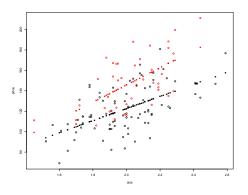


Is this good or bad news for the plaintiff?

Brick-Size Interaction

Let's see if the brick and size variables interact in the housing data:

$$Price_i = \beta_0 + \beta_1 size_i + \beta_2 brickdum_i + \beta_3 size_i \times brickdum_i + \epsilon_i$$



Here is the regression outure where sbint = *size* \times *brickdum*.

```
Call:
lm(formula = price ~ ., data = ddf)
Residuals:
    Min
            10 Median
                                  Max
-38.406 -14.091 -1.405 14.962 46.488
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept)
              4 448
                        19.397
                                0.229
                                         0.819
size
             59.074
                       9.693
                                6 094 1 28e-08 ***
                       37.234 -0.730
brickdum
            -27.193
                                         0.467
             25.130 18.387 1.367
                                         0.174
sbint
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 19.58 on 124 degrees of freedom
Multiple R-squared: 0.4817, Adjusted R-squared: 0.4692
F-statistic: 38.41 on 3 and 124 DF, p-value: < 2.2e-16
```

What does the output tell you about the relationship between price and brick??

It would be a brutal error to drop both brickdum and sbint !!

In general we can add in a *product term* by creating a x variable which is product of two others.

This is often called an interaction term:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon.$$

With the interaction term, the effect on y and changing on x depends on the other.

You can have a combination of powers and interactions:

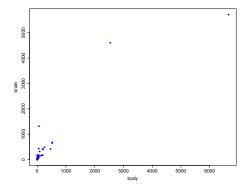
$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + \epsilon.$$

6. The Log, Outliers and Standardized Residuals

Body weight vs. brain weight...

X = body weight of a mammal in kilograms

Y = brain weight of a mammal in grams



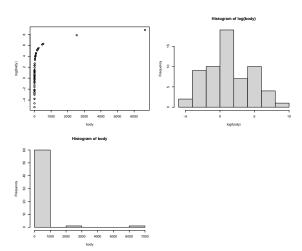
Do you feel like running a linear regression with this data?

Both the brain and body numbers are heavily right-skewed.

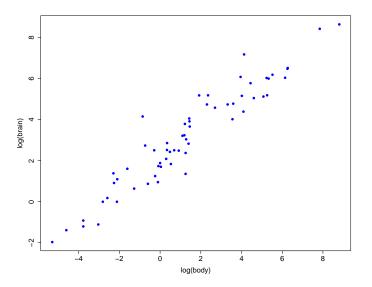
In this case it can help to transform the variable by taking the log.

Here is what happens when we take the log of the body weights.

The log pulls the big ones in!



Here is the plot of log(body) vs. log(brain).



Standardized Residuals

In our model $\epsilon \sim N(0, \sigma^2)$

The residuals e are a proxy for ϵ and $\hat{\sigma}$ is an estimate for σ

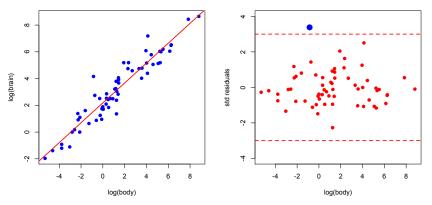
Call $z_i=rac{\epsilon_i-0}{\sigma}pprox e_i/\hat{\sigma}$, the standardized residuals... We should expect

$$z \approx N(0,1)$$

(How often should we see an observation of |z| > 2?)

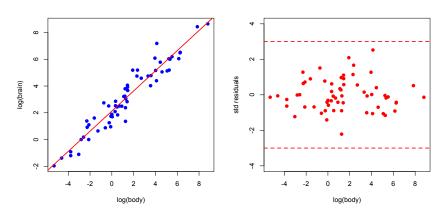
Sometimes we plot the standardized resids instead of resids because it is easier to think about what a "big one" is.

Regression fit and standardized residuals.



Looks good!! But we see a large and positive potential outlier... the Chinchilla!

It turns out that the data had the brain of a Chinchilla weighting 64 grams!! In reality, it is 6.4 grams... after correcting it:



How to Deal with Outliers

When should you delete outliers?

Only when you have a really good reason!

There is nothing wrong with running regression with and without potential outliers to see whether results are significantly impacted.

Any time outliers are dropped the reasons for removing observations should be clearly noted.

7. Trees

We have seen that we can fit nonlinear relationships using transformed variables and multiple regression.

This is very powerfull but it can also be very confusing. How do you decide what transformations to use ???!!

One popular approach is to throw in tons of transformed variable and then use some sophisticated form of variable selection to see which ones matter, the "kitchen sink" approach.

Other approaches which are popular in modern statistcs/Machine Learning/Data Science/Artificial Intelligence are Neural Networks and methods based on binary trees.

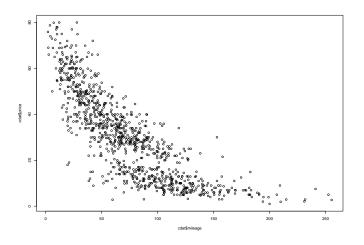
Since they are simple and powerful (my favorite combination) let's have a look at binary trees.

Let's use the used cars data in which try to predict the price of a used car.

```
> dim(cdat)
Γ17 1000
> summarv(cdat)
    price
                             isOneOwner
                                           mileage
                    trim
                                                                vear
 Min.
        : 0.995
                 430 :143
                             f:841
                                               : 1.997
                                                          Min.
                                                                 :1994
                                        1st Qu.: 40.133
 1st Qu.:12.995
                 500 :127
                             t:159
                                                          1st Qu.:2004
Median :29.800
                 550 :591
                                        Median : 67,919
                                                          Median:2007
       :30.583
                 other:139
                                        Mean : 73.652
                                                                : 2007
 Mean
                                                          Mean
3rd Qu.:43.992
                                         3rd Qu.:100.138
                                                          3rd Qu.:2010
       .79 995
                                               .255.419
 Max
                                         Max
                                                          Max
                                                                 :2013
    color
             displacement
Black :415
            4.6 :137
other :227
            5.5 .476
 Silver:213
             other:387
White :145
```

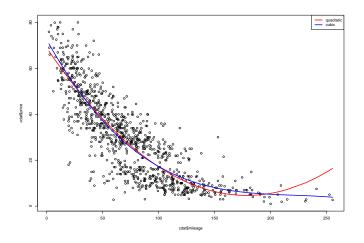
mileage in thousands of miles. price in thousands of dollars.

Let's start by having a look at how x=mileage and y=price looks.



nonlinear !!

Let's try a quadratic and cubic fit.



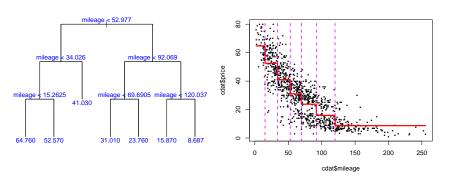
We needed the cubic model to get a good looking fit:

price =
$$\beta_0 + \beta_1 m + \beta_2 m^2 + \beta_3 m^3 + \epsilon$$

This is a *tree* fit to the data.

At each *interior node* there is a decision rule of the form $\{x < c\}$. If x < c you go left, otherwise you go right.

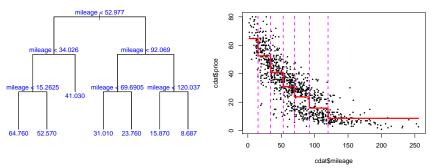
Each observation is sent down the tree until it hits a bottom node or *leaf* of the tree.



The set of bottom nodes gives us a partition of the predictor (x) space into disjoint intervals.

The vertical lines display the interval boundaries.

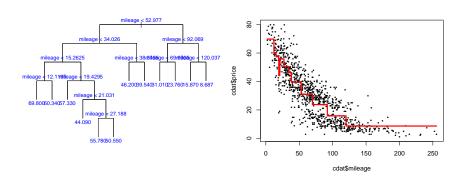
Within each interval we compute the average of the y values for the subset of data in the region. This gives us the step function fit to the data. The \bar{y} values are also printed at the bottom nodes (left plot).



To predict, we just use our step function estimate of f(x).

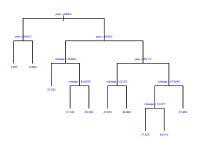
Equivalently, we drop x down the tree until it lands in a leaf and then predict the average of the y values for the training observations in that leaf (or bottom node).

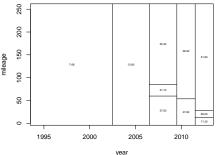
We can choose how big to build the tree.

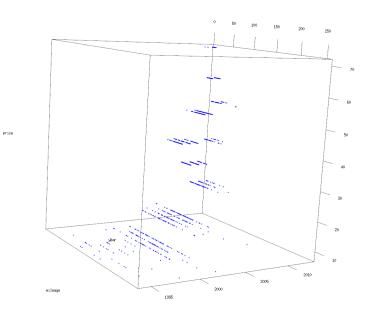


We can use more than one x variable.

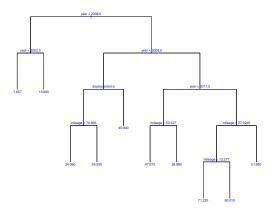
Now each rule involves a choice of cut point and a choice of which x variable to use.







This scheme works with any number of x's !!!! Let's use all the x's.



Notice the form of the rule for the categorical variable displacement.

It tell us which categories get sent left.

In this case the second ("b") category goes left and all the others go right.

Trees can automatically figure out nonlinearity !!!

Trees can automatically figure out interactions !!!

Trees can decide which variable to use !!!

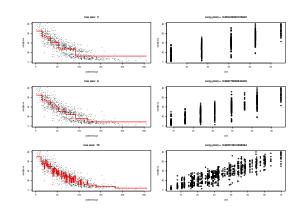
Trees can use both categorical and numeric x simply !!!

Choosing the size of the tree (number of bottom nodes or leaves) is tricky!!

At left is the tree.

At right is \hat{y} vs. y, the fits vs. y.

Which of these three sizes (5, 8, or 70 leaves) do you like the best?



Even though the tree with 70 nodes gives us the best fit in terms of the \hat{y} vs. y plot, we don't like it!!!

We don't believe the true relationship can't be that complex.

We say we have *overfit* the data.

The tree with 5 bottom nodes (or leaves) might be too simple. The resulting step-function is too crude.

Maybe the size 8 tree is a reasonable choice.

Train and Test:

We may not want to just look at the fit and pick one we like.

With many x's this is very difficult.

A key observation is that we cannot just pick the tree size which gives us the best fit !!!

We would always just pick the biggest tree.

Assuming our goal is make a prediction we:

- Randomly split our data into two subsets, the train and test data.
- Fit trees using the training data.
- ► For each tree fit obtained using the training data, we predict on the test data.
- Measure the prediction accuracy using (for example) root mean squared error (rmse).

$$rmse = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_i)^2}$$

This is called the *out of sample* rmse. It is the rmse on data **not** used to fit the model.

I randomly split the data into 750 training data observation and 250 test observations.

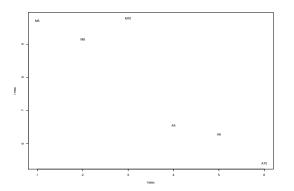
For tree sizes 5, 8, and 70 if fit a tree of that size using just mileage and all the variables and the training data.

For each of the 2*3=6 fitted tree models I predicted on the 250 test observations and computed the rmse.

Out of Sample rmse for different tree models

M: just using mileage.

A: all the variables.



With just mileage our intuition was right, 8 is the best choice of the three.

With all the variables a more complex tree works!! Notice how much smaller our rmse is using all the variables.

Note:

With only 1,000 observations, I worry that my results depend on the random split.

I actually repeated the process several times (changing the seed!!) and I got similar results each time.

Fit, but don't over-fit !!!!

$$Y = f(x) + \epsilon$$

 $Y = \text{signal} + \text{noise}$

You want the model complicated enough to capture f but not so complicated that you fit ϵ !!!

If you fit ϵ it will be misleading when you go to predict because new data has a new ϵ .

Modern computational data science is *exploding* with new techniques!!!

Regression and trees are two of the major players.

All the methods have pros and cons, e.g.

Trees Pro: don't have to think about what transformations to use (unlike regression).

Trees Con: difficult to assess uncertainty (no confidence intervals as in regression).

Trees Pro: small trees are interpretable.

Trees Con: big trees are not interpretable.