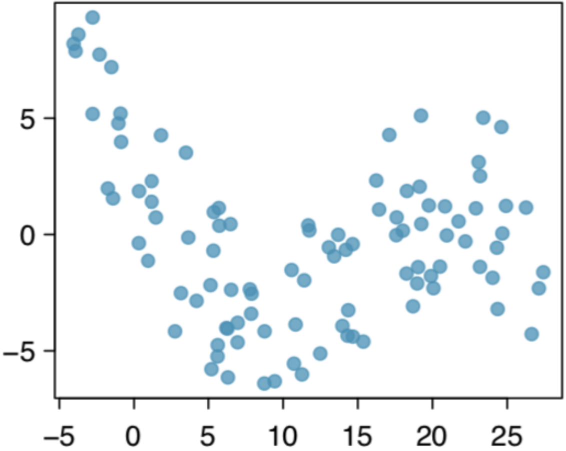
Nonlinear Trends and Multiple Regression Case Study

November 20, 2019

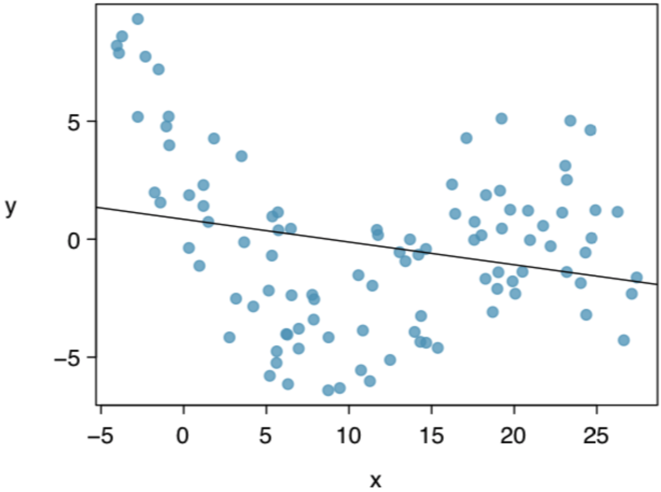
Fitting a Polynomial Curve

Consider the following data:



Fitting a Polynomial Curve

...with the best fitting straight line:



Fitting a Polynomial Curve

- Clearly, the straight line does not fit well.
- If we drew a curve following the apparent relationship, the variance would be approximately **homoskedastic**.
    - homoskedastic = constant (same) variance
- This is a good sign that we want to fit a curve rather than transforming y.

Fitting a Polynomial Curve

In order to fit a curve, we generate what's called a **polynomial basis of $\boldsymbol{x}$**.

All this means is that we take x and create

- $x_1 = x$
- $x_2 = x^2$
- $x_3 = x^3$
- etc.

Fitting a Polynomial Curve

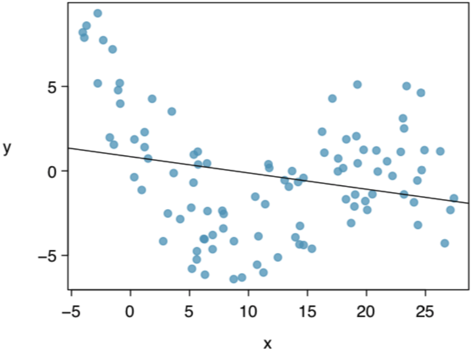
We will then use these variables in the multiple regression model.

Note:

- It is uncommon to use terms beyond x^2.
- It is very rare to use terms beyond x^3.

The Linear Model

Let's start by looking at the best fitting straight line from



$$\hat{y} = 0.8441 - 0.0964x$$

The Linear Model

	Estimate	Std Error	t value	Pr(> |t|)
(Intercept)	0.8441	0.5799	1.46	0.1487
x1	-0.0964	0.0397	-2.43	0.0169

Why is this model inappropriate for the data?

Fitting a Polynomial Curve

Let's try adding another variable to the model: $x_2 = x^2$.

- Generally, when we fit polynomial terms, we include *both variables* in the model.
- This is in contrast to a transformation, where we include only the transformed variable.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

Example

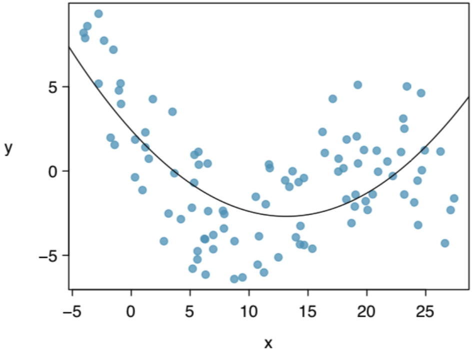
The model is summarized by

	Estimate	Std Error	t value	Pr(> |t|)
(Intercept)	2.4252	0.5079	4.78	0.0000
x1	-0.7769	0.0956	-8.13	0.0000
x2	0.0295	0.0039	7.55	0.0000

Write out the regression model.

Fitting a Polynomial Curve

Based on the scatterplot overlaid with the polynomial curve,



a quadratic model is still insufficient.

Cubic Terms

Let's try including a cubic term. This model looks like

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

where $x_3 = x^3$.

- Note that we again include x_3 *and* the lower order polynomial terms x_1 and x_2.

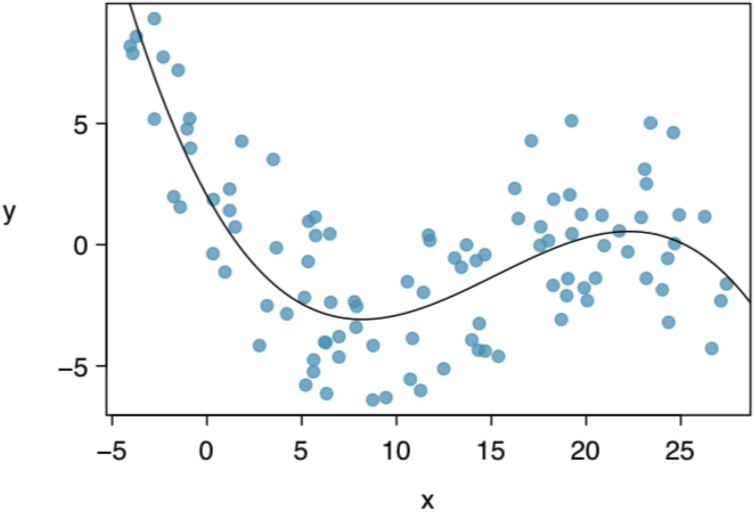
Example

This model is summarized by

	Estimate	Std Error	t value	Pr(> |t|)
(Intercept)	2.0187	0.4242	4.76	0.0000
x1	-1.4202	0.1236	-11.49	0.0000
x2	0.1187	0.0136	8.75	0.0000
x3	-0.0026	0.0004	-6.77	0.0000

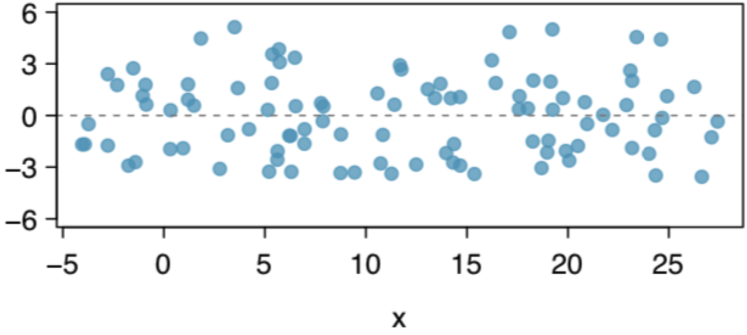
Write out the regression model.

Example



Example

This model has residual plot



A Word of Caution

- Start with x^2 and use x^3 only as necessary.
- If a cubic polynomial doesn't work, be very cautious of using higher order polynomials.
  - We don't want to force the data to fit!
  - There are other approaches to modeling that can help deal with this.
- Extrapolation is already problematic, but can be much worse for models with transformed data or polynomial terms.

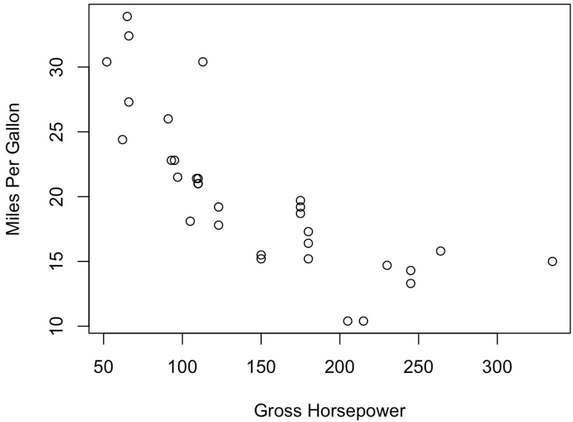
Multiple Regression Case Study: Motor Trend Cars

The `mtcars` data in `R` has data on 10 aspects of car design and performance for 32 automobiles:

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46	0	1	4	4
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02	0	1	4	4
Datsun 710	22.8	4	108	93	3.85	2.320	18.61	1	1	4	1
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.460	20.22	1	0	3	1

Example

Let's start with examining horsepower and miles per gallon.



A Simple Linear Model

It's hard to tell whether this relationship is linear or not. Let's start with the simple linear model.

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept) 30.09886    1.63392  18.421  < 2e-16 ***
hp          -0.06823    0.01012  -6.742 1.79e-07 ***

Multiple R-squared:  0.6024,Adjusted R-squared:  0.5892
```

Write the regression model. Interpret the coefficients.

A Quadratic Model

Now let's try a model with a quadratic term.

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept)     20.091      0.544  36.931  < 2e-16 ***
hp1            -26.046      3.077  -8.464 2.51e-09 ***
hp2             13.155      3.077   4.275 0.000189 ***

Multiple R-squared:  0.7561,Adjusted R-squared:  0.7393
```

Write the regression model.

Multiple Linear Regression

Now, we know that other variables may be useful... so let's try adding them in. The summary of full model (with $\texttt{hp}^2$ included) is

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	13.982035	18.988291	0.736	0.470
cyl	0.044743	1.041147	0.043	0.966
disp	0.008652	0.018070	0.479	0.637
hp1	-11.877106	8.753289	-1.357	0.190
hp2	4.959203	4.072697	1.218	0.238
drat	0.430521	1.643201	0.262	0.796
wt	-2.967539	1.971111	-1.506	0.148
qsec	0.510263	0.766336	0.666	0.513
vs	-0.190406	2.122169	-0.090	0.929
am	1.748014	2.130010	0.821	0.422
gear	0.927728	1.493229	0.621	0.541
carb	-0.469657	0.848911	-0.553	0.586

How many predictors are in this model? What does β_4 represent?

Example

- The estimated coefficient for `hp`^{2} in the smaller model was 13.155
- In the full model, this coefficient is 4.959.

Why might this difference occur?

Let's do a backward selection based on p-values.

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	13.982035	18.988291	0.736	0.470
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What variable do we remove first?

Model Selection

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	14.516933	13.994971	1.037	0.311
disp	0.008873	0.016907	0.525	0.605
hp1	-11.796710	8.345344	-1.414	0.172
hp2	4.937641	3.944451	1.252	0.224
drat	0.413058	1.553865	0.266	0.793
wt	-2.979803	1.903425	-1.565	0.132
qsec	0.503152	0.730261	0.689	0.498
vs	-0.216661	1.983443	-0.109	0.914
am	1.728754	2.032237	0.851	0.405
gear	0.904345	1.357122	0.666	0.512
carb	-0.460509	0.802022	-0.574	0.572

Model Selection

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	14.922119	13.187937	1.131	0.270
disp	0.009315	0.016044	0.581	0.567
hp1	-11.914838	8.087022	-1.473	0.155
hp2	4.832406	3.738113	1.293	0.210
drat	0.401197	1.514859	0.265	0.794
wt	-2.985060	1.859596	-1.605	0.123
qsec	0.474635	0.666511	0.712	0.484
am	1.774822	1.942840	0.914	0.371
gear	0.874993	1.300039	0.673	0.508
carb	-0.440539	0.763170	-0.577	0.570

Model Selection

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	16.176651	12.056492	1.342	0.193
disp	0.009256	0.015714	0.589	0.562
hp1	-12.340452	7.763871	-1.589	0.126
hp2	5.071981	3.552934	1.428	0.167
wt	-3.018258	1.817474	-1.661	0.110
qsec	0.471422	0.652791	0.722	0.477
am	1.848385	1.883611	0.981	0.337
gear	0.953887	1.239606	0.770	0.449
carb	-0.424462	0.745215	-0.570	0.574

Model Selection

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  13.41166   10.87958   1.233  0.22961
disp          0.01510    0.01174   1.286  0.21057
hp1         -14.31438    6.84901  -2.090  0.04739 *
hp2           4.62330    3.41540   1.354  0.18846
wt           -3.76861    1.23435  -3.053  0.00547 **
qsec          0.67281    0.54097   1.244  0.22562
am            2.00853    1.83611   1.094  0.28486
gear          0.67669    1.12392   0.602  0.55277
```

Model Selection

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  16.62533    9.35861   1.776  0.08783 .
disp          0.01200    0.01041   1.152  0.26006
hp1         -13.19944    6.50931  -2.028  0.05337 .
hp2           4.79117    3.36032   1.426  0.16629
wt           -3.66706    1.20708  -3.038  0.00551 **
qsec          0.64249    0.53171   1.208  0.23822
am            2.52789    1.60007   1.580  0.12671
```

Model Selection

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  20.2315     8.8754   2.280  0.03108 *
hp1         -11.5546     6.3908  -1.808  0.08219 .
hp2           4.5925     3.3770   1.360  0.18553
wt           -2.7832     0.9379  -2.967  0.00637 **
qsec          0.4486     0.5075   0.884  0.38492
am            1.9866     1.5392   1.291  0.20817
```

Model Selection

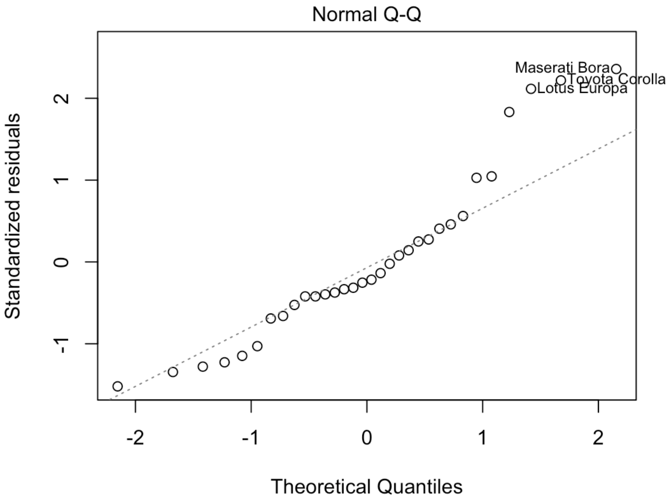
```
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  27.5420     3.2037   8.597 3.27e-09 ***
hp1         -16.2337     3.5647  -4.554 0.000101 ***
hp2           6.1579     2.8635   2.151 0.040628 *  
wt           -2.4839     0.8711  -2.851 0.008242 ** 
am            1.3289     1.3419   0.990 0.330791    
```

Model Selection

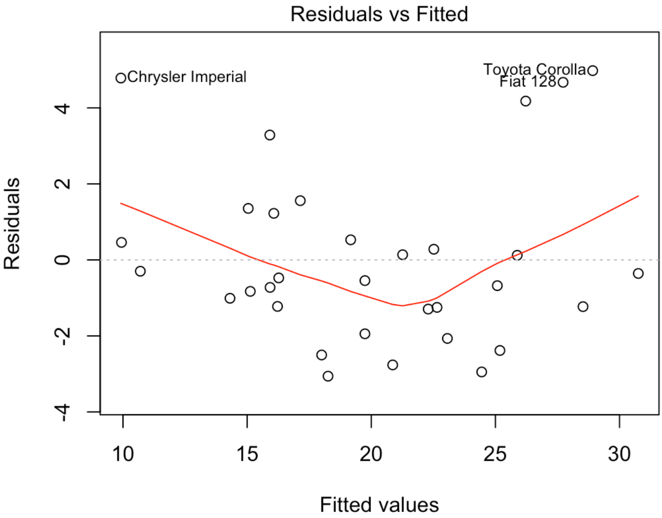
```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)   29.8389     2.2093  13.506 8.72e-14 ***
hp1          -15.1717     3.3984  -4.464  0.00012 ***
hp2            6.8997     2.7628   2.497  0.01867 *
wt            -3.0300     0.6741  -4.495  0.00011 ***
```

Write out the final model.

Now that we have a final model, we should check our regression diagnostics.



Diagnostics: Constant Variance



Diagnostics: Residuals vs. Predictors