SLR: Model Evaluation and Diagnostics

Nicky Wakim

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Learning Objectives

1. Use visualizations and cut off points to flag potentially influential points using residuals, leverage, and Cook's distance
2. Handle influential points and assumption violations by checking data errors, reassessing the model, and making data transformations.
3. Implement a model with data transformations and determine if it improves the model fit.

Let's remind ourselves of the model that we have been working with

- We have been looking at the association between life expectancy and female literacy rate
- We used OLS to find the coefficient estimates of our best-fit line

pop model $Y = \beta_0 + \beta_1 X + \epsilon$

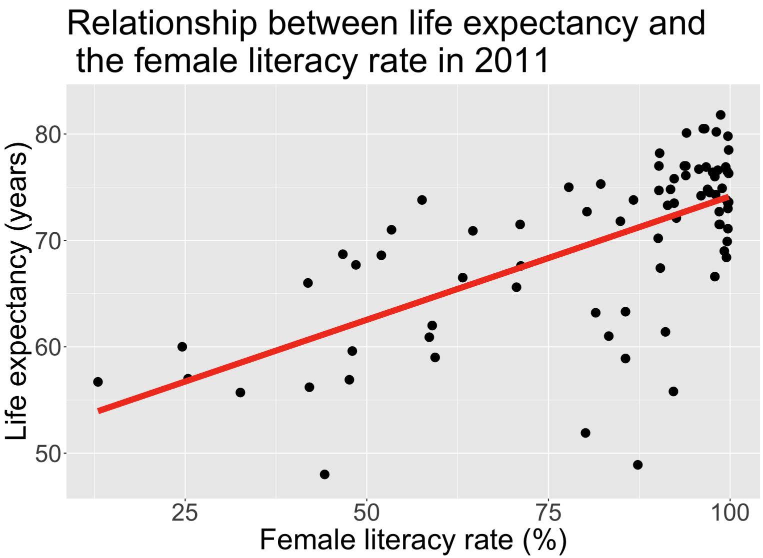
fit

term	estimate	std.error	statistic	p.value
(Intercept)	50.93	2.66	19.14	0.00
female_literacy_rate_2011	0.23	0.03	7.38	0.00

$$\widehat{Y} = \widehat{\beta}_0 + \widehat{\beta}_1 \cdot X$$

$$\text{life } \widehat{\text{expectancy}} = 50.9 + 0.232 \cdot \text{female literacy rate}$$

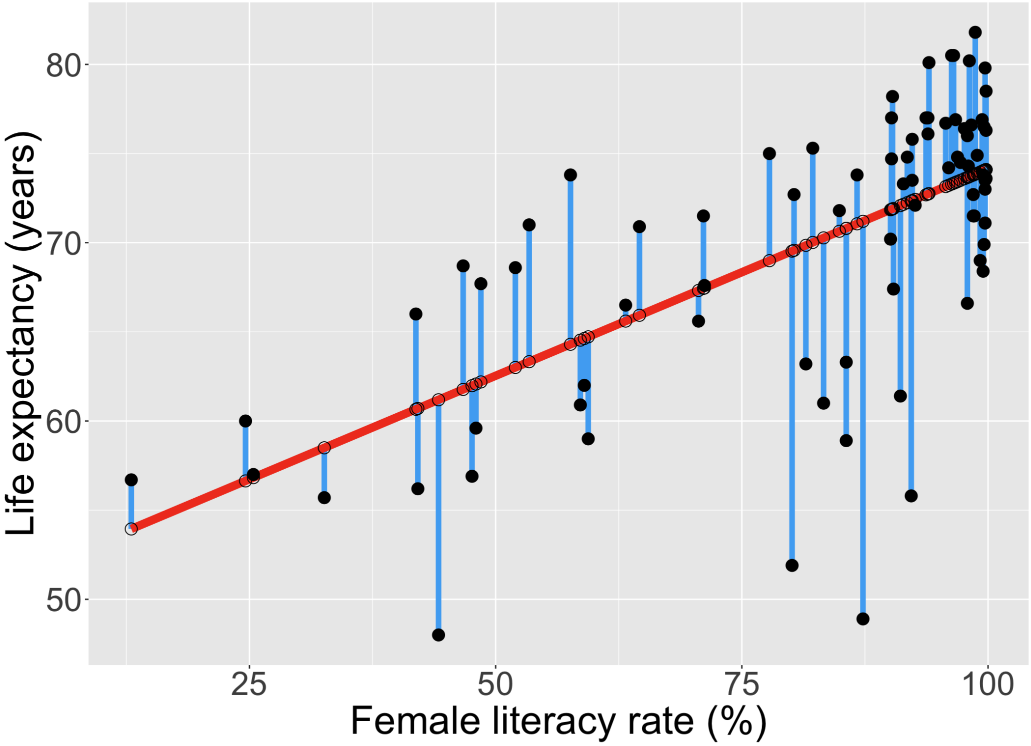
fitted model line



Our residuals will help us a lot in our diagnostics!

- The **residuals** $\hat{\epsilon}_i$ are the vertical distances between
  - the observed data (X_i, Y_i)
  - the fitted values (regression line) $\widehat{Y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 X_i$

$$\hat{\epsilon}_i = Y_i - \widehat{Y}_i, \text{ for } i = 1, 2, \ldots, n$$



`augment()`: getting extra information on the fitted model

- Run `model1` through `augment()` (`model1` is input)
  - So we assigned `model1` as the output of the `lm()` function (`model1` is output)
- Will give us values about each observation in the context of the fitted regression model
  - cook's distance (`.cooksd`), fitted value (`.fitted`, $\widehat{Y}_i$), leverage (`.hat`), residual (`.resid`), standardized residuals (`.std.resid`)

```
aug1 <- augment(model1)
glimpse(aug1)
```

```
Rows: 80
Columns: 9
$ .rownames                  <chr> "1", "2", "5", "6", "7", "8", "14", "22", "…
$ life_expectancy_years_2011 <dbl> 56.7, 76.7, 60.9, 76.9, 76.0, 73.8, 71.0, 7…
$ female_literacy_rate_2011  <dbl> 13.0, 95.7, 58.6, 99.4, 97.9, 99.5, 53.4, 9…
$ .fitted                    <dbl> 53.94643, 73.14897, 64.53453, 74.00809, 73.…
$ .resid                     <dbl> 2.7535654, 3.5510294, -3.6345319, 2.8919074…
$ .hat                       <dbl> 0.13628996, 0.01768176, 0.02645854, 0.02077…
$ .sigma                     <dbl> 6.172684, 6.168414, 6.167643, 6.172935, 6.1…
$ .cooksd                    <dbl> 1.835891e-02, 3.062372e-03, 4.887448e-03, 2…
```

observation

RDocumentation on the `augment()` function.

Revisiting our LINE assumptions

[L] Linearity of relationship between variables

Check if there is a linear relationship between the mean response (Y) and the explanatory variable (X)

[I] Independence of the Y values

Check that the observations are independent

[N] Normality of the Y's given X (residuals)

Check that the responses (at each level X) are normally distributed

- Usually measured through the residuals

[E] Equality of variance of the residuals (homoscedasticity)

Check that the variance (or standard deviation) of the responses is equal for all levels of X

- Usually measured through the residuals

Not Y alone

$\boxed{Y | X}$ @ each X level

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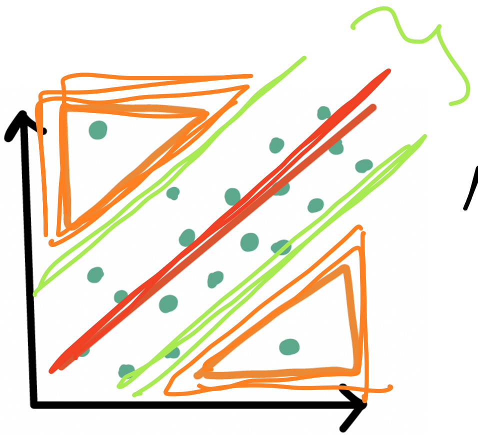
Influential points

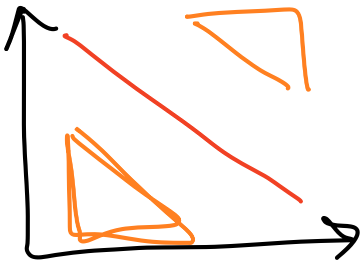
Outliers

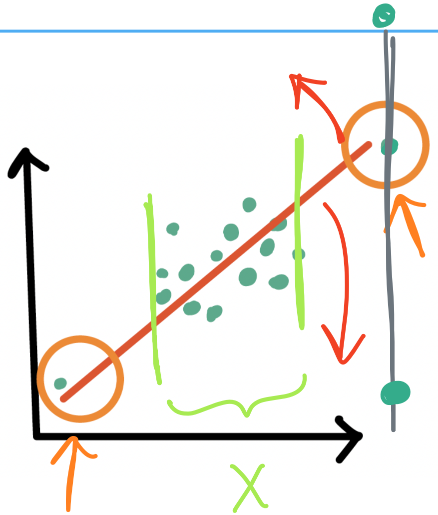
- An observation (X_i, Y_i) whose response Y_i does not follow the general trend of the rest of the data

High leverage observations

- An observation (X_i, Y_i) whose predictor X_i has an extreme value
- X_i can be an extremely high or low value compared to the rest of the observations







Outliers

- An observation (X_i, Y_i) whose response Y_i does not follow the general trend of the rest of the data
- How do we determine if a point is an outlier?
  - Scatterplot of Y vs. X
  - Followed by evaluation of its residual (and standardized residual)

- Use the internally standardized residual (aka studentized residual) to determine if an observation is an outlier

$$\text{std } \widehat{\text{residual}} \sim N(0, \underline{1})$$

$$\widehat{\text{residual}} \sim N(0, \underline{\hat{\sigma}^2})$$

Poll Everywhere Question 1

Identifying outliers

pts / obs

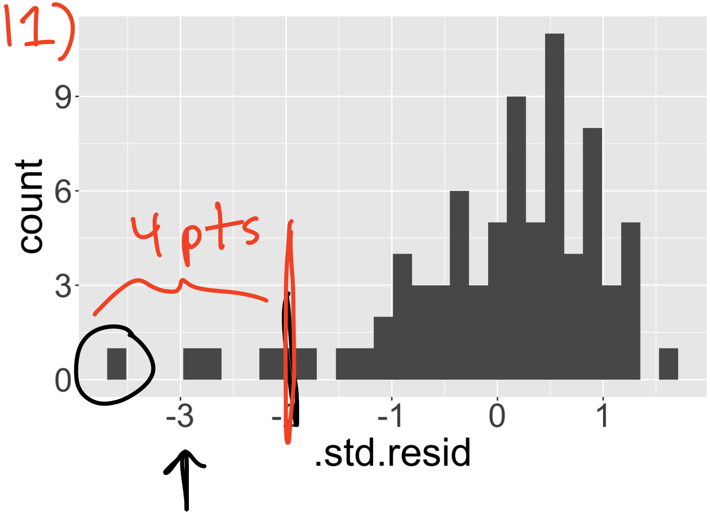
Internally standardized residual

$$r_i = \frac{\hat{\epsilon}_i}{\sqrt{\hat{\sigma}^2(1 - h_{ii})}}$$

- We flag an observation if the standardized residual is "large"
  - Different sources will define "large" differently
  - PennState site uses $|r_i| > 3$ if + $r_i > 3$ if − $r_i < -3$
  - `autoplot()` shows the 3 observations with the highest standardized residuals
  - Other sources use $|r_i| > 2$, which is a little more conservative

aug1 = augment(model1)

```
ggplot(data = aug1) +
  geom_histogram(aes(x = .std.resid))
```



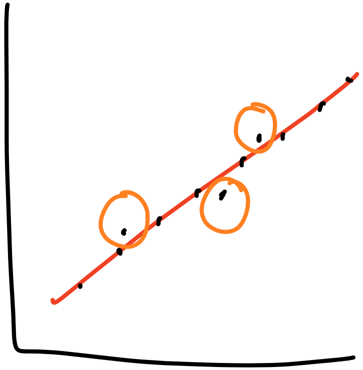
Countries that are outliers ($|r_i| > 2$)

- We can identify the countries that are outliers

$|r_i|$ > 2

```
aug1 %>%
  filter(abs(.std.resid) > 2)
```

```
# A tibble: 4 × 10
  .rownames country      life_expectancy_year…¹ female_literacy_rate…² .std.resid
  <chr>     <chr>                         <dbl>                  <dbl>      <dbl>
1 33        Central Af…                    48                     44.2      -2.20
2 152       South Afri…                    55.8                   92.2      -2.71
3 161       Swaziland                      48.9                   87.3      -3.65
4 187       Zimbabwe                       51.9                   80.1      -2.89
# ℹ abbreviated names: ¹life_expectancy_years_2011, ²female_literacy_rate_2011
# ℹ 5 more variables: .fitted <dbl>, .resid <dbl>, .hat <dbl>, .sigma <dbl>,
#   .cooksd <dbl>
```



High leverage observations

- An observation (X_i, Y_i) whose response X_i is considered "extreme" compared to the other values of X

- How do we determine if a point has high leverage?
  - Scatterplot of Y vs. X
  - Calculating the leverage of each observation

Leverage h_i

$[h_{11} h_{12} \quad]$

H : matrix hat matrix

★ what does diff in magnitude

- Values of leverage are: $0 \leq h_i \leq 1$ higher means more leverage
- We flag an observation if the leverage is "high"
  - Different sources will define "high" differently
  - Some textbooks use $h_i > 4/n$ where n = sample size → $\frac{4}{80}$ (LE)
  - Some people suggest $h_i > 6/n$ → $6/80$ (LE)
  - PennState site uses $h_i > 3p/n$ where p = number of regression coefficients

$Y = \beta_0 + \beta_1 X + \varepsilon$

$h_i > \frac{3(2)}{n} = \frac{3(2)}{80}$ LE

```
aug1 = aug1 %>% relocate(.hat, .after = female_literacy_rate_2011)
aug1 %>% arrange(desc(.hat))
```

SLR

highest h_i to lowest h_i

.hat

```
# A tibble: 80 × 10
  .rownames country          life_expectancy_year…¹ female_literacy_rate…²   .hat
  <chr>     <chr>                             <dbl>                  <dbl>  <dbl>
1 1         Afghanistan                        56.7                   13   0.136
2 104       Mali                               60                     24.6 0.0980
3 34        Chad                               57                     25.4 0.0956
4 146       Sierra Leone                       55.7                   32.6 0.0757
5 62        Gambia                             66                     41.9 0.0540
6 70        Guinea-Bissau                      56.2                   42.1 0.0536
7 33        Central Afric…                     48                     44.2 0.0493
```

Countries with high leverage ($h_i > 4/n$)

- We can look at the countries that have high leverage

```
aug1 %>%
  filter(.hat > 4/80) %>%
  arrange(desc(.hat))
```

$h_i > 4/n = 4/80 = 0.05$

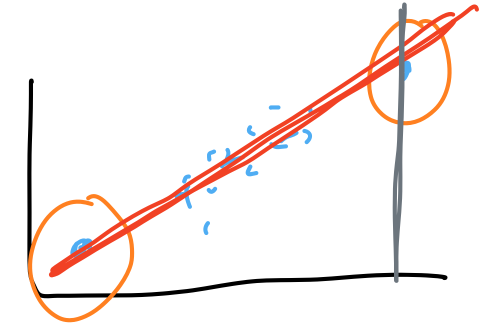
```
# A tibble: 6 × 10
  .rownames country        life_expectancy_years_…¹ female_literacy_rate…²   .hat
  <chr>     <chr>                             <dbl>                  <dbl>  <dbl>
1 1         Afghanistan                        56.7                   13   0.136
2 104       Mali                               60                     24.6 0.0980
3 34        Chad                               57                     25.4 0.0956
4 146       Sierra Leone                       55.7                   32.6 0.0757
5 62        Gambia                             66                     41.9 0.0540
6 70        Guinea-Bissau                      56.2                   42.1 0.0536
# ℹ abbreviated names: ¹life_expectancy_years_2011, ²female_literacy_rate_2011
```

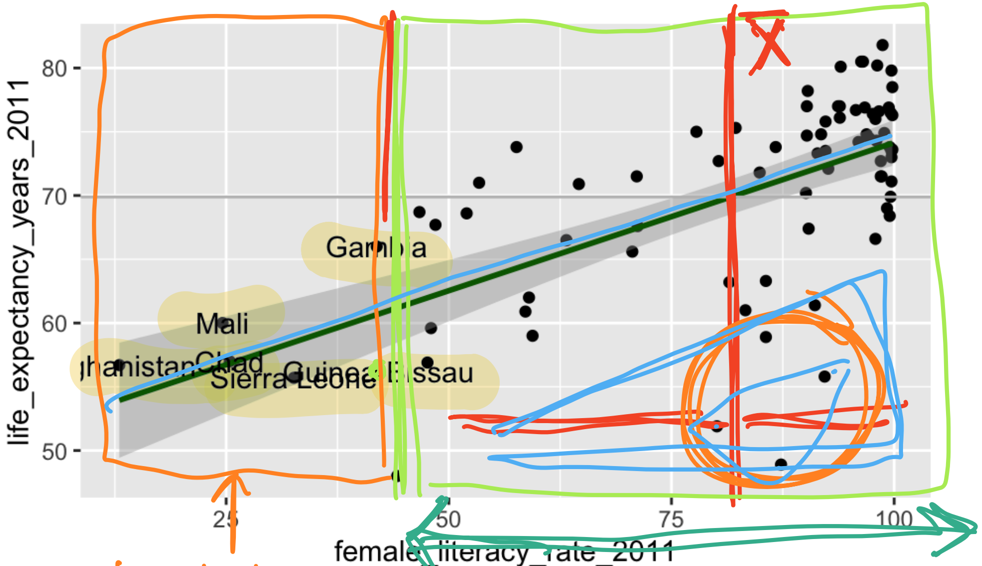
Poll Everywhere Question 2

Countries with high leverage ($h_i > 4/n$)

Label only countries with large leverage:

```
ggplot(aug1, aes(x = female_literacy_rate_2011, y = life_expectancy_years_2011,
                 label = country)) +
  geom_point() +
  geom_smooth(method = "lm", color = "darkgreen") +
  geom_text(aes(label = ifelse(.hat > 0.05, as.character(country), ''))) +
  geom_vline(xintercept = mean(aug1$female_literacy_rate_2011), color = "grey") +
  geom_hline(yintercept = mean(aug1$life_expectancy_years_2011), color = "grey")
```





high leve

What does the model look like without the high leverage points?

Sensitivity analysis removing countries with high leverage

```r
model1_lowlev <- lm(life_expectancy_years_2011 ~ female_literacy_rate_2011,
                    data = aug1_lowlev)
tidy(model1_lowlev) %>% gt() %>% # Without high-leverage points
  tab_options(table.font.size = 40) %>%
  fmt_number(decimals = 3)
```

w/out hL

term	estimate	std.error	statistic	p.value
(Intercept)	49.563	3.888	12.746	0.000
female_literacy_rate_2011	0.247	0.044	5.562	0.000

```r
tidy(model1) %>% gt() %>% # With high leverage points
  tab_options(table.font.size = 40) %>%
  fmt_number(decimals = 3)
```

w/ hL

term	estimate	std.error	statistic	p.value
(Intercept)	50.928	2.660	19.143	0.000
female_literacy_rate_2011	0.232	0.031	7.377	0.000

- still sig.
- sign of $\hat{\beta}_1$ does not change
- magnitude change of $\hat{\beta}_1$ is not drastic

Cook's distance

- Measures the overall influence of an observation

- Attempts to measure how much influence a single observation has over the fitted model
  - Measures how all fitted values change when the ith observation is removed from the model
  - Combines leverage and outlier information

coeff est.
resid. variance est.

Identifying points with high Cook's distance

$0.5 < d_i < 1$ - check it out

The Cook's distance for the i^{th} observation is

$$d_i = \frac{h_i}{2(1-h_i)} \cdot r_i^2$$

where h_i is the leverage and r_i is the studentized residual

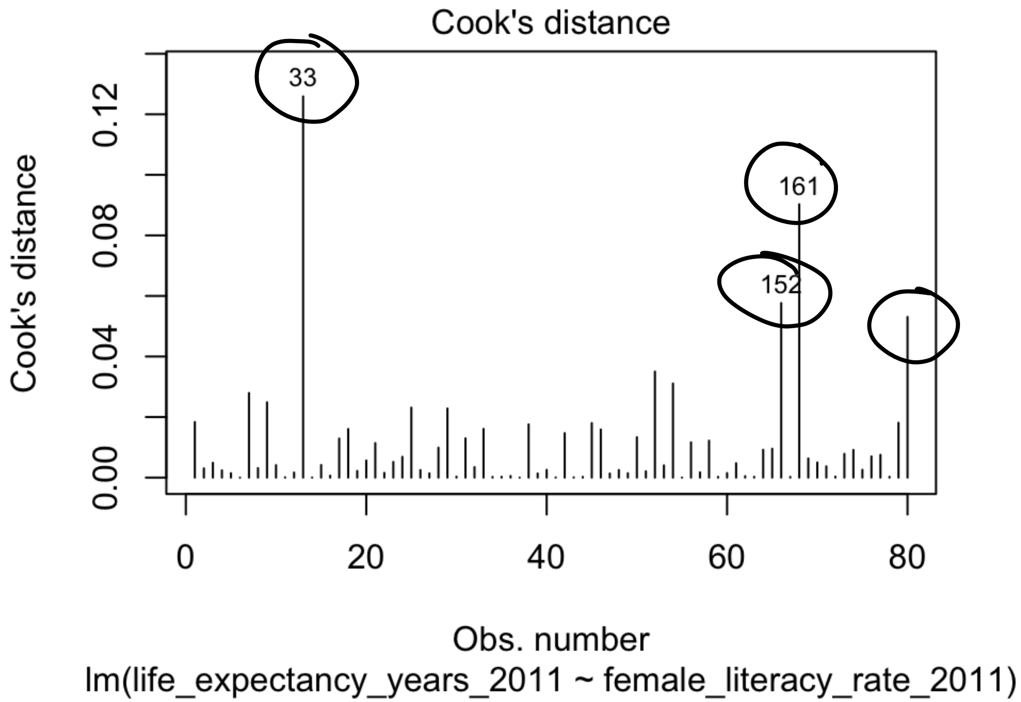
- Another rule for Cook's distance that is not strict:
  - Investigate observations that have $d_i > 1$
- Cook's distance values are already in the augment tibble: `.cooksd`

```
aug1 = aug1 %>% relocate(.cooksd, .after = female_literacy_rate_2011)
aug1 %>% arrange(desc(.cooksd))
```

```
# A tibble: 80 × 10
  .rownames country      life_expectancy_year…¹ female_literacy_rate…² .cooksd
  <chr>     <chr>                         <dbl>                  <dbl>   <dbl>
1 33        Central Afri…                  48                     44.2  0.126
2 161       Swaziland                      48.9                   87.3  0.0903
3 152       South Africa                   55.8                   92.2  0.0577
4 187       Zimbabwe                       51.9                   80.1  0.0531
5 114       Morocco                        73.8                   57.6  0.0350
6 118       Nepal                          68.7                   46.7  0.0311
7 14        Bangladesh                     71                     53.4  0.0280
```

Plotting Cook's Distance

```r
# plot(model) shows figures similar to autoplot()
# adds on Cook's distance though
plot(model1, which = 4)
```



Model without those 4 points: QQ Plot, Residual plot

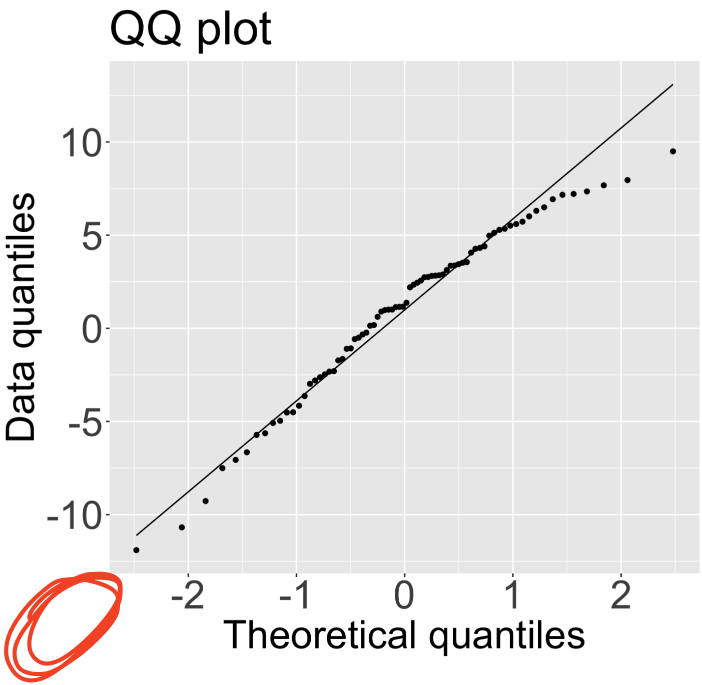
```r
model1_lowcd <- lm(life_expectancy_years_2011 ~ female_literacy_rate_2011,
                    data = aug1_lowcd)
tidy(model1_lowcd) %>% gt() %>% # Without high-leverage points
 tab_options(table.font.size = 40) %>%
 fmt_number(decimals = 3)
```

term	estimate	std.error	statistic	p.value
(Intercept)	52.388	2.078	25.208	0.000
female_literacy_rate_2011	0.226	0.024	9.208	0.000

```r
tidy(model1) %>% gt() %>% # With high leverage points
 tab_options(table.font.size = 40) %>%
 fmt_number(decimals = 3)
```

term	estimate	std.error	statistic	p.value
(Intercept)	50.928	2.660	19.143	0.000
female_literacy_rate_2011	0.232	0.031	7.377	0.000

Model without those 4 points: QQ Plot, Residual plot



I am okay with this!

- And don't forget: we may want more variables in our model!
- You do not need to produce plots with the influential points taken out

Summary of how we identify influential points

- Use scatterplot of Y vs. X to see if any points fall outside of range we expect
- Use standardized residuals, leverage, and Cook's distance to further identify those points
- Look at the models run with and without the identified points to check for drastic changes
  - Look at QQ plot and residuals to see if assumptions hold without those points
  - Look at coefficient estimates to see if they change in sign and large magnitude

- Next: how to handle? *It's a little wishy washy*

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How do we deal with influential points?

- It's always weird to be using numbers to help you diagnose an issue, but the issue kinda gets unresolved
- If an observation is influential, we can check data errors:
  - Was there a data entry or collection problem?
  - If you have reason to believe that the observation does not hold within the population (or gives you cause to redefine your population)
- If an observation is influential, we can check our model:
  - Did you leave out any important predictors?
  - Should you consider adding some interaction terms?
  - Is there any nonlinearity that needs to be modeled? → transformation
- Basically, deleting an observation should be justified outside of the numbers!
  - If it's an honest data point, then it's giving us important information!
- A really well thought out explanation from StackExchange

When we have detected problems in our model…

- We have talked about influential points
- We have talked about identifying issues with our LINE assumptions

What are our options once we have identified issues in our linear regression model?

- See if we need to add predictors to our model
  - Nicky's thought for our life expectancy example
- Try a transformation if there is an issue with linearity or normality
- Try a transformation if there is unequal variance
- Try a weighted least squares approach if unequal variance (might be lesson at end of course)
- Try a robust estimation procedure if we have a lot of outlier issues (outside scope of class)

→ end of class

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Transformations

- When we have issues with our LINE (mostly linearity, normality, or equality of variance) assumptions
  - We can use transformations to improve the fit of the model
- Transformations can...
  - Make the relationship more linear
  - Make the residuals more normal
  - "Stabilize" the variance so that it is more constant
  - It can also bring in or reduce outliers ⇒ potential consequence
- We can transform the dependent (Y) variable of the independent (X) variable
  - Usually we want to try transforming the X first

- **Requires trial and error!!**
- **Major drawback:** interpreting the model becomes harder!

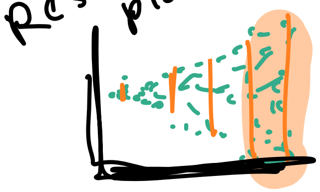
Common transformations

density plot of X alone

or Y|X

Y|X

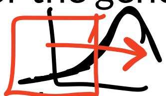
resid



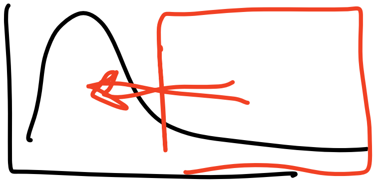
- Tukey's transformation (power) ladder
  - Use R's `gladder()` command from the `describedata` package

Power p	-3	-2	-1	-1/2	0	1/2	1	2	3
	$\frac{1}{x^3}$	$\frac{1}{x^2}$	$\frac{1}{x}$	$\frac{1}{\sqrt{x}}$	$\log(x)$	$\sqrt{x}$	x	x^2	x^3

- How to use the power ladder for the general distribution shape



  - If data are skewed left, we need to compress smaller values towards the rest of the data
    - Go "up" ladder to transformations with power > 1
  - If data are skewed right, we need to compress larger values towards the rest of the data
    - Go "down" ladder to transformations with power < 1



- How to use the power ladder for heteroscedasticity
  - If higher X values have more spread
    - Compress larger values towards the rest of the data
    - Go "down" ladder to transformations with power < 1
  - If lower X values have more spread
    - Compress smaller values towards the rest of the data
    - Go "up" ladder to transformations with power > 1

Poll Everywhere Question 3

Transform dependent variable? Y

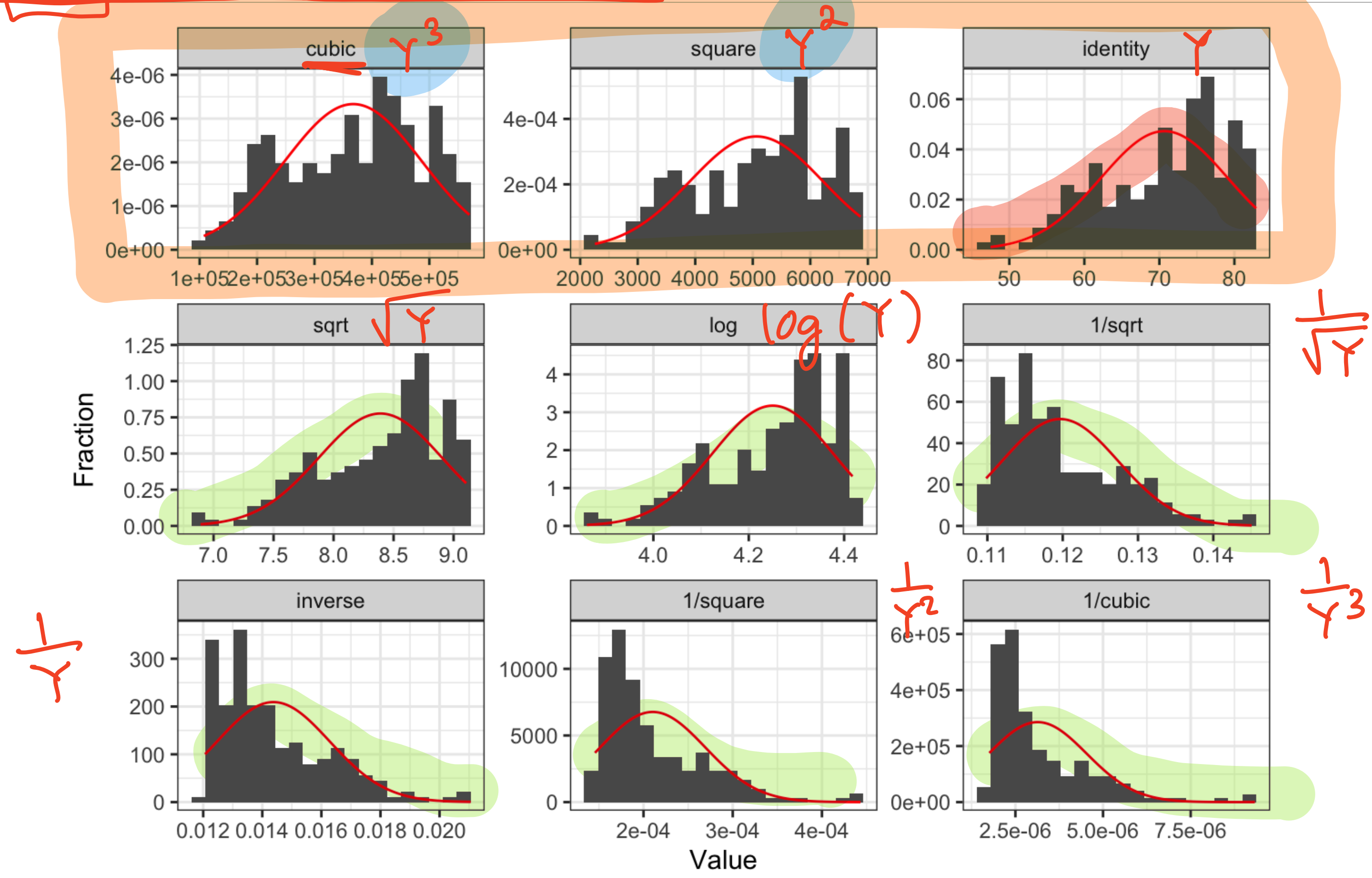
```
ggplot(gapm, aes(x = life_expectancy_years_2011)) +
  geom_histogram()
```

`gladder()` of life expectancy

want it less skewed

```
1  gladder(gapm$life_expectancy_years_2011)
```

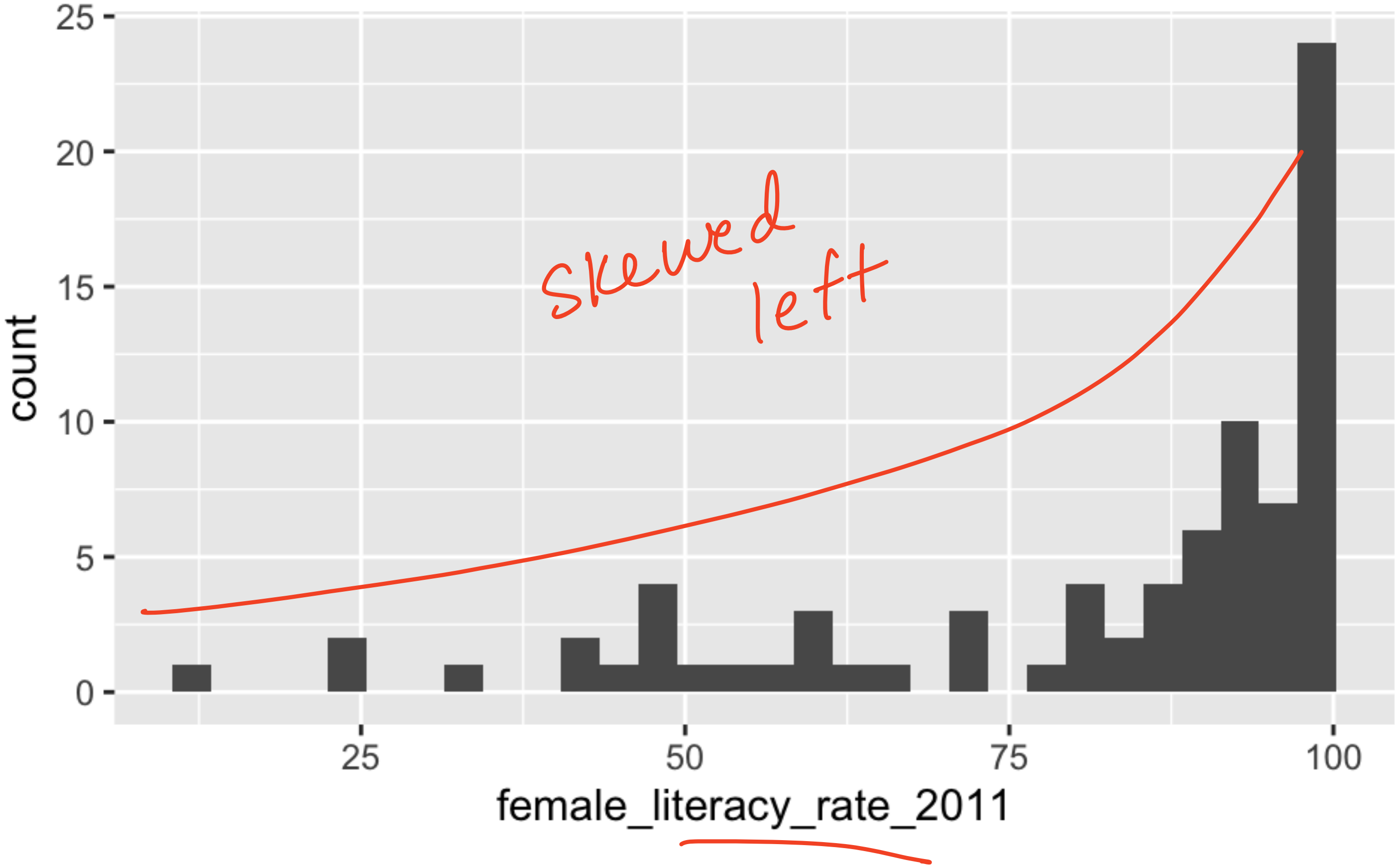
Y



Transform independent variable? X

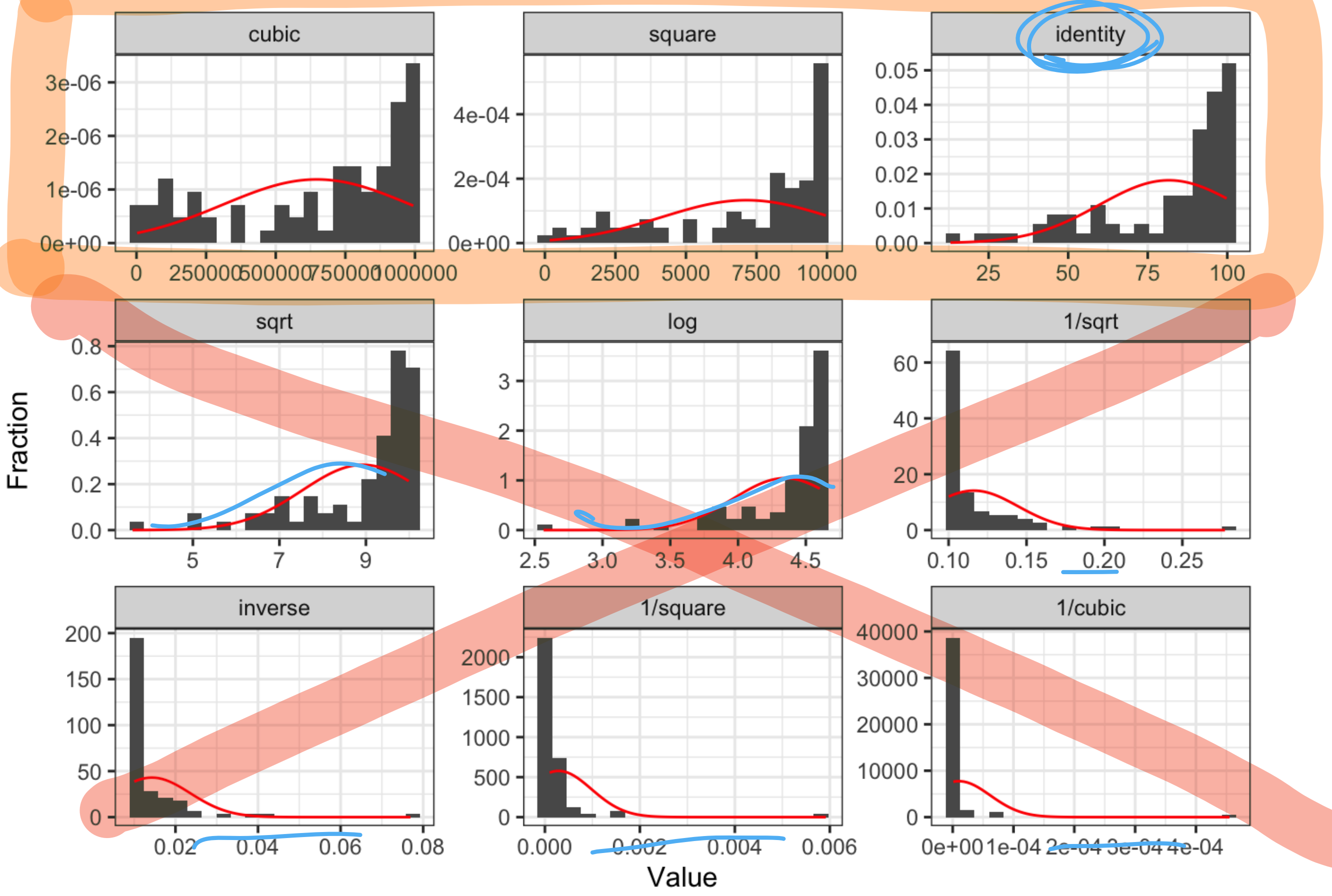
Y|X or residual

```
1 ggplot(gapm, aes(x = female_literacy_rate_2011)) +
2   geom_histogram()
```



`gladder()` of female literacy rate

```
1  gladder(gapm$female_literacy_rate_2011)
```



Tips

- Recall, assessing our LINE assumptions are not on Y alone!!
  - We can use `gladder()` to get a sense of what our transformations will do to the data, but we need to check with our residuals again!!
- Transformations usually work better if all values are positive (or negative)
- If observation has a 0, then we cannot perform certain transformations
- Log function only defined for positive values
  - We might take the $log(X+1)$ if X includes a 0 value
- When we make cubic or square transformations, we MUST include the original X
  - We do not do this for Y though

X^3 : X, X^2, X^3

X^2 : X, X^2

Add quadratic and cubic transformations to dataset

- Helpful to make a new variable with the transformation in your dataset

```
gapm <- gapm %>%
  mutate(LE_2 = life_expectancy_years_2011^2,
         LE_3 = life_expectancy_years_2011^3,
         FLR_2 = female_literacy_rate_2011^2,
         FLR_3 = female_literacy_rate_2011^3)

glimpse(gapm)
```

```
Rows: 188
Columns: 8
$ country                     <chr> "Afghanistan", "Albania", "Algeria", "Andor…
$ life_expectancy_years_2011 <dbl> 56.7, 76.7, 76.7, 82.6, 60.9, 76.9, 76.0, 7…
$ female_literacy_rate_2011  <dbl> 13.0, 95.7, NA, NA, 58.6, 99.4, 97.9, 99.5,…
$ .rownames                   <chr> "1", "2", "3", "4", "5", "6", "7", "8", "9"…
$ LE_2                        <dbl> 3214.89, 5882.89, 5882.89, 6822.76, 3708.81…
$ LE_3                        <dbl> 182284.3, 451217.7, 451217.7, 563560.0, 225…
$ FLR_2                       <dbl> 169.00, 9158.49, NA, NA, 3433.96, 9880.36, …
$ FLR_3                       <dbl> 2197.0, 876467.5, NA, NA, 201230.1, 982107.…
```

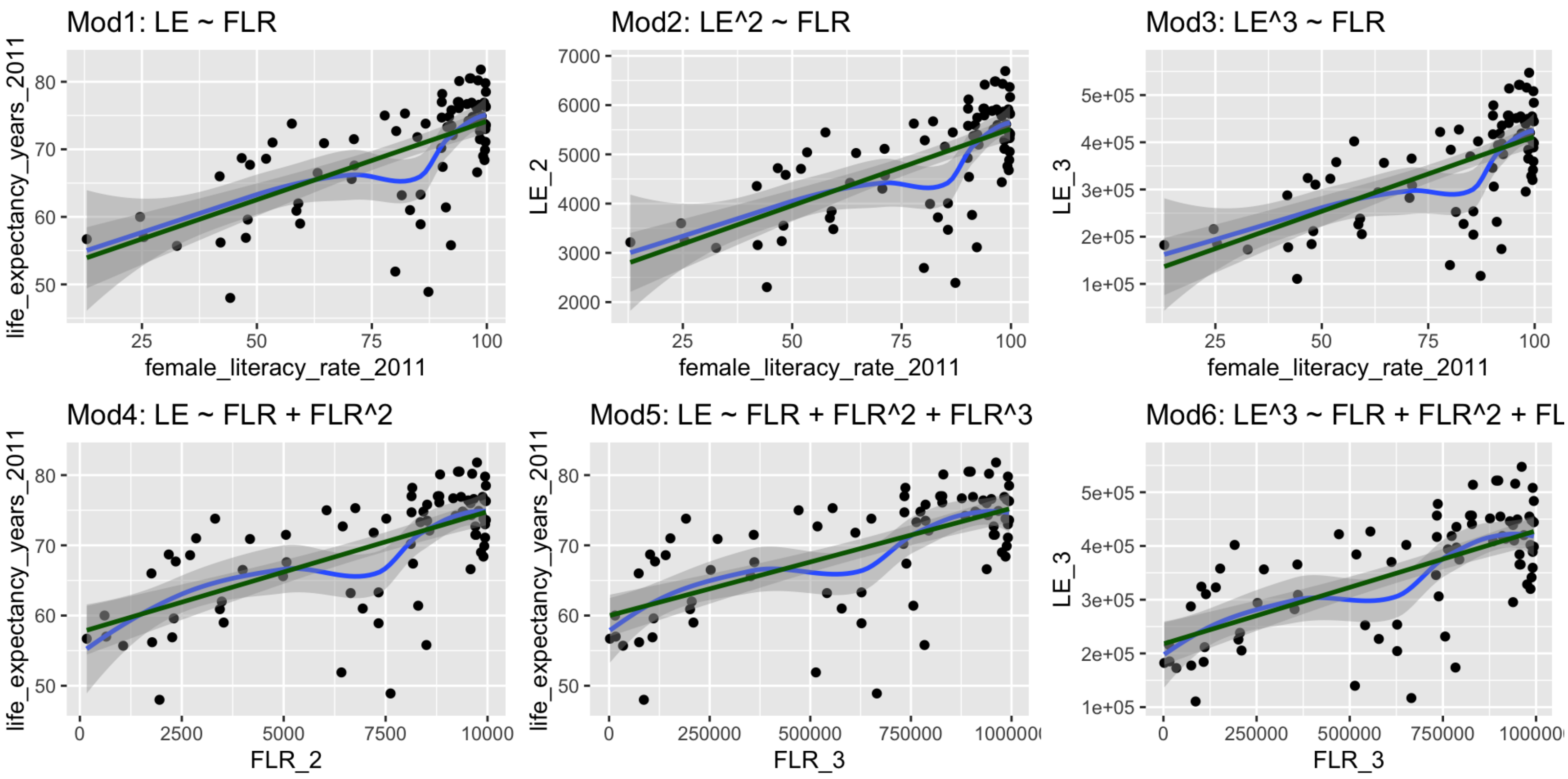
We are going to compare a few different models with transformations

We are going to call life expectancy LE and female literacy rate FLR

- Model 1: $LE = \beta_0 + \beta_1 FLR + \epsilon$
- Model 2: $LE^2 = \beta_0 + \beta_1 FLR + \epsilon$
- Model 3: $LE^3 = \beta_0 + \beta_1 FLR + \epsilon$
- Model 4: $LE = \beta_0 + \beta_1 FLR + \beta_2 FLR^2 + \epsilon$
- Model 5: $LE = \beta_0 + \beta_1 FLR + \beta_2 FLR^2 + \beta_3 FLR^3 + \epsilon$
- Model 6: $LE^3 = \beta_0 + \beta_1 FLR + \beta_2 FLR^2 + \beta_3 FLR^3 + \epsilon$

Poll Everywhere Question 4

Compare Scatterplots: does linearity improve?



Run models with transformations: examples

Model 2: $LE^2 = \beta_0 + \beta_1 FLR + \epsilon$

```r
model2 <- lm(LE_2 ~ female_literacy_rate_2011,
                data = gapm)
```

term	estimate	std.error	statistic	p.value
(Intercept)	2,401.272	352.070	6.820	0.000
female_literacy_rate_2011	31.174	4.166	7.484	0.000

0.23

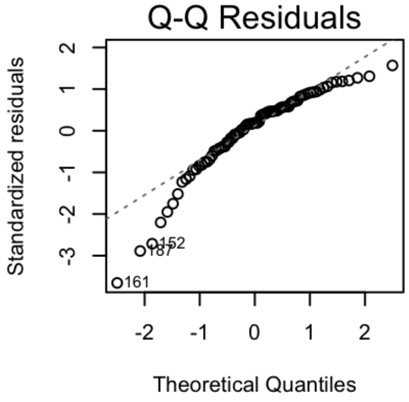
Model 6: $LE^3 = \beta_0 + \beta_1 FLR + \beta_2 FLR^2 + \beta_3 FLR^3 + \epsilon$

```r
model6 <- lm(LE_3 ~
                  female_literacy_rate_2011 + FLR_2 + FLR_3,
                data = gapm)
```

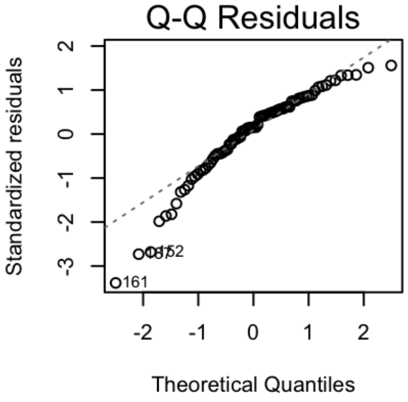
term	estimate	std.error	statistic	p.value
(Intercept)	67,691.796	149,056.945	0.454	0.651
female_literacy_rate_2011	8,092.133	8,473.154	0.955	0.343
FLR_2	−128.596	147.876	−0.870	0.387
FLR_3	0.840	0.794	1.059	0.293

Normal Q-Q plots comparison

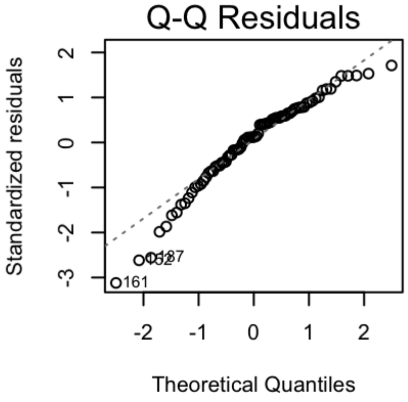
Model 1



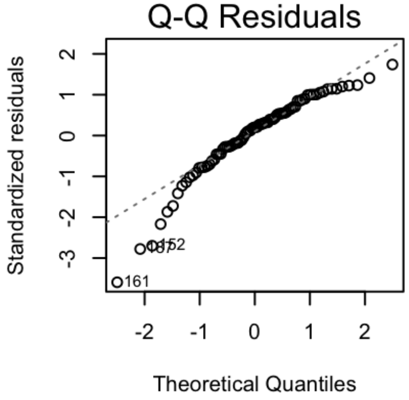
2



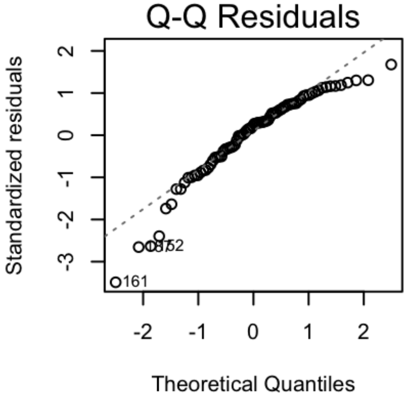
3



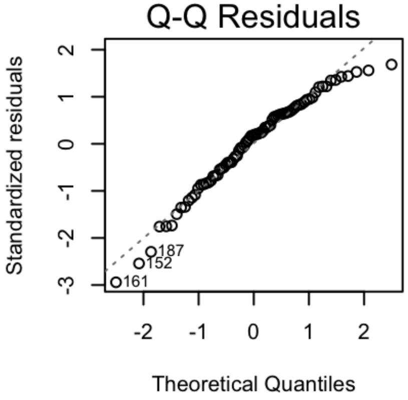
4



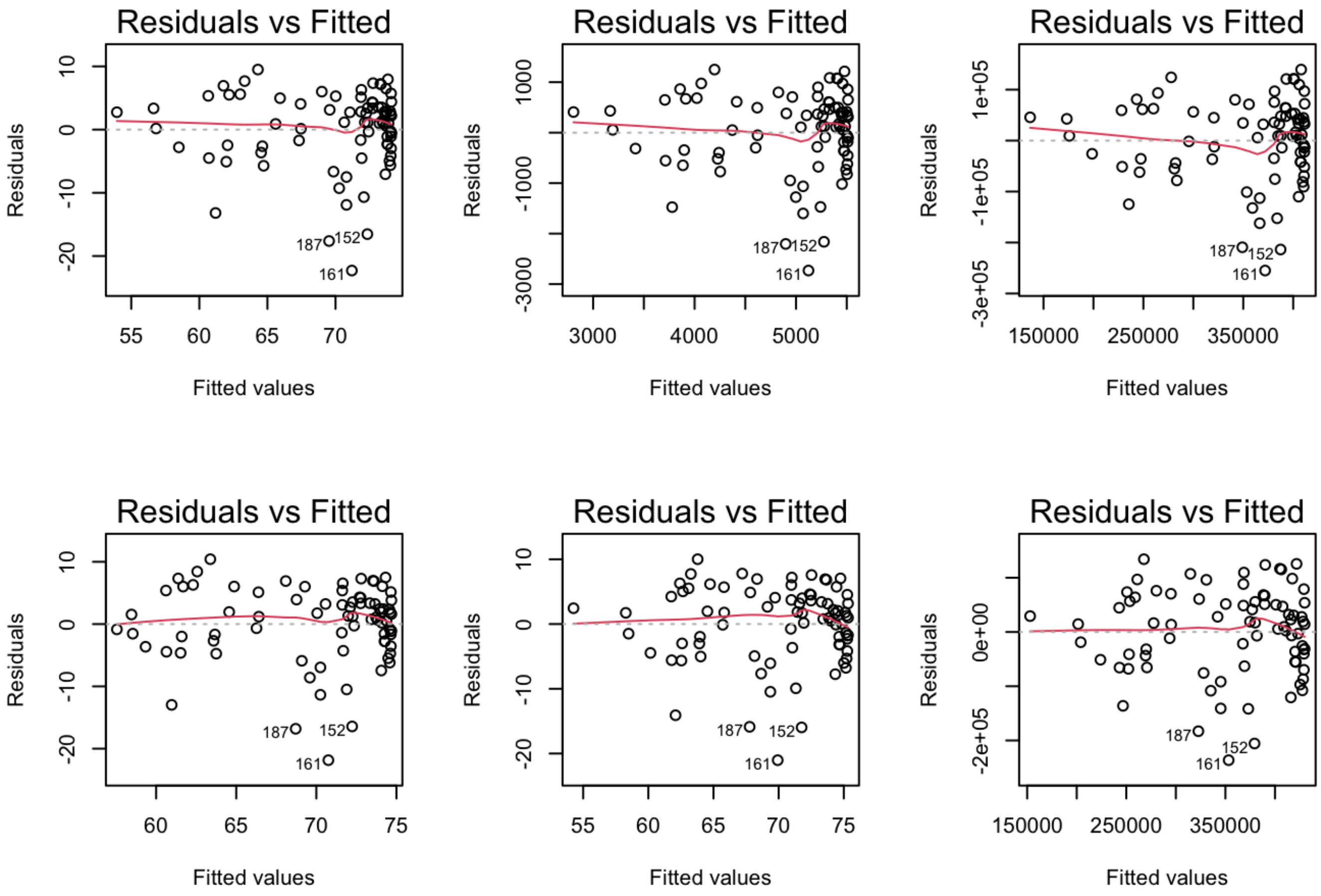
5



6



Residual plots comparison



Summary of transformations

- If the model without the transformation is blatantly violating a LINE assumption
  - Then a transformation is a good idea
- If the model without a transformation is not following the LINE assumptions very well, but is mostly okay
  - Then try to avoid a transformation
  - Think about what predictors might need to be added
  - Especially if you keep seeing the same points as influential
- If interpretability is important in your final work, then transformations are not a great solution

Reference: all run models

Model 2: $LE^2 = \beta_0 + \beta_1 FLR + \epsilon$

```r
model2 <- lm(LE_2 ~ female_literacy_rate_2011,
             data = gapm)

tidy(model2) %>% gt()
```

term	estimate	std.error	statistic	p.value
(Intercept)	2401.27207	352.069818	6.820443	1.726640e-09
female_literacy_rate_2011	31.17351	4.165624	7.483514	9.352191e-11

Model 3: $LE^3 \sim FLR$

```r
model3 <- lm(LE_3 ~ female_literacy_rate_2011,
             data = gapm)

tidy(model3) %>% gt()
```

term	estimate	std.error	statistic	p.value
(Intercept)	95453.189	35631.6898	2.678885	9.005716e-03
female_literacy_rate_2011	3166.481	421.5875	7.510853	8.285324e-11

Model 4: $LE \sim FLR + FLR^2$

```r
model4 <- lm(life_expectancy_years_2011 ~
               female_literacy_rate_2011 + FLR_2,
             data = gapm)

tidy(model4) %>% gt()
```

term	estimate	std.error	statistic	p.value
(Intercept)	57.030875456	6.282845592	9.07723652	8.512585e-14
female_literacy_rate_2011	0.019348795	0.201021963	0.09625215	9.235704e-01
FLR_2	0.001578649	0.001472592	1.07202008	2.870595e-01

Model 5: $LE \sim FLR + FLR^2 + FLR^3$

```r
model5 <- lm(life_expectancy_years_2011 ~
                 female_literacy_rate_2011 + FLR_2 + FLR_3,
               data = gapm)

tidy(model5) %>% gt()
```

term	estimate	std.error	statistic	p.value
(Intercept)	4.732796e+01	1.117939e+01	4.2335001	6.373341e-05
female_literacy_rate_2011	6.517986e-01	6.354934e-01	1.0256576	3.083065e-01
FLR_2	-9.952763e-03	1.109080e-02	-0.8973895	3.723451e-01
FLR_3	6.245016e-05	5.953283e-05	1.0490038	2.975008e-01

Model 6: $LE^3 \sim FLR + FLR^2 + FLR^3$

```r
model6 <- lm(LE_3 ~
                 female_literacy_rate_2011 + FLR_2 + FLR_3,
               data = gapm)

tidy(model6) %>% gt()
```

term	estimate	std.error	statistic	p.value
(Intercept)	67691.7963283	1.490569e+05	0.4541338	0.6510268
female_literacy_rate_2011	8092.1325988	8.473154e+03	0.9550320	0.3425895
FLR_2	-128.5960879	1.478757e+02	-0.8696230	0.3872447
FLR_3	0.8404736	7.937625e-01	1.0588477	0.2930229