Stat 608 Chapter 3

STARTED @ 36:59 mark

Monday 11/1/22 (Week 3, Lecture 6)

Introduction: Checking Assumptions

Summary

- Chapter 2:
  - Set up model:
    - Inferences about model parameters & regression line
    - Dummy (categorical) variable regression
- Chapter 3:
  - Check the model assumptions: **L**inear, **I**ndependent, **N**ormal, **E**rrors have constant variance:
    - Residual plots
    - Leverage & Influence
    - Transformations

Usual Assumptions

Four assumptions:

L: Y and x are **Linearly** related. (The model must be valid! If we should be fitting a parabola, all bets are off.)

I: The errors are **Independent** of each other (e.g. random samples or randomized experiments)

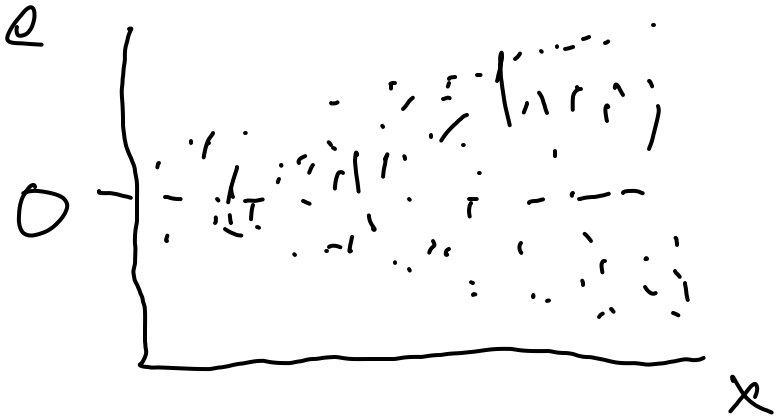
N: The errors are **Normally** distributed with mean 0. For larger sample sizes, this is less necessary, as we can use the CLT.

E: **Equal** variance of the errors, σ^2.

Anscombe's Data Sets

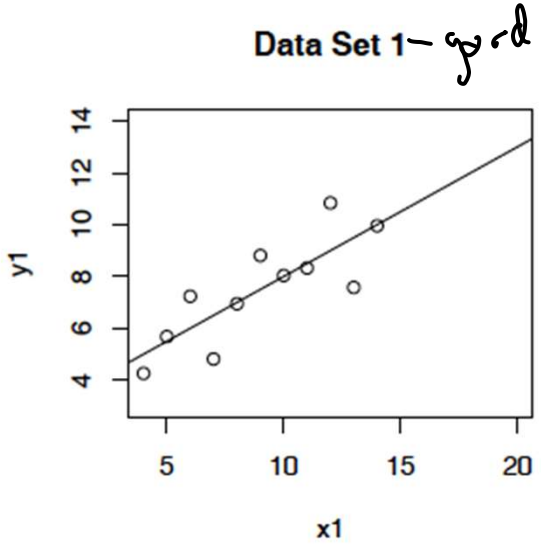
- Valid Model
  - Is the mean structure correct?
    - For valid models, $E[Y \mid X = x] = \beta_0 + \beta_1 x$

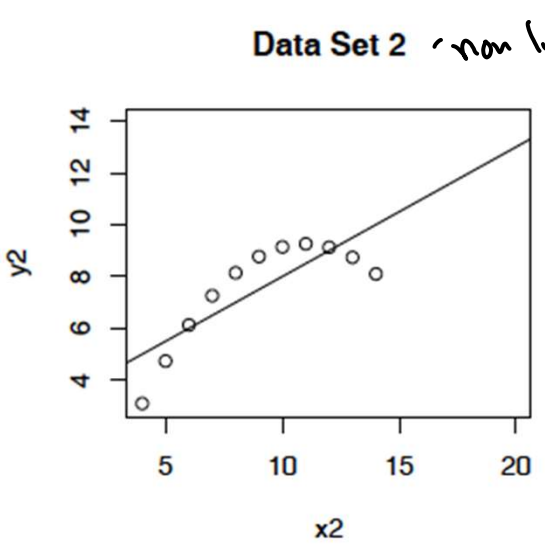
  - Is the variance structure correct?
    - The most common assumption is $Var(Y \mid X = x) = \sigma^2$.

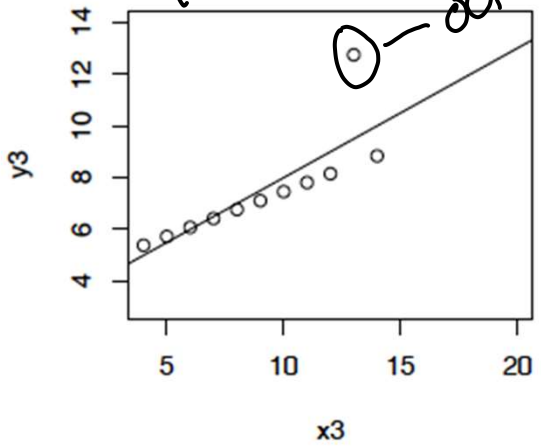


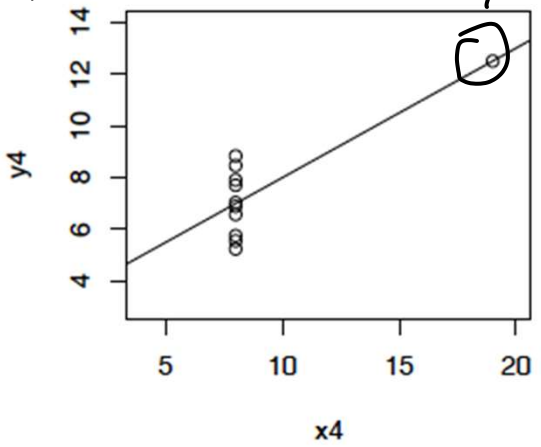
Anscombe's Data Sets

- Is SLR a valid model for any of these datasets?
  - Same slope
  - Same intercept
  - Same R^2
  - Same s.e.
  - Same p-values









Using Residuals

- Plot residuals:
  - No pattern => model could be valid
  - Pattern => residual plot gives information on what to do

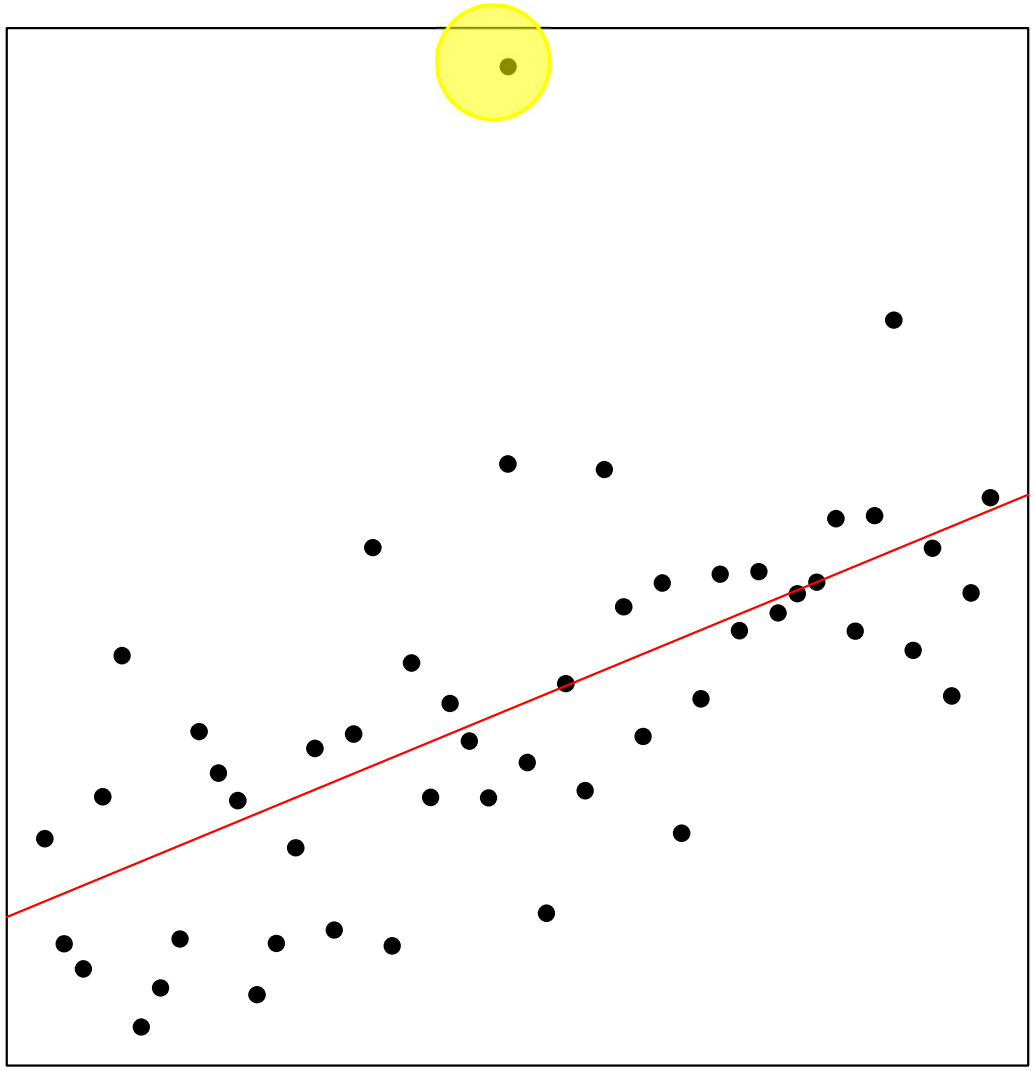
- Look at individual points:
  - **Outliers** don't follow the pattern of the rest of the data, after taking into account the model. Outliers will change p-values and correlation, and will change them both substantially without larger sample sizes.
  - **Bad Leverage** points are outliers which also have an unusually large effect on the estimated regression model itself. (Does the slope change much when a single point is removed?)

STOP Monday 1/31/22 (week 3, lecture 6)

START Wed 2/2/22 (week 3, lecture 7)

Outliers, Leverage, and Influence

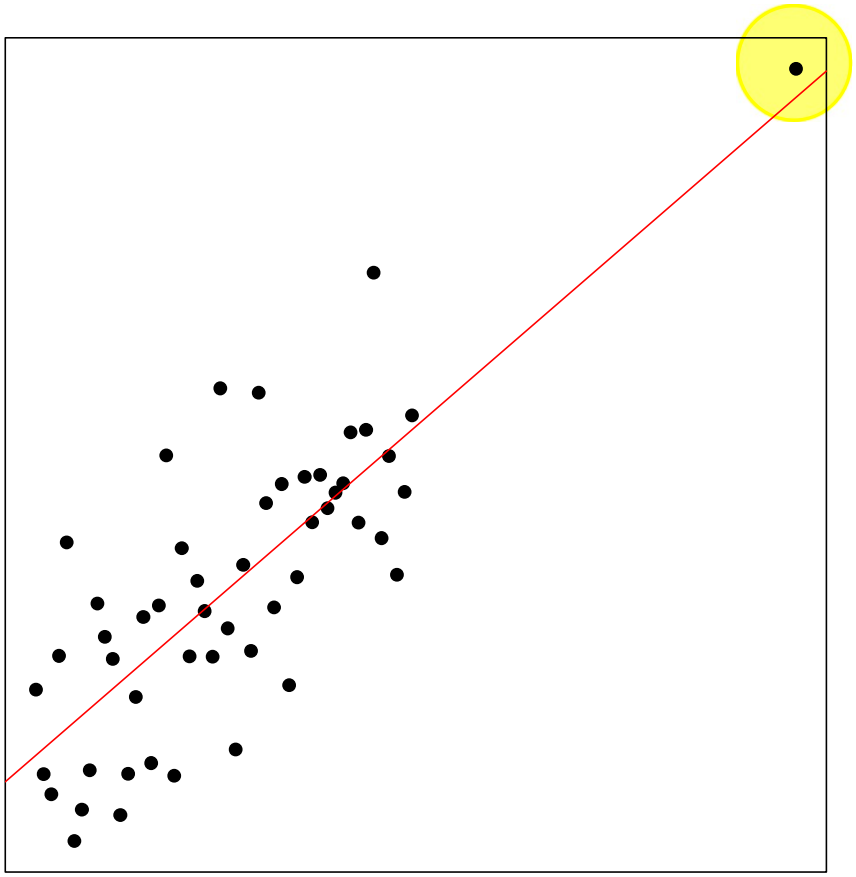
Outlier, But Not a Leverage Point



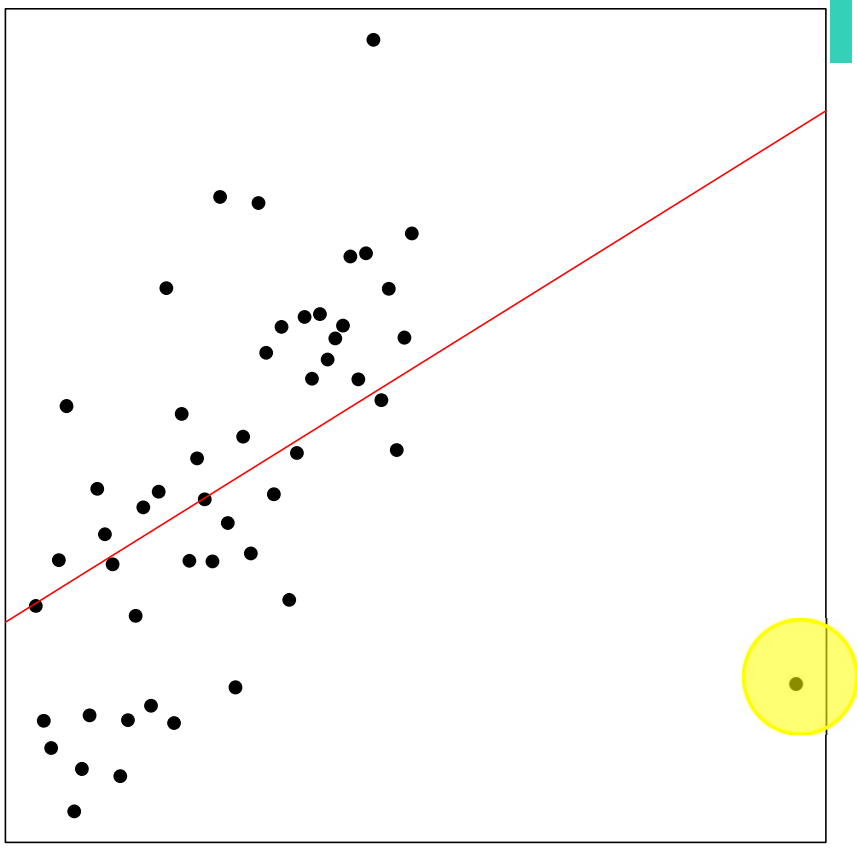
Outlier is not an outlier in the x-direction.

The slope is unchanged whether we add or remove this point.

Leverage Points



Good leverage point:
Slope is unchanged.
(P-value and correlation still changed.



Bad leverage point:
Slope is drastically changed.

Leverage Points

A **leverage point** is a point whose x-value is far from the other x-values in the data set.

"Bad" Leverage Points

- Y-value does not follow the pattern set by the other points
- Regression outlier
- Changes slope drastically
- Probably changes correlation and p-value
- Also called "Influential" points

"Good" Leverage Points

- Y-value does follow the pattern set by the other points
- Outlier, but not regression outlier
- Does not change slope drastically: model predictions unchanged
- Increases correlation in absolute value and R-squared, and decreases p-value for slope and correlation.

h_{ii} = "Leverage" of the i^{th} point

Leverage

- The leverage of the ith point is the ith diagonal value of **H**:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y}$$

- We can write the predicted value for each point as a linear combination (or weighted average) of the values of y:

$$\hat{y}_i = \sum_{j=1}^{n} h_{ij} y_j$$

- Which weights are probably highest?

$$h_{ij} = \frac{1}{n} + \frac{(x_i - \bar{x})(y_j - \bar{x})}{ssx}$$

highest weights when x_i is far from the mean.

Leverage

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \mathbf{H}\mathbf{y}$$

$h_{ii} = i^{th}$ diagonal of $\mathbf{H}$ = leverage of i^{th} point.

$$\sum_{i=1}^{n} h_{ii} = \text{trace}(H)$$

$$= \text{trace}\left(X(X'X)^{-1}X'\right)$$

$$= \text{trace}\left((X'X)^{-1}X'X\right)$$

$$= \text{trace}(I_{p+1})$$

NOTE: $\text{Trace}(AB) = \text{Trace}(BA)$

Leverage Rule

- Leverage of i^{th} point = h_{ii}
- A popular rule is to classify the i^{th} point as a leverage point in a multiple linear regression model with p predictors (and one intercept, so that the design matrix has p+1 columns) if:

$$h_{ii} > 2 \times \text{average}(h_{ii}) = 2 \times \frac{p+1}{n}$$

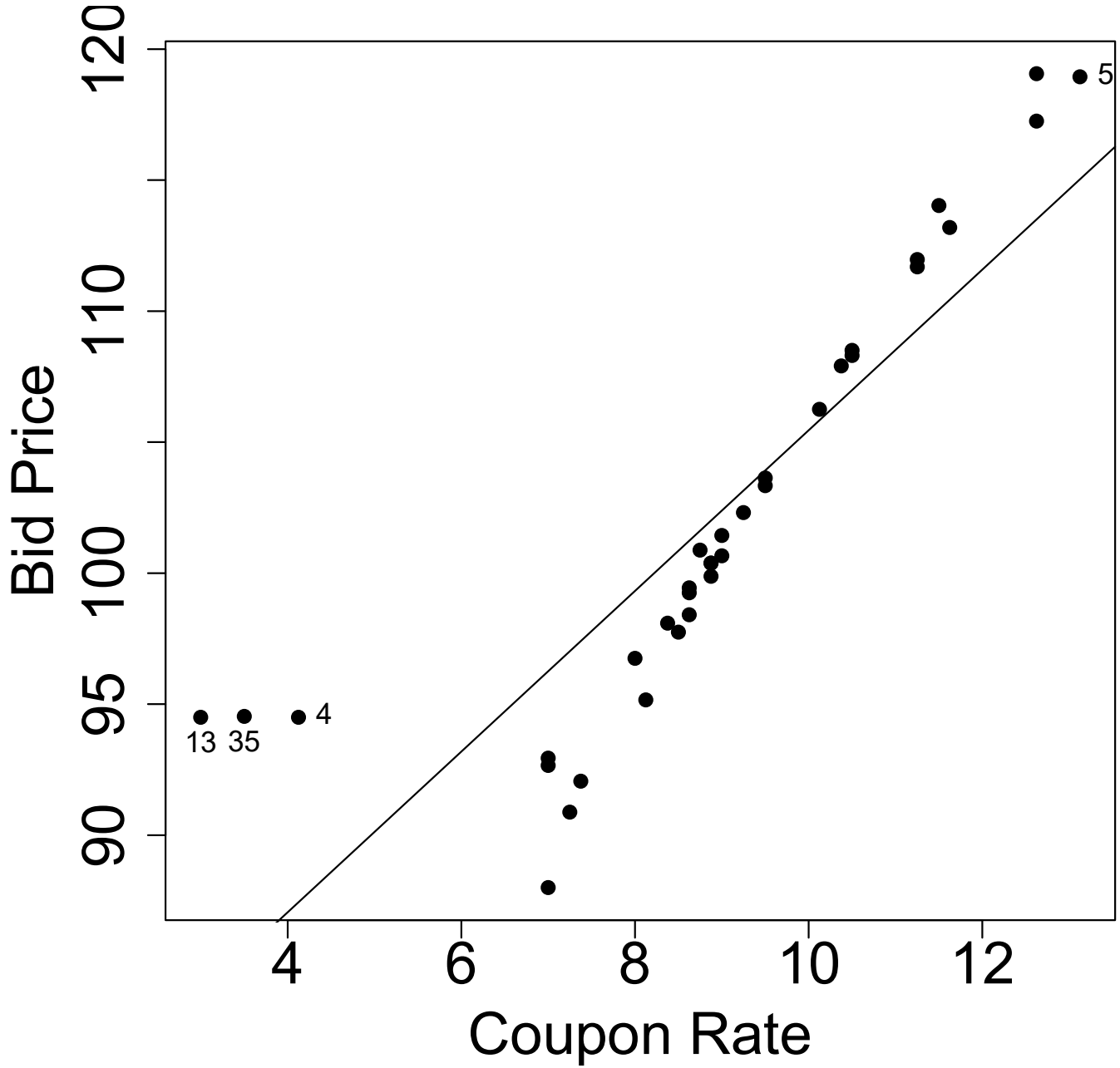
- In a simple linear regression, the i^{th} point is a leverage point if $h_{ii} > 4/n$.

Treasury Bonds

U.S. Treasury bonds maturing between 1994 and 1998.

Half the coupon rate is paid every six months (e.g. a 7% bond pays $3.50 every six months) until maturity, at which time it pays $100.

Treasury Bonds: Regression Line



Treasury Bonds: Leverage Points

$$n = 35$$

$$4/35 = 0.11$$

- Cases 4, 5, 13, and 35 all have leverage values greater than 0.11.

```
> hatvalues(my.lm)
        1         2         3         4         5         6         7
0.04850372 0.02860476 0.04850372 0.15277805 0.12397083 0.03315530 0.02873009
        8         9        10        11        12        13        14
0.10262572 0.03037870 0.03639225 0.06803392 0.02904583 0.21787629 0.04202499
       15        16        17        18        19        20        21
0.05784582 0.03018347 0.03997869 0.05784582 0.10262572 0.02858307 0.04202499
       22        23        24        25        26        27        28
0.02904583 0.03037870 0.06446917 0.02858307 0.04148268 0.04365431 0.02904583
       29        30        31        32        33        34        35
0.02953029 0.02858307 0.03199597 0.02860476 0.02915429 0.04850372 0.18725657
```

Strategies for bad leverage points

1. Remove invalid data points

Are these data unusual or different in some systematic way from the rest of the model? If so, should we use a different model for these data? Our three worst leverage points correspond to flower bonds, which have tax advantages over other bonds.

2. Fit a different regression model

Has an incorrect model been fit to the data? Consider a different model:

- Add predictor variables
- Transform Y and / or x.

Leverage Properties

$$h_{ii} = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{SXX}$$

- What happens to leverage if the point is farther from the rest of the data in the x-direction?

- Does whether a point has high leverage depend on the value of y for that point?

Standardized Residuals

$\hat{e}_i = y_i - \hat{y}_i$ standardizing a R.V.

$\Rightarrow \dfrac{r.v._i - \text{mean}(r.v.)}{SD(r.v.)}$

For standardized residual:

How about: $\dfrac{\hat{e}_i - 0}{RMSE}$? ← NOT quite right ($RMSE = \hat{\sigma}$, but $sd(\hat{e}_i) \neq \hat{\sigma}$, $SD(e_i) = \sigma$)

$var(\hat{y}) = var(X(X'X)^{-1}X'y) = X(X'X)^{-1}X'\,\sigma^2 I\, X(X'X)^{-1}X'$

$= \sigma^2 X(X'X)^{-1}X'$

$var(y|X) = \sigma^2 I = var(e)$

$var(\hat{e}) = var(y - \hat{y}) = \sigma^2(I - H)$

$$r_i = \frac{\hat{e}_i}{s\sqrt{1 - h_{ii}}} \leftarrow \text{est. } SD(\hat{e}_i)$$

STOP Wednesday 2/2/22 (week 3, lecture 7)

START Friday 2/4/22 (Week 3, Lecture 8)

Standardized Residuals

$$r_i = \frac{\hat{e}_i}{s\sqrt{1 - h_{ii}}}$$

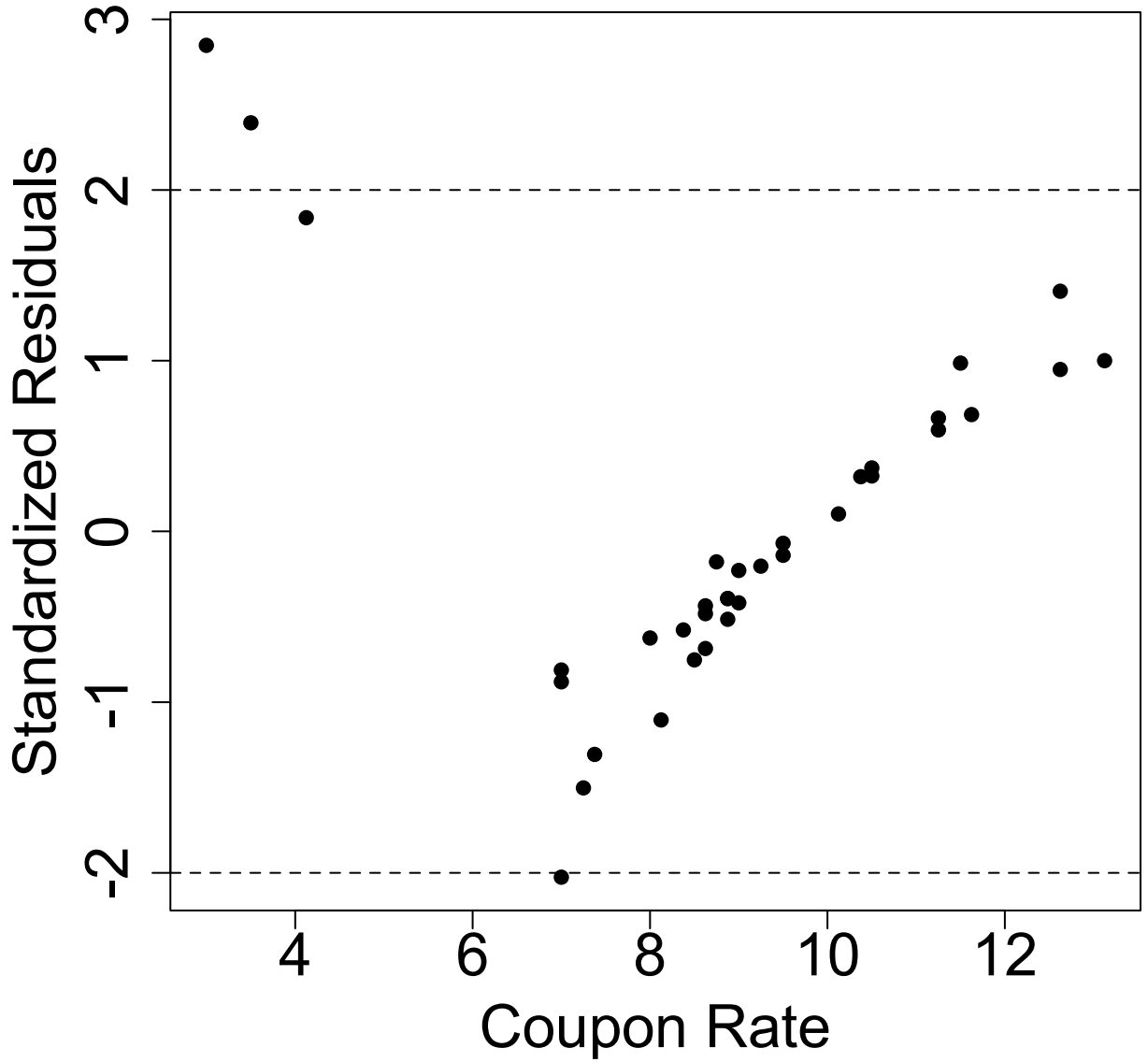
- Two advantages to standardizing (taking z-scores of) residuals:
  1. Residuals (sample) will have nonconstant variance, even if the errors (population) have constant variance, in the presence of high leverage.
  2. The standardization immediately tells us how many standard deviations any point is away from the fitted regression model. If the errors are normally distributed, 95% of them should be within 2 standard deviations of 0; for small data sets, this is our rule of thumb for outliers. For very large data sets, we expand this rule to +/- 4 standard deviations.

Rule

Recall that a bad leverage point is a leverage point which is also an outlier. Thus, a bad leverage point is a leverage point whose standardized residual falls outside the interval from –2 to 2.

On the other hand, a “good” leverage point is a leverage point whose standardized residual falls inside the interval from –2 to 2 .

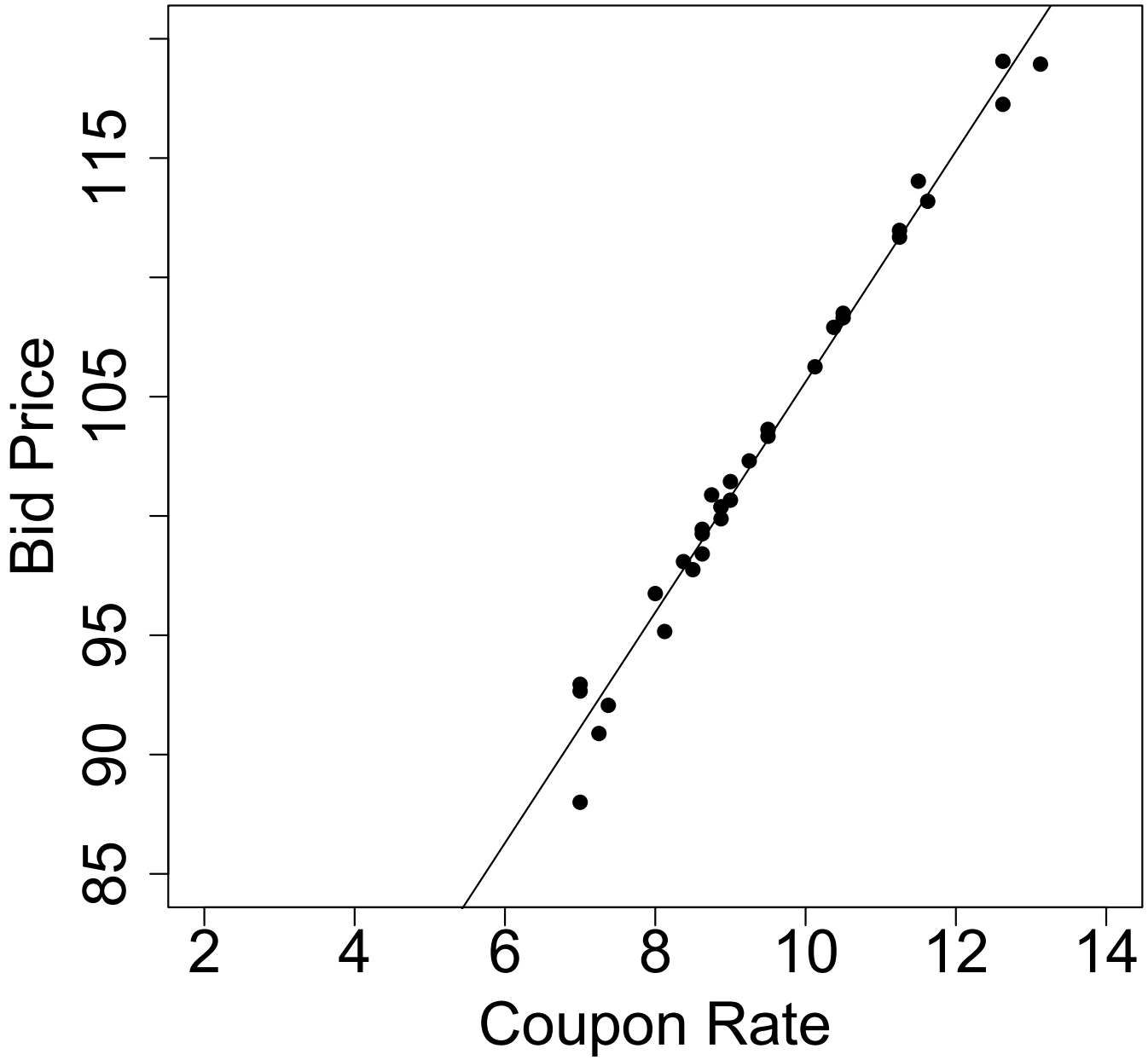
Treasury Bonds: Residuals



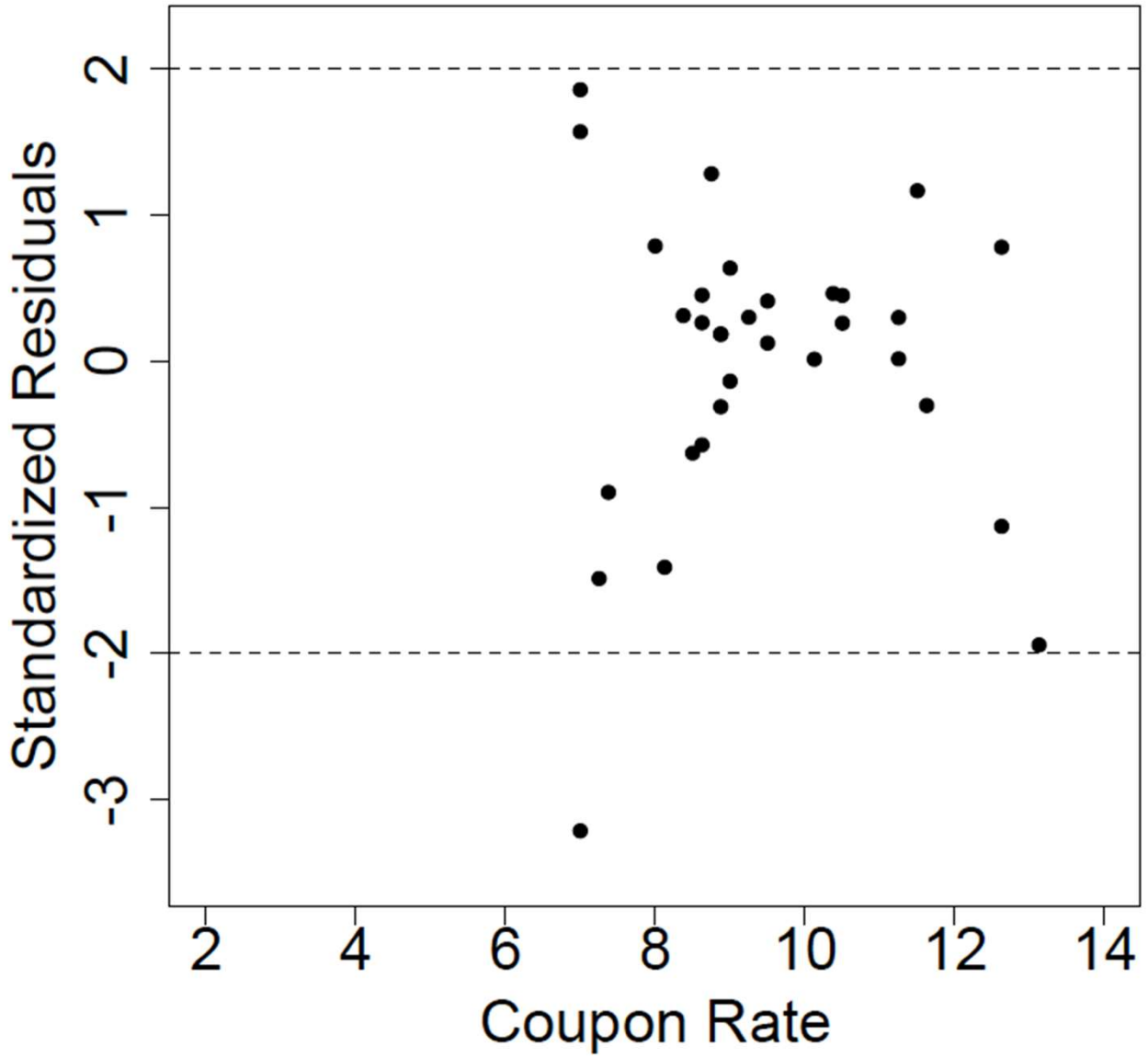
Treasury Bonds: Residuals

- First, the pattern of residuals is not a random scatter, so our model is not valid.
- We saw earlier that cases 4, 5, 13, and 35 could be classified as leverage points.
- Cases 13, 35, and 34 have standardized residual values greater than -2, and case 4 has standardized residual equal to -1.8.
- Cases 13 and 35 (and to a lesser extent, case 4) are thus of high leverage that are also outliers; thus, they are **bad leverage points**.

Treasury Bonds: New Model



Treasury Bonds: New Model



Recommendations for Handling Outliers and Leverage Points

- Points shouldn't be routinely deleted just because they do not fit the model!
- Outliers often point to an alternative model. Including one or more dummy variables is one way of coping with outliers that point to an important feature.

Correlation between estimated errors

There is a small amount of correlation present in standardized residuals, even if the errors are independent. In fact it can be shown that

$$\text{Cov}(\hat{e}_i, \hat{e}_j) = -h_{ij}\sigma^2 \, (i \neq j)$$

$$\text{Corr}(\hat{e}_i, \hat{e}_j) = \frac{-h_{ij}}{\sqrt{(1-h_{ii})(1-h_{jj})}} \, (i \neq j)$$

However, the size of the **correlations inherent in the least squares residuals** are generally so small in situations in which correlated errors is an issue (e.g., data collected over time) that they can be effectively ignored in practice.

Assessing Influence

- Leverage (x-direction) $\times$ standardized residual (y-direction) $\approx$ influence
- Influence measures by how much a point changes (influences) the slope of a regression line.
- Bad outliers will have too much influence over the location of the line.

Assessing Influence

Cook's D:

$$D_i = \frac{\sum_{j=1}^{n}(\hat{y}_{j(i)} - \hat{y}_i)^2}{(p+1)S^2} = \frac{r_i^2}{(p+1)}\frac{h_{ii}}{(1-h_{ii})}$$

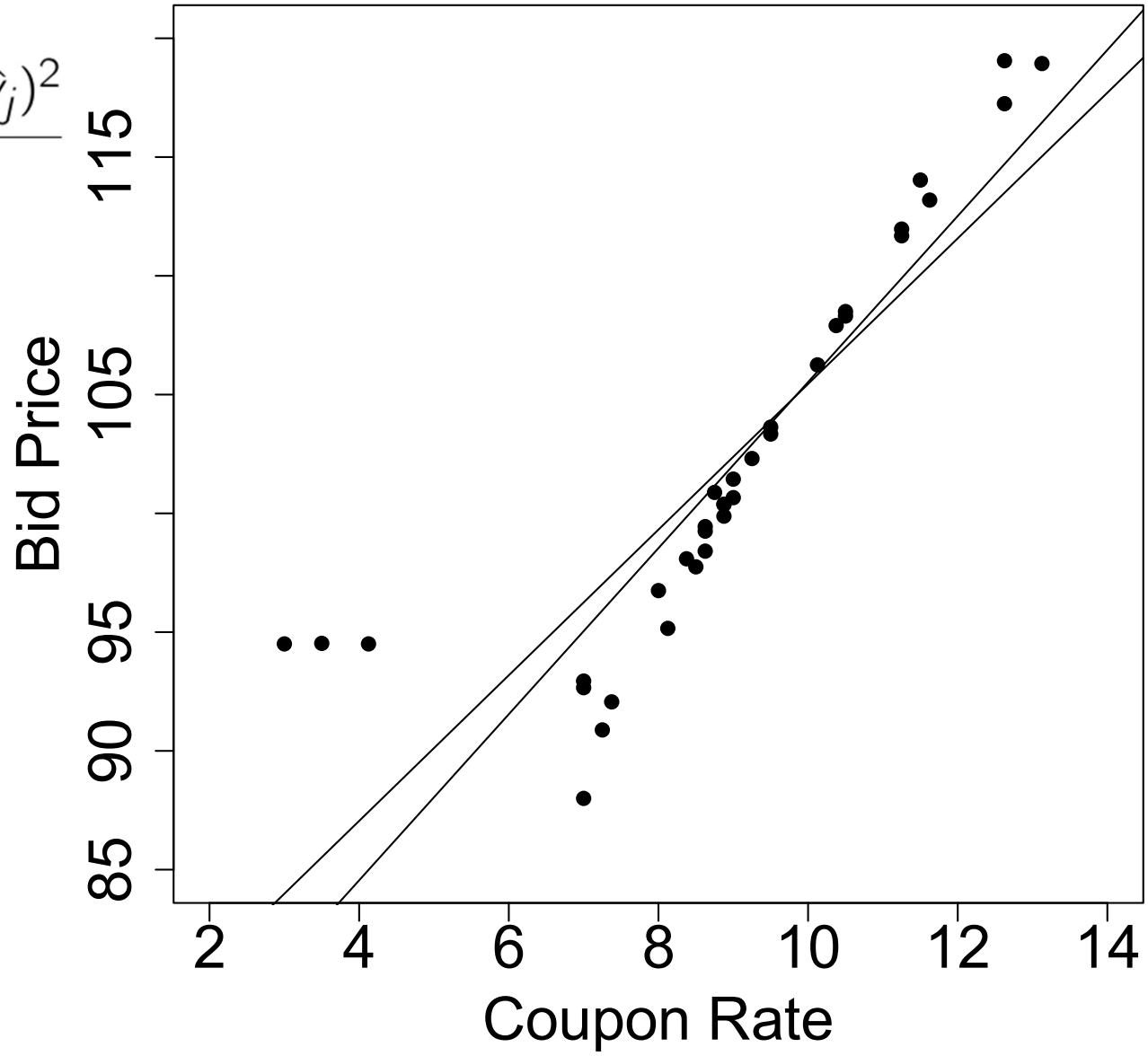
- The notation j(i) means the value of y-hat with the i^{th} observation deleted.
- When is D_i large?
- One rule of thumb is to classify an observation as noteworthy if D_i is greater than 4/(n-2).
- In practice, look at gaps in the D_i values.

SMLT Monday 2/7/22 (week 4, lecture 9)

Assessing Influence

$$D_i = \frac{\sum_{j=1}^{n}(\hat{y}_{j(i)} - \hat{y}_j)^2}{(p+1)S^2}$$

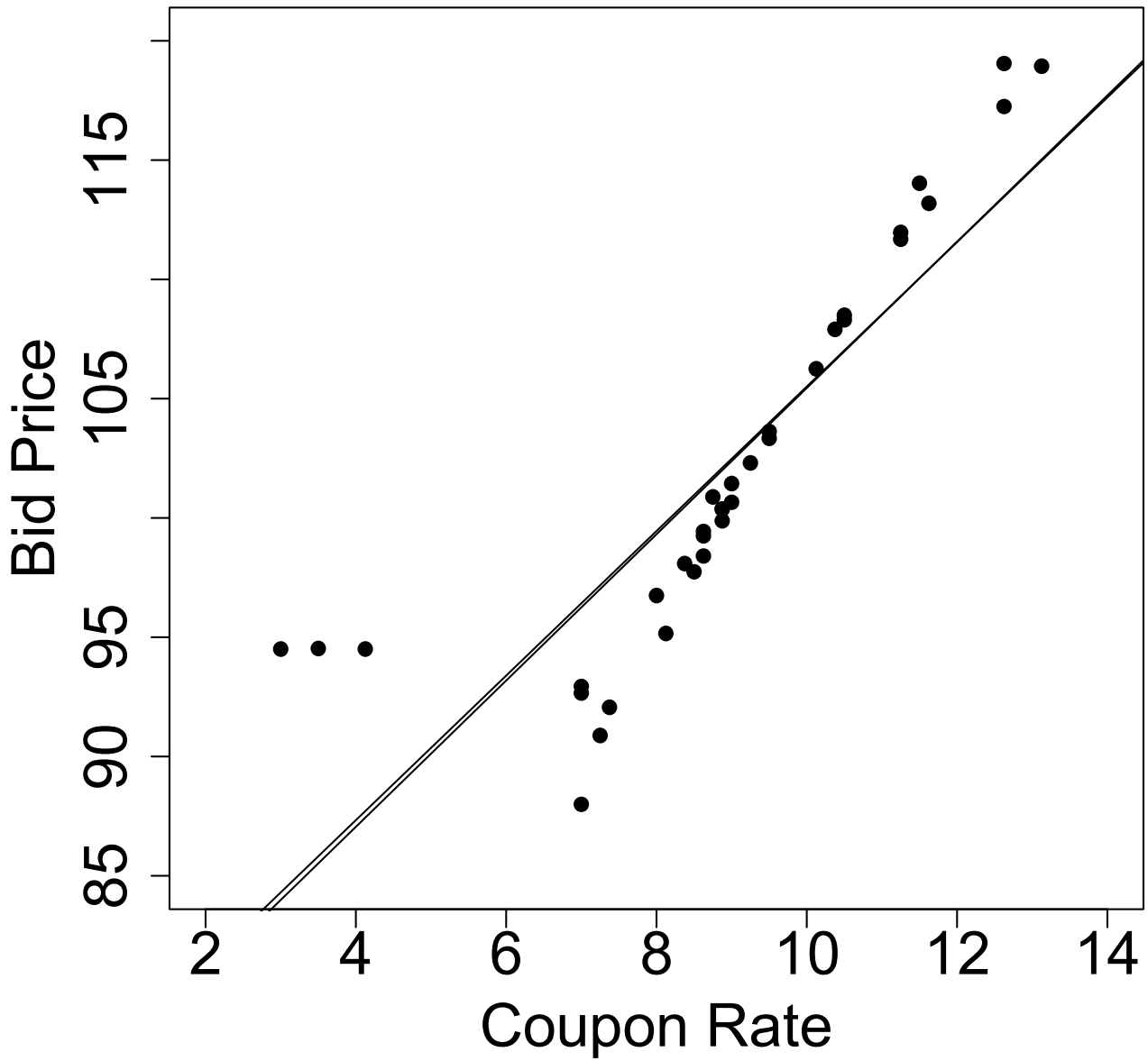
Remove point #13 and compare



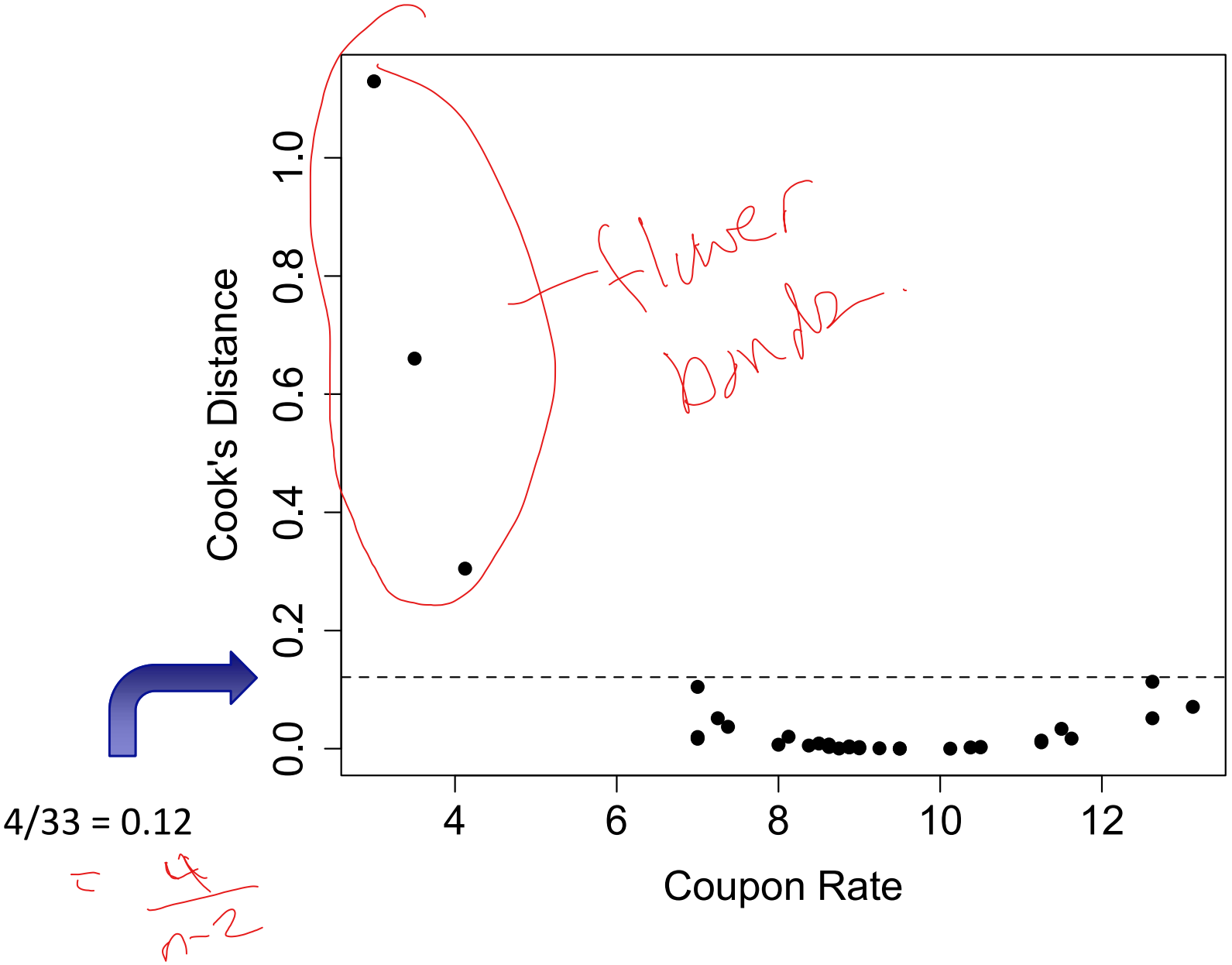
Assessing Influence

Remove point #1:

Small Cook's D



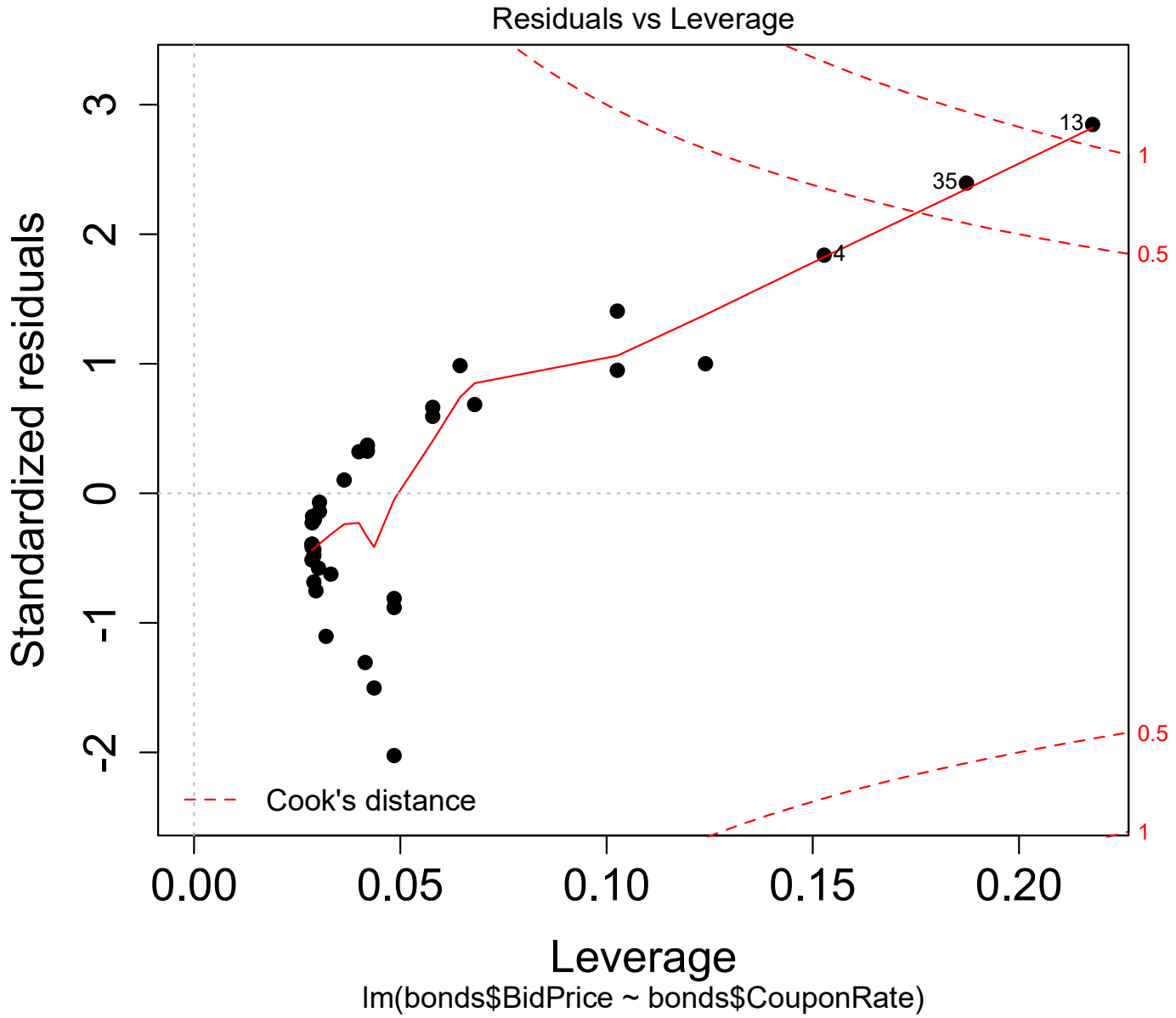
Cook's D: Bond data



4/33 = 0.12

$= \frac{4}{n-2}$

Cook's D: Bond data (default plot)



Normality of the Errors

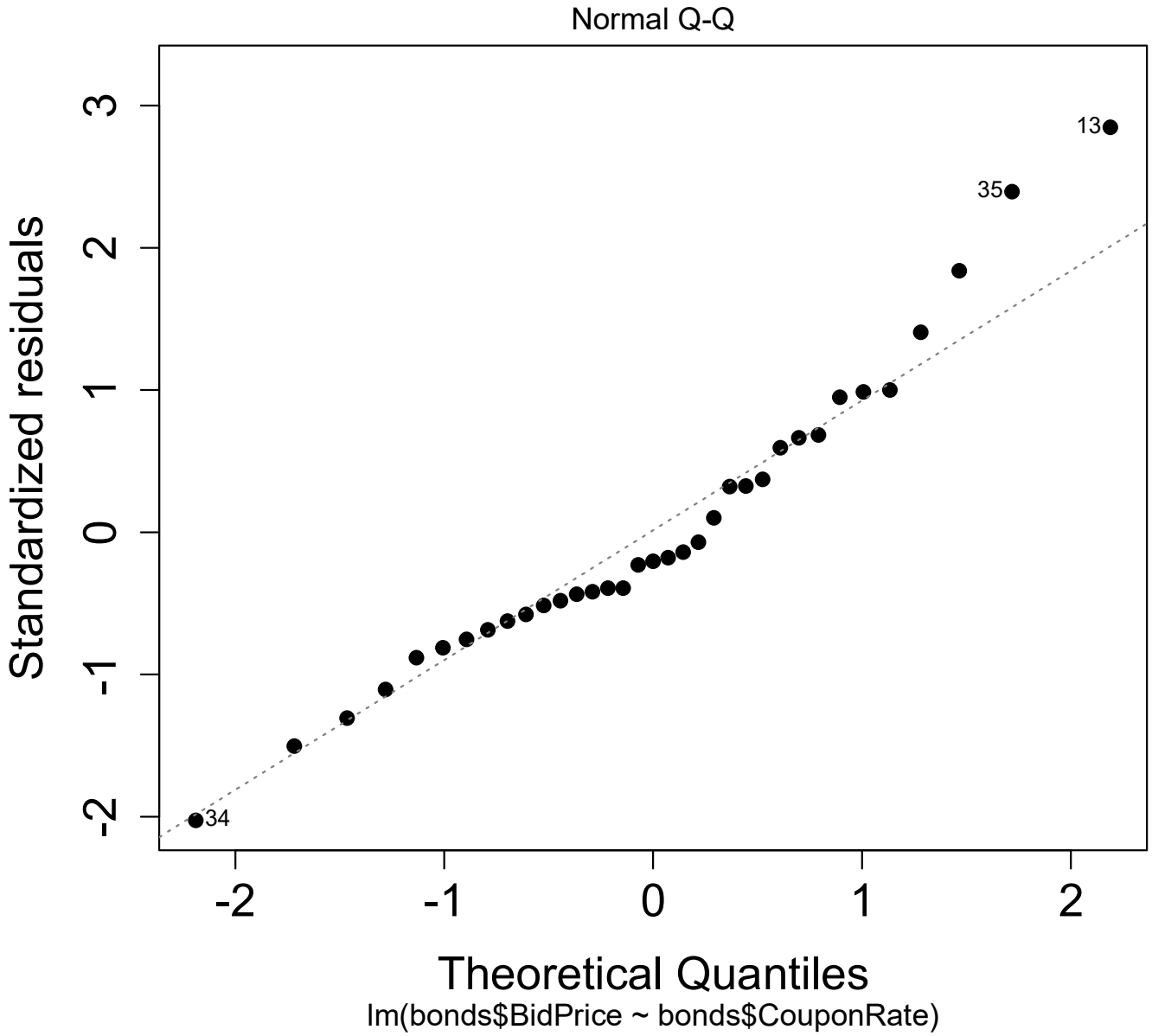
Necessary for:

- Small sample sizes: Hypothesis tests and confidence intervals for the regression parameters and regression line (for larger n, CLT applies for slope and CI for the mean of y at a particular x).
- All sample sizes: Prediction intervals (distribution of *individual* values of y at each x assumed normal); otherwise, bootstrap

To check:

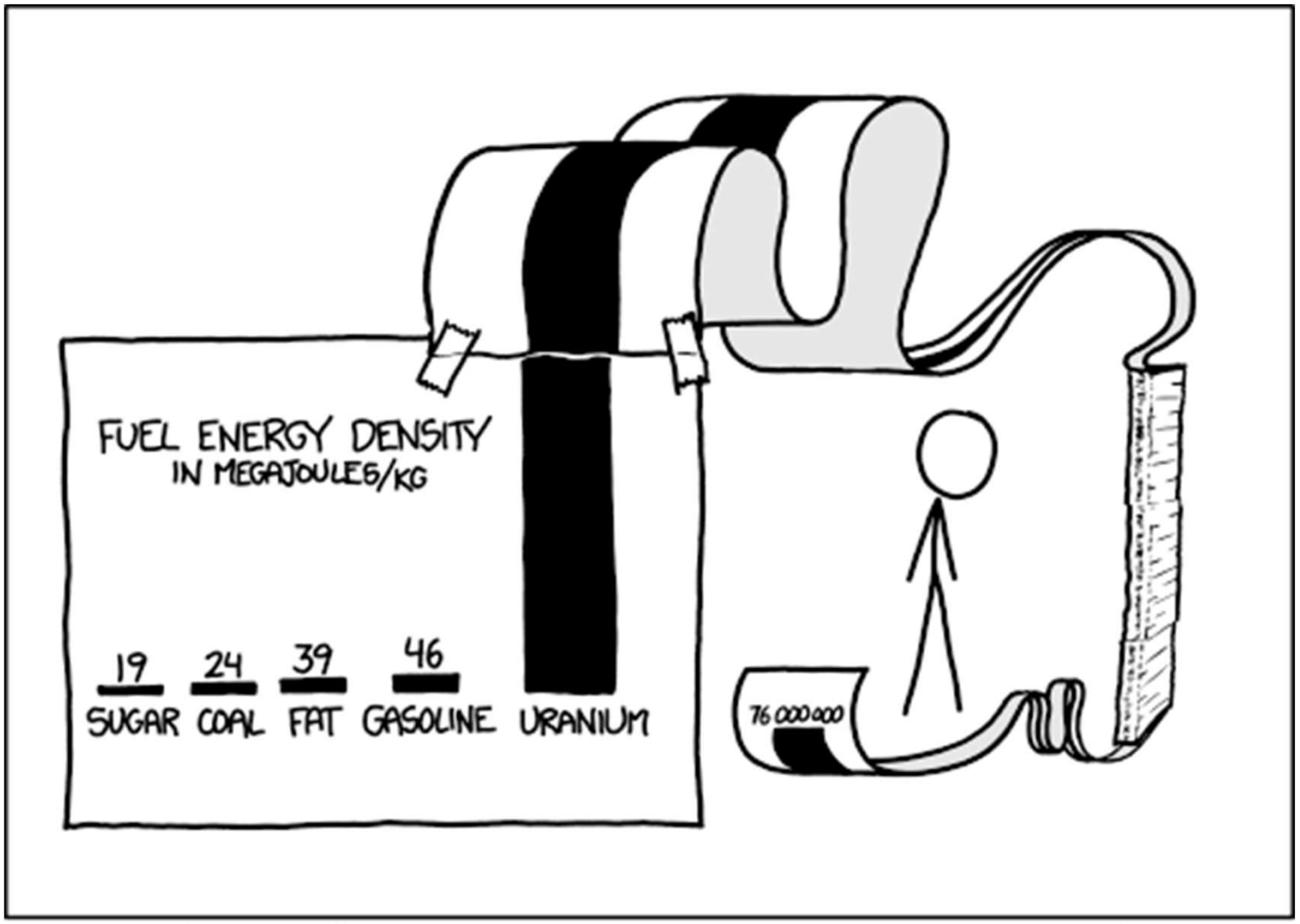
- Q-Q plots of residuals (Warning: residuals appear normal though errors are not normal)
- Formal tests of normality (Anderson-Darling, but remember significance is not the same as practical importance)

Q-Q Plot: Bonds Data (default)



Transformations

Transformations



SCIENCE TIP: LOG SCALES ARE FOR QUITTERS WHO CAN'T FIND ENOUGH PAPER TO MAKE THEIR POINT *PROPERLY.*

Constant Variance

If we have nonconstant variance we can do transformations to make variance constant approx

Necessary for inference

Tools to assess constant variance (homoskedasticity):

- Plots
- Formal tests (e.g. White, 1980)

Tools to deal with non-constant variance (heteroskedasticity):

- Transformations
- Weighted least squares (Chapter 4)

Constant variance: Plots

An effective plot to diagnose nonconstant error variance is a plot of

$|\text{Residuals}|^{0.5}$ against x

or

$|\text{Standardized Residuals}|^{0.5}$ against x

Typically use this

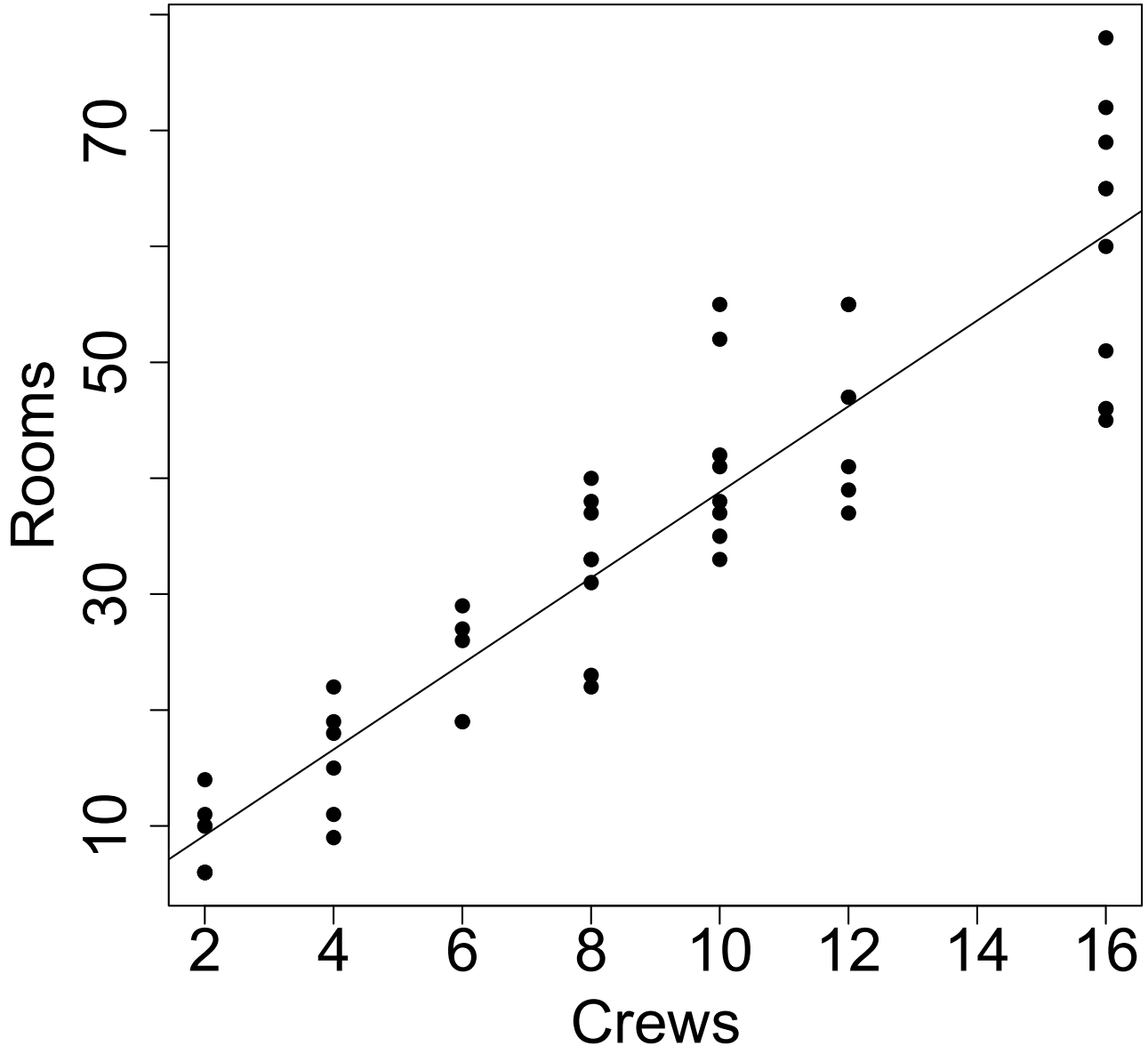
(The square root is taken to reduce skewness in the absolute values.)

Constant Variance: Example

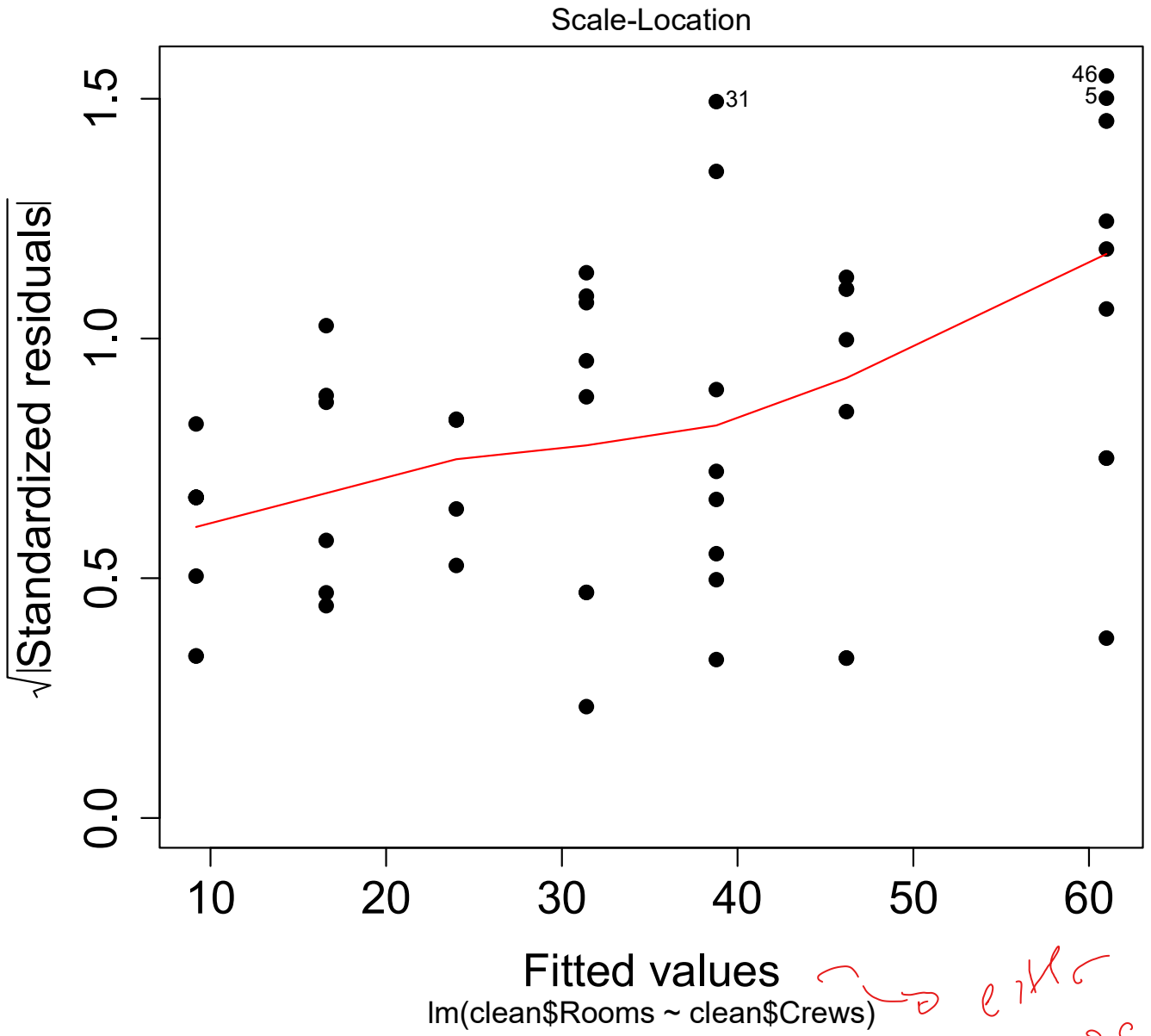
Developing a bid on contract cleaning

- Goal: Bid on a contract to clean offices.
- Costs proportional to # cleaning crews needed.
- 53 days of records: # crews & # rooms cleaned

Constant Variance: Example



Constant Variance: Example (default)



either x val of
in this case, fitted values
can be used as
X-axis.

Transformations

Transformations can be used to:

- Overcome problems due to nonconstant variance
- Estimate percentage effects — log transform 2.
- Overcome problems due to nonlinearity
  - reduce influence of outliers

Transformations: Count Data

Count data are often modeled using the Poisson distribution. Suppose that *Y* follows a Poisson distribution with mean λ. Then the variance of *Y* is also equal to λ. In this case, the appropriate transformation of Y for stabilizing variance is square root.

Justification: Consider the following Taylor series expansion around μ:

$$f(Y) = f(E(Y)) + f'(E(Y))(Y - E(Y)) + \ldots$$

The well-known delta rule for calculating first-order variance terms is obtained by considering just the terms given in this last expansion. In particular, taking the variance of each side of this equation gives:

$$\mathrm{Var}(f(Y)) \simeq \left[f'(\mathrm{E}(Y))\right]^2 \mathrm{Var}(Y).$$

Transformations: Count Data

Suppose $f(Y) = \sqrt{Y}$ and $Var(Y) = \lambda = E[Y]$.

$f'(\lambda) = \frac{1}{2}\lambda^{-1/2} = \frac{1}{2\sqrt{\lambda}}$

$var(\sqrt{y}) \approx [(\frac{1}{2\sqrt{\lambda}})^2] * var(y) = \frac{1}{4}$ (constant w.r.t λ)

doesn't increase as mean increases.

- In our crew cleaning example, both # crews and # rooms cleaned are count data, so try the square root transformation on both variables.
- It's natural to use the same transformation on both variables when they are measured in the same units.

Cleaning Data: Intervals

Table 3.7 Predictions and 95% prediction intervals for the number of rooms

x, Crews	Prediction	Lower limit	Upper limit
4 (transformed data)	16 $=(4.003^2)$	8 $=(2.790^2)$	27$=(5.217^2)$
4 (raw data)	17	2	32
16 (transformed data)	61 $=(7.806^2)$	43 $=(6.582^2)$	82 $=(9.031^2)$
16 (raw data)	61	46	76

- Note: When using confidence or prediction intervals after transforming, back-transform the endpoints to get an interval in the original units.
- Correction factor for confidence intervals coming soon.

Using Logarithms to Estimate Percentage Effects

$$log(Y) = \beta_0 + \beta_1 log(x) + e$$

$$\begin{aligned}
\beta_1 &= \frac{\Delta log(Y)}{\Delta log(x)} \\
&= \frac{log(Y_2) - log(Y_1)}{log(x_2) - log(x_1)} \\
&= \frac{log(Y_2/Y_1)}{log(x_2/x_1)} \\
&\approx \frac{Y_2/Y_1 - 1}{x_2/x_1 - 1} \text{(using } log(1+z) \approx z \text{ and assuming } \beta_1 \text{ is small)} \\
&= \frac{100(Y_2/Y_1 - 1)}{100(x_2/x_1 - 1)} \\
&= \frac{\%\Delta Y}{\%\Delta x}
\end{aligned}$$

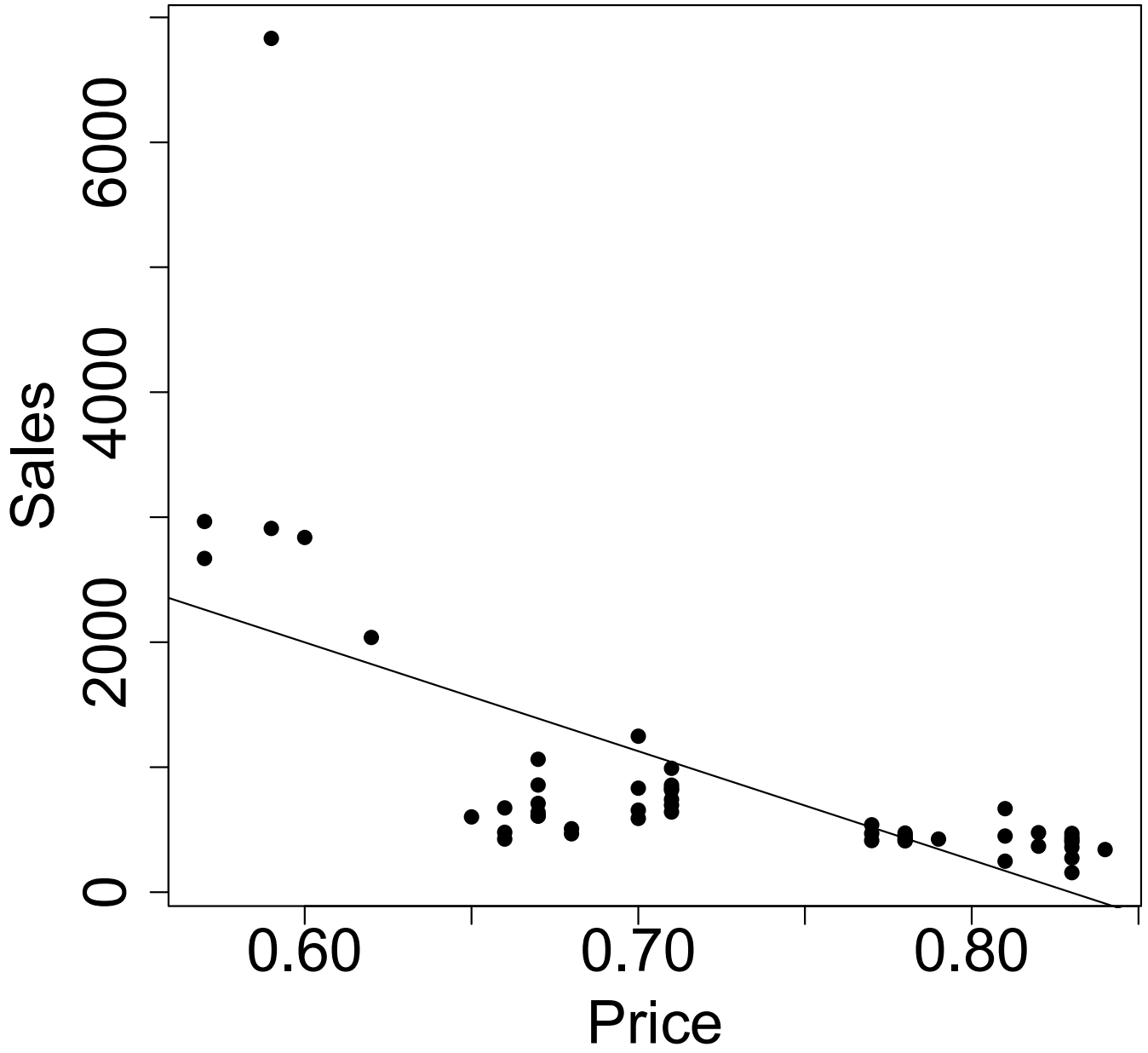
Remember:
Log is always natural log!

Business & Marketing

- Elasticity: If we increase supply by 1%, what happens to demand (in percentages)?
- A manager of Consolidated Foods, Inc. wants to know the relationship between price (P) and the quantity sold (Q).
- First we develop the model

$$Q = \beta_0 + \beta_1 P + e$$

Log Transformation Example



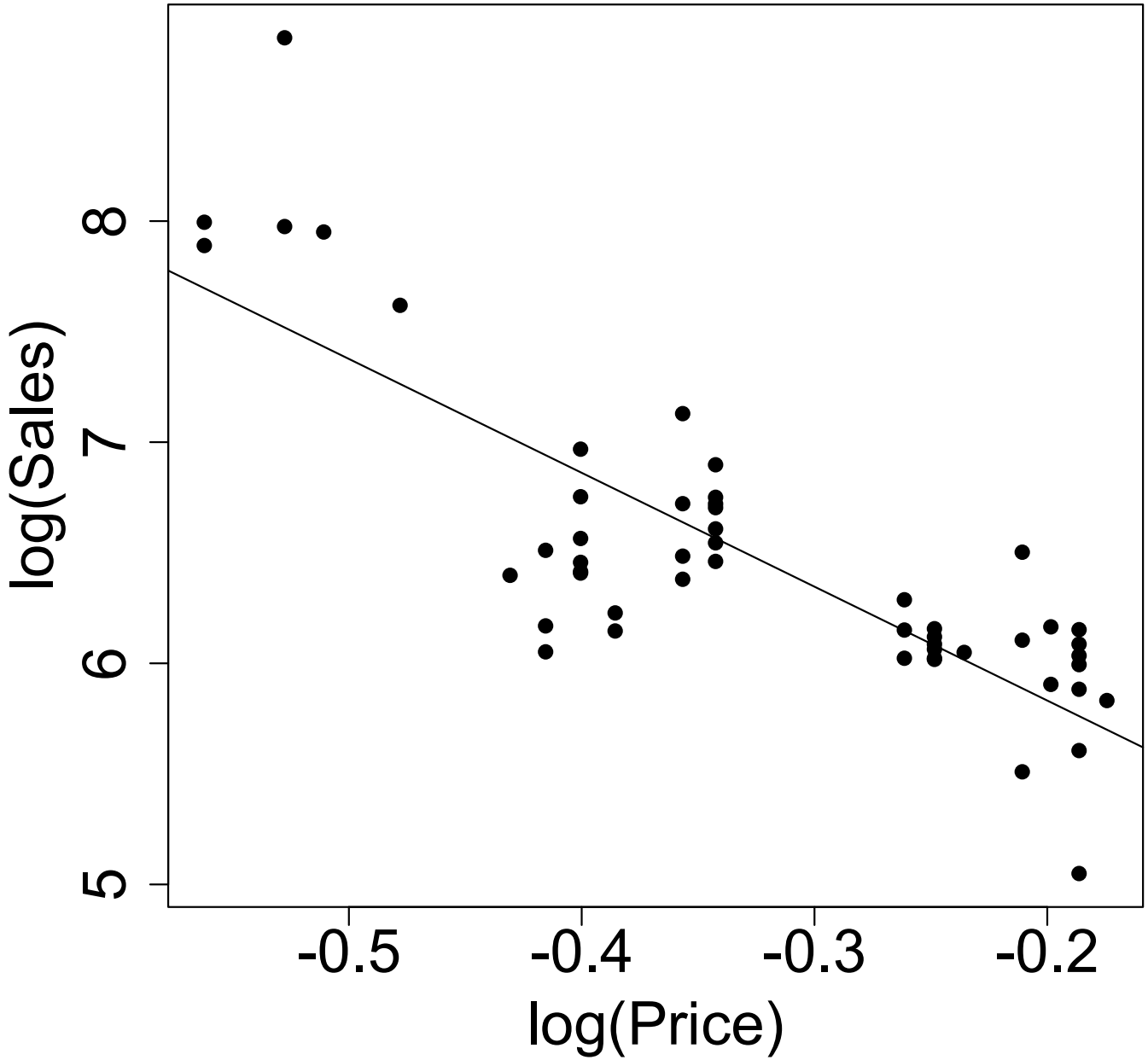
Business & Marketing

- To study the relationship between a 1% increase in price and the percent change on quantity sold, we take the logarithms of both variables.
- So we try out the model

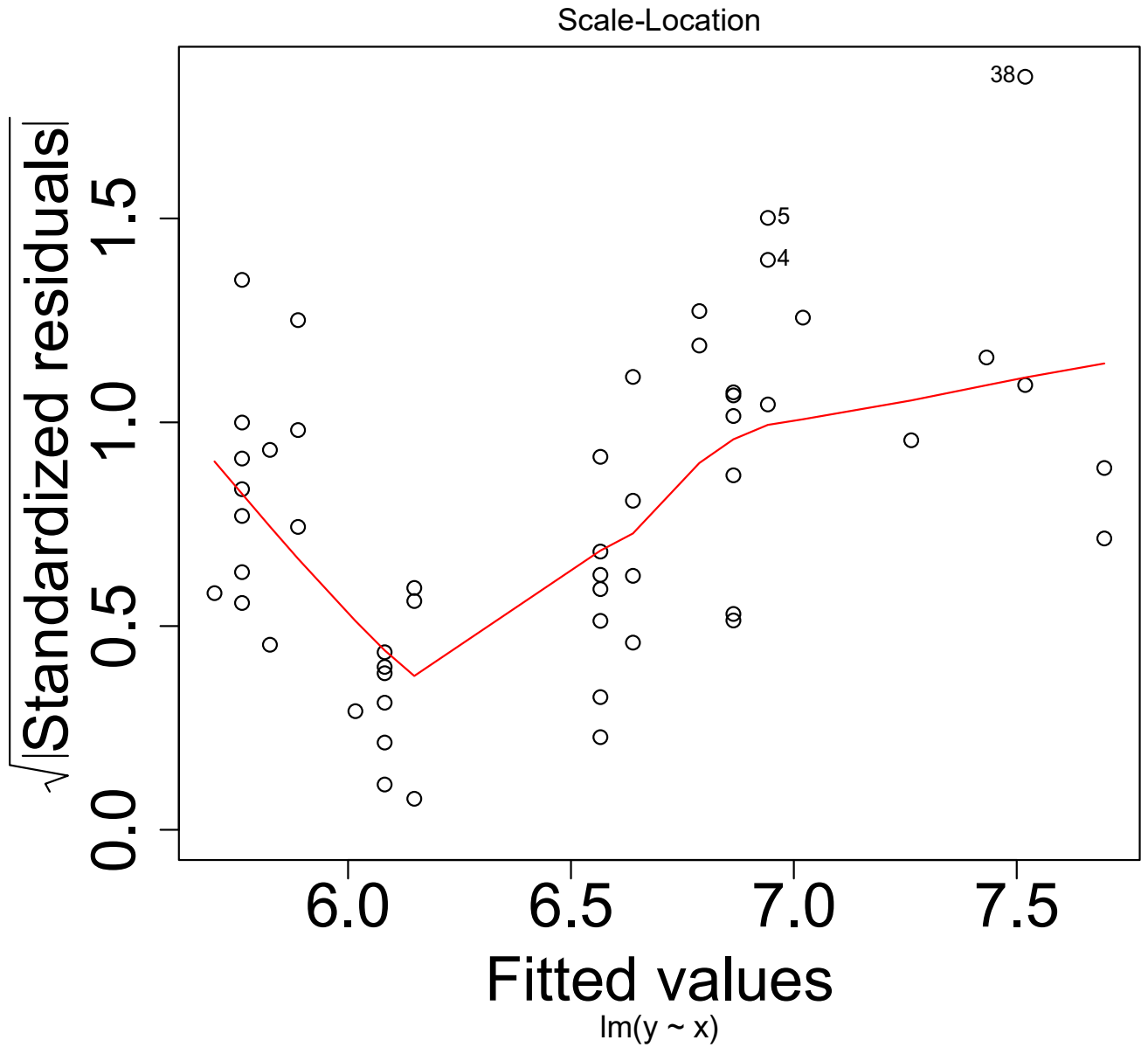
$$log(Q) = \beta_0 + \beta_1 log(P) + e$$

- The estimated slope is -5.14. Interpret in context:

Log Transformation Example



Log Transformation Example



Using Transformations to Overcome Problems due to Nonlinearity

We've discussed transformations to stabilize variance and estimate percentage effects. Next we attempt to overcome **nonlinearity in the relationship between x and y**. Two methods to do this are:

- Inverse response plots
- Box-Cox procedure

There are three main situations to be considered:

- Only the response variable needs to be transformed
- Only the predictor variable needs to be transformed
- Both need to be transformed.

Transforming only the response variable Y using inverse regression

Suppose that the true regression model between Y and X is:

$$Y = g(\beta_0 + \beta_1 x + e)$$

where *g* is some unknown function. We can turn this model into a simple linear regression model by transforming Y by g^{-1}, since:

$$g^{-1}(Y) = \beta_0 + \beta_1 x + e$$

For example, if:

$$Y = (\beta_0 + \beta_1 x + e)^3$$

Then the inverse transformation would be:

$$g(Y) = Y^3, \text{and so } g^{-1}(Y) = Y^{1/3}$$

Transforming Y

Randomly generated example:

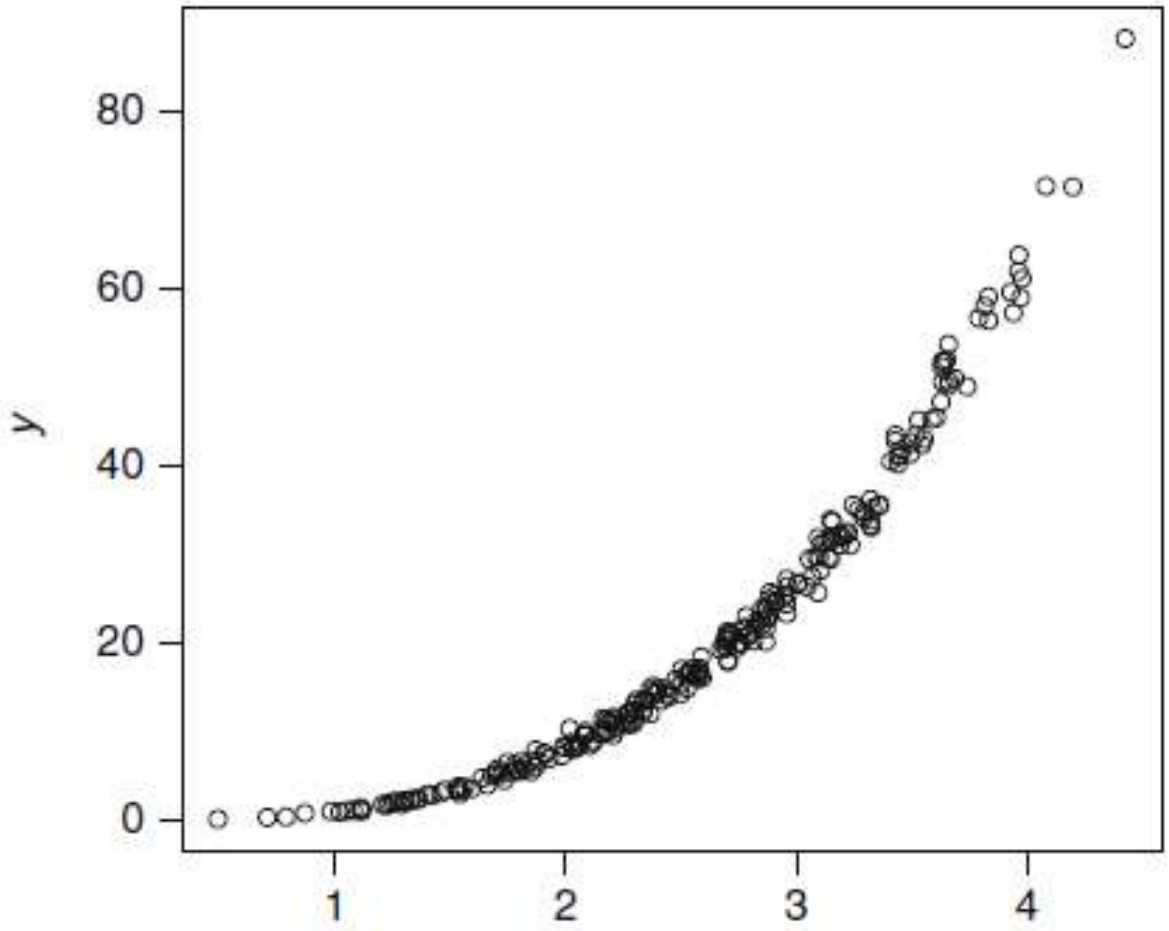
$$Y = (\beta_0 + \beta_1 x + e)^3$$

x and e both normally distributed.

Goal: figure out g(Y). Let's start with fitting a simple linear regression model and see how terrible it is.

$$Y = \beta_0 + \beta_1 x + e$$

Transforming Y



Transforming Y

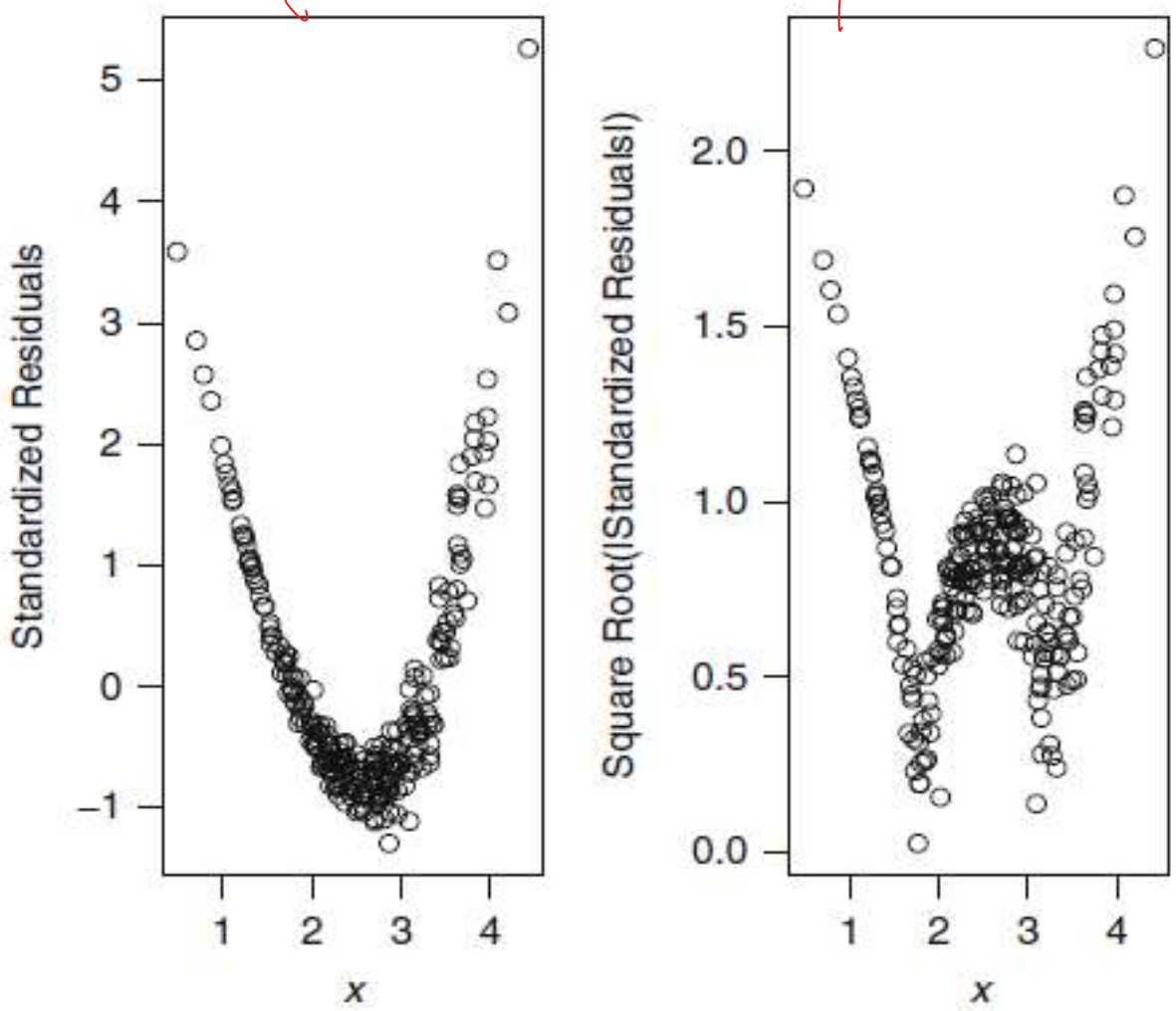


Figure 3.26 Diagnostic plots for model (3.2)

Transforming Y: Inverse Response Plots

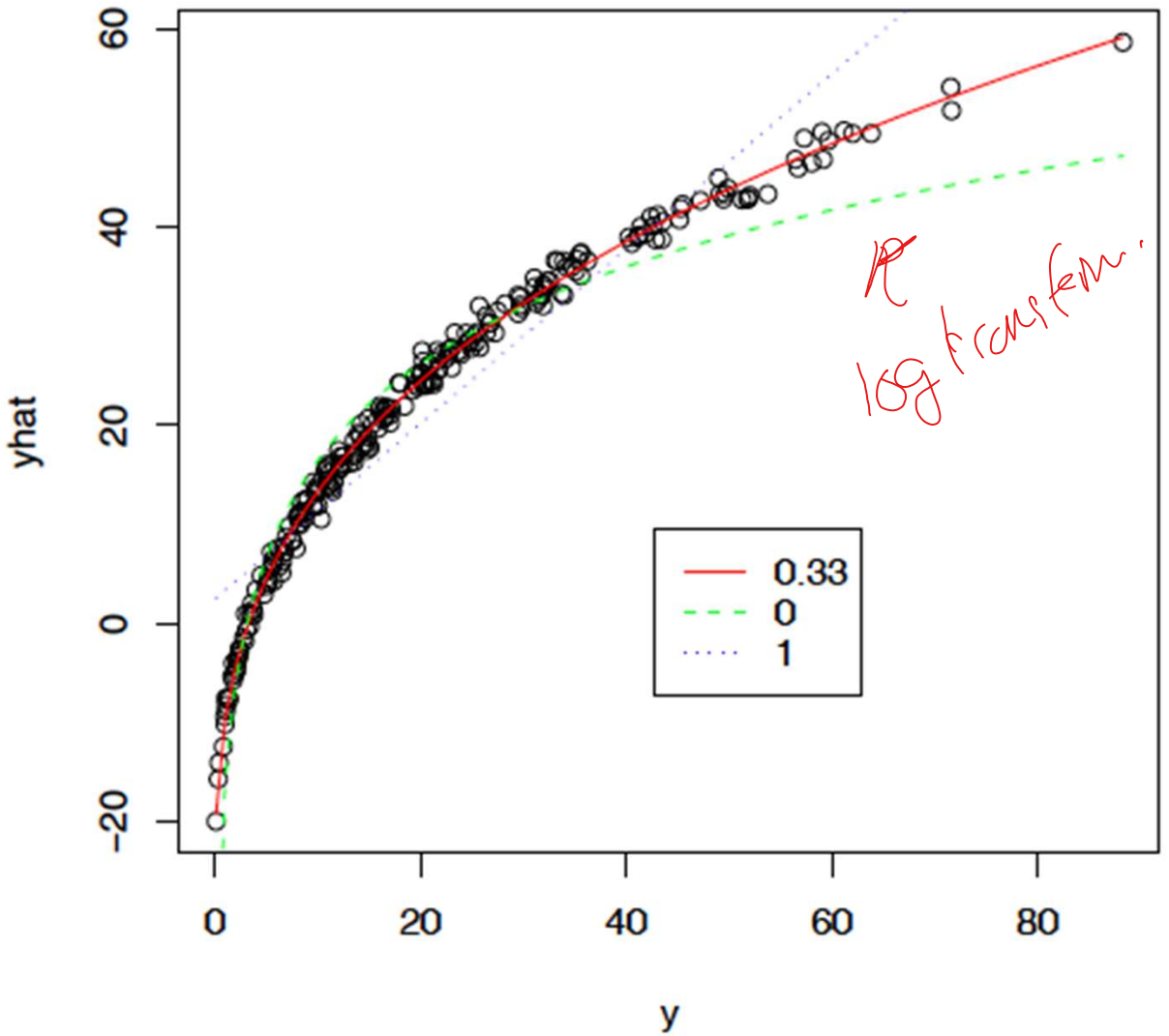
Recall that:

$$Y = g(\beta_0 + \beta_1 x + e)$$

$$g^{-1}(Y) = \beta_0 + \beta_1 x + e$$

So if we plot Y on the x-axis and $\beta_0 + \beta_1 x$ on the Y- axis, we should discover the shape of g^{-1}.

Inverse Response Plot



R
log transform.

STOP Monday 2/7/22 (week 4 (lecture 9))

START Wednesday 2/9/22 (week 4 lecture 10).

Transforming Y: Box Cox

STARTED by looking at bonds.r file.

- The relationship between normal random variables is guaranteed to be linear.
- We may want to transform both the predictor and response to a normal random variable, if possible, to find a linear relationship between them.
- The Box-Cox method searches for the power transformation that transforms variables most closely to normality.

Transforming Y: Box Cox

- To estimate $g^{-1}(Y)$, the power transformation, we consider the following family of scaled power transformations, defined only for *strictly positive Y*, by:

$$\Psi_S(Y,\lambda) = \begin{cases} (Y^\lambda - 1)/\lambda \text{ if } \lambda \neq 0 \\ \log(Y) \text{ if } \lambda = 0 \end{cases}$$

- Remember: log always means natural log!

Transforming Y: Box Cox

- The (natural) log transformation is a member of this family, since:

$$\lim_{\lambda \to 0} \Psi_S(Y, \lambda) = \lim_{\lambda \to 0} \frac{(Y^\lambda - 1)}{\lambda} = \log(Y)$$

- Scaled transformations preserve the direction of the association (positive or negative): if X and Y are positively related, then X and $\Psi_S(y, \lambda)$ are also positively related for all values of λ.

Transforming Y: Box Cox

$$E[\hat{y}|Y = y] = \alpha_0 + \alpha_1 \psi(y, \lambda)$$

The explanatory variable in the model above is the transformed y, and the response variable is $\hat{y}$ from the simple linear regression model.

We fit the model above for a range of values λ and choose an estimated optimal value of λ that minimizes the residual sum of squares RSS(λ).

Usually choosing a λ from {-1, -1/2, -1/3, -1/4 0, 1/4, 1/3, 1/2, 1} is adequate. Why? → for interpretation purposes.

Transforming Y: Box-Cox

- Box-Cox assumes there exists a power transformation g(Y) such that the transformed version of Y is **normally distributed**.
- If X and Y are normally distributed, the relationship between them will be _____linear_____.
- We're not as concerned with the distribution of the residuals as we are with the relationship between x and y.

Transforming Y: Box-Cox

Box and Cox multiply the function $\psi_S(x, \lambda)$ by a factor to get $\psi_M(x, \lambda)$, the goal being to keep all units the same for all values of λ. The method is based on the maximum likelihood estimates for Y. Maximizing the likelihood with respect to λ is equivalent to minimizing RSS(λ) with respect to λ.

$$RSS(\lambda) = \sum_{i=1}^{n} (\psi_M(y_i, \lambda) - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

This time, the response variable is the transformed y and the explanatory variable is x.

Transformations: Caution

- Transformations don't perform well in every situation.
- X may not explain Y very well, no matter what transformation is used.
  - Ex. Important predictors not included.
- Box-Cox might result in a transformed variable that is not very close to normally distributed.
  - Ex. heavy tails on both sides… consider turning into a categorical variable.

Transforming X

- Try scaled power transformations, as for Y.

$$\psi_S(X,\lambda) = \begin{cases} (X^\lambda - 1)/\lambda & \text{if } \lambda \neq 0 \\ log(X) & \text{if } \lambda = 0 \end{cases}$$

$$E[Y|X = x] = \alpha_0 + \alpha_1 \psi_S(x,\lambda)$$

Choose the value of λ that minimizes the residual sum of squares from fitting the above model.

- The Box-Cox method can also be directly applied to X.

Transforming both the response and the predictor variables

Approach 1:

1. Transform X to $\psi(x, \lambda)$ so that the distribution of the transformed version of X is as normal as possible. Univariate Box-Cox is one way to do this.
2. Consider a simple linear regression model of the form $Y = g(\beta_0 + \beta_1 \psi(x, \lambda) + e)$. Use an inverse response plot to decide on the transformation g^{-1} for Y.

Approach 2:

Transform X and Y simultaneously to joint normality using multivariate Box-Cox.

Many times, the two approaches lead to the same answer. Approach 1 is more robust, and may give reasonable answers when approach 2 fails.

Interpreting the slope

- Two common reasons people choose a parametric model are its ability to be interpreted in context and its power.
- Instead of transforming, would a nonparametric regression, bootstrap regression, or neural net work better?
- Nonparametric and bootstrap models lose power, but at large sample sizes, that becomes less important.

STOP Wednesday 2/9/22 (Week 4, Lecture 10)

Transformation Corrections

START Friday 2/11/22 (week 4, Lecture 11)

Transformations: Confidence and Prediction Intervals

Suppose we are interested in the middle 95% of a distribution (as in a confidence or prediction interval).

What happens if we shift the interval to the left or right?

Transformations: Confidence and Prediction Intervals

If the relationship between Y and some transformation g(Y) were linear, then it would be true that E[g(Y)] = g(E[Y]). But if the relationship between X and g(Y) were linear, and the relationship between g(Y) and Y were linear, then the relationship between X and Y would be linear.

Moral: g(Y) is non-linear. Linear transformations are mostly useless.

$$
\begin{aligned}
E[X] &= \int g(x)f(x)dx = \int (ax+b)f(x)dx \\
&= \int ax\,f(x)dx + \int b\,f(x)dx \\
&= a\int x\,f(x)dx + b\int f(x)dx \\
&= a\,E[X] + b
\end{aligned}
$$

we're trying to reshape the curve of Y vs X or reshape the axis terms

Review

$$
\begin{aligned}
Var(X) &= E[(X-\mu)^2] \\
&= E[X^2 - 2X\mu + \mu^2] \\
&= E[X^2] - 2\mu\, E[X] + \mu^2 \\
&= E[X^2] - 2\mu^2 + \mu^2 \\
&= E[X^2] - \mu^2
\end{aligned}
$$

$$E[X^2] = \mu^2 + Var(X)$$

correction factor

back transformation

Transformations: Confidence and Prediction Intervals

We sometimes want to be able to find confidence intervals and prediction intervals for the least squares regression line in models with transformed X and Y.

Remember, we're modeling the mean of Y using x:

$$\mu_Y = \beta_0 + \beta_1 x$$

But in order to get a linear relationship between X and Y, we had to transform Y, so we had:

$$g(Y) = W, \mu_W = \beta_0 + \beta_1 x$$

If we also found that g(Y) was normally distributed, then to go back and find the mean of Y at each value of x*, we would need:

$$E[g^{-1}(W)]$$

Example: Square Root Transformation

Square root transformation to stabilize variance (e.g. Cleaning. Everything is conditional on X):

$$g(Y) = \sqrt{Y} = W$$

$$\begin{aligned} E[g^{-1}(Y)] &= E[W^2] \\ &= E[W]^2 + Var(W) \\ &= \mu_W^2 + \sigma_W^2 \\ &= (\beta_0 + \beta_1 x)^2 + \sigma_W^2 \end{aligned}$$

σ_W^2 ~

$(\beta_0 + \beta_1 x)^2$ ↳ back transform

σ_W^2 ↳ correction factor.

The variance of W, given X, is the variance of the errors. So we would estimate the confidence or prediction interval (if W were normal) by transforming the endpoints of the usual confidence or prediction interval using W plus MSE.

Example: Square Root Transformation

Square root transformation to stabilize variance (Everything is conditional on X):

$$E[g^{-1}(Y)] = (\beta_0 + \beta_1 x)^2 + \sigma_W^2$$

- The correction to the confidence interval endpoints, then, is (endpoint)^2 + MSE.
- Adding the correction factor, the variance of the errors, is less important when it is small.
- In general, if we don't add the correction factor, simply transforming the endpoints leads to terribly biased intervals that do not contain the population mean the advertised percentage of the time.

Example: Log Transformation

Suppose now that log(Y) is normally distributed. Then Y has the log normal distribution.

The mean of the lognormal distribution is:

$$E[Y] = e^{\mu+\sigma^2/2}$$

So the correction is exp(endpoint + MSE/2).

Example: Inverse Transformation

Suppose we take W = g(Y) = 1/Y, which is normally distributed. Then the inverse transformation is also $g^{-1}(W) = 1/W$. If W is normally distributed, finding the distribution of 1/W becomes more complicated; let's try a Taylor series expansion:

$$g^{-1}(W) \approx \frac{1}{\mu} + (W-\mu)\frac{-1}{\mu^2} + \frac{1}{2}(W-\mu)^2\frac{2}{\mu^3}$$

$$E[g^{-1}(W)] \approx \frac{1}{\mu_W} + 0 + \sigma_W^2\frac{1}{\mu_W^3}$$

$$= \frac{1}{\mu_W}\left(1 + \frac{\sigma_W^2}{\mu_W^2}\right)$$

Back Transformation Adjustments

Transformation	Transformed Model	Back Transformation with Adjustment
Logarithmic	$log(Y) = \beta_0 + \beta_1 X + e$	$\hat{E}[Y] = exp(\hat{\beta}_0 + \hat{\beta}_1 X + \frac{\hat{\sigma}^2}{2})$
Square Root	$\sqrt{Y} = \beta_0 + \beta_1 X + e$	$\hat{E}[Y] = (\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2$
Inverse	$\frac{1}{Y} = \beta_0 + \beta_1 X + e$	$\hat{E}[Y] = \frac{1}{\hat{\beta}_0 + \hat{\beta}_1 X}\left(1 + \frac{\hat{\sigma}^2}{(\hat{\beta}_0 + \hat{\beta}_1 X)^2}\right)$
Inverse Square Root	$\frac{1}{\sqrt{Y}} = \beta_0 + \beta_1 X + e$	$\hat{E}[Y] = \frac{1}{(\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2}\left(1 + \frac{2\hat{\sigma}^4 + 4(\hat{\beta}_0 + \hat{\beta}_1 X)^2\hat{\sigma}^2}{\left[(\hat{\beta}_0 + \hat{\beta}_1 X)^2 + \hat{\sigma}^2\right]^2}\right)$

Back Transformation Adjustments

- What if we want to use some other transformation?

  Bootstrap.

- What about prediction intervals?

  Bootstrap.

R^2 Rant

High R^2 does not imply valid model

- R^2 (the square of the correlation) is often defined as the proportion of the variability in the random variable Y explained by the regression model.

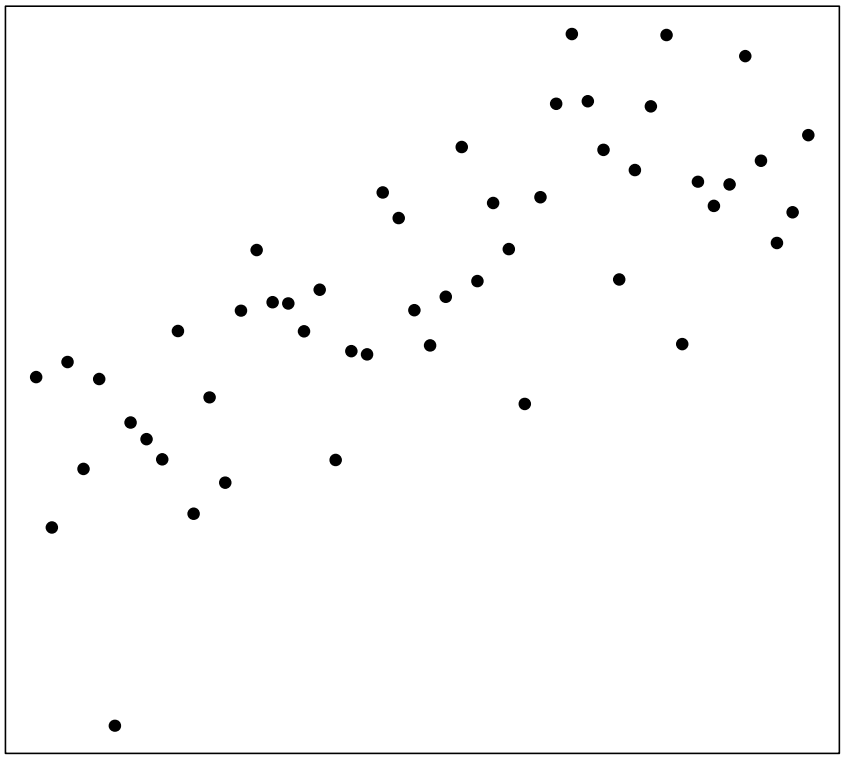
$$SSreg + RSS = SST$$

$$R^2 = \frac{SSreg}{SST} = 1 - \frac{RSS}{SST}$$

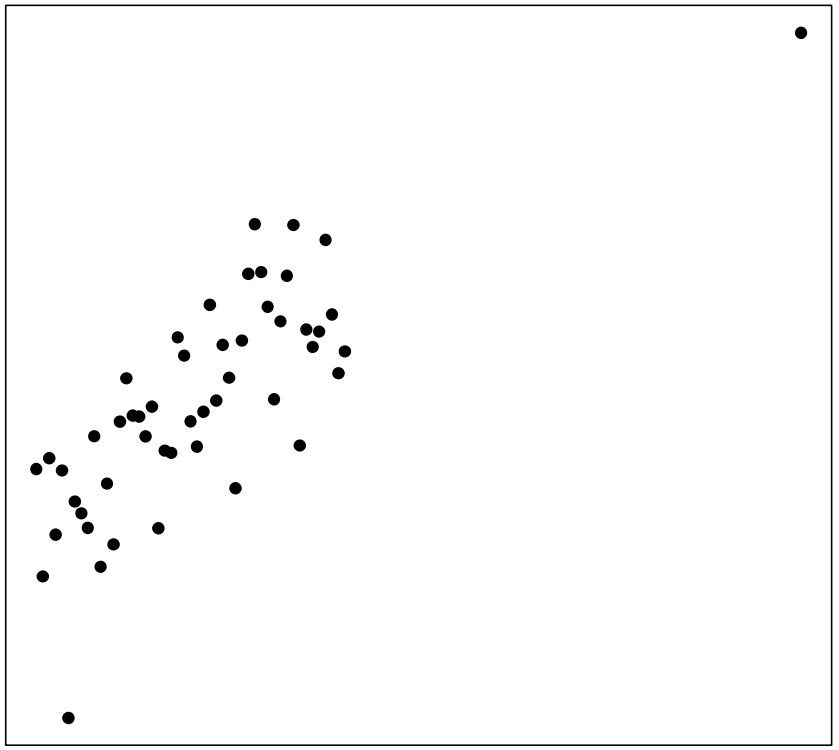
R^2: Outliers

- R^2 is not robust to outliers.

r = 0.75



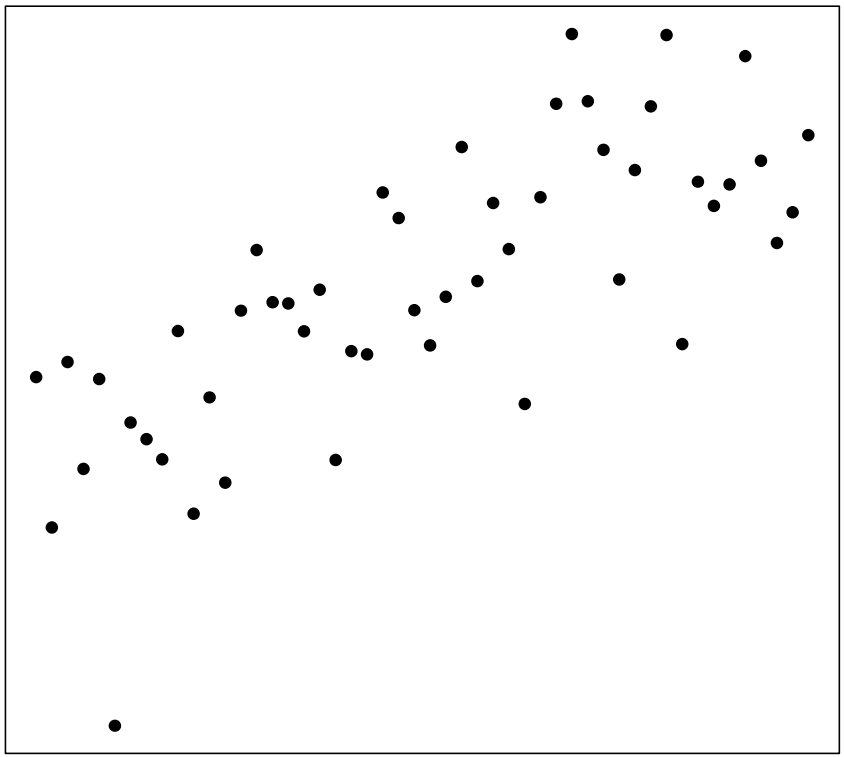
r = 0.80



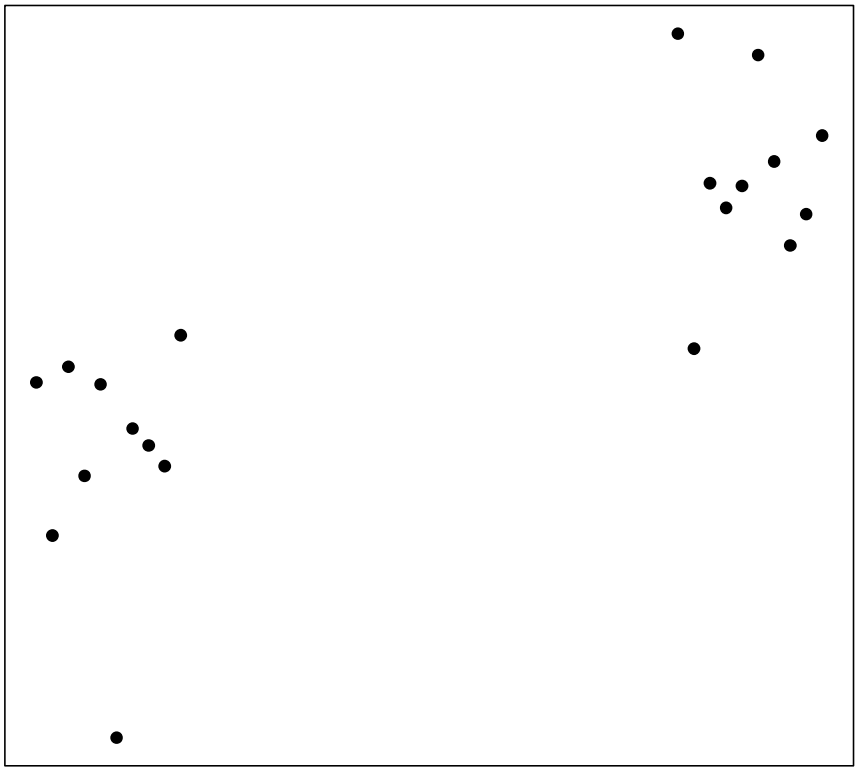
R^2: Stratification

- R^2 takes different values when different values of X are observed.

r = 0.75



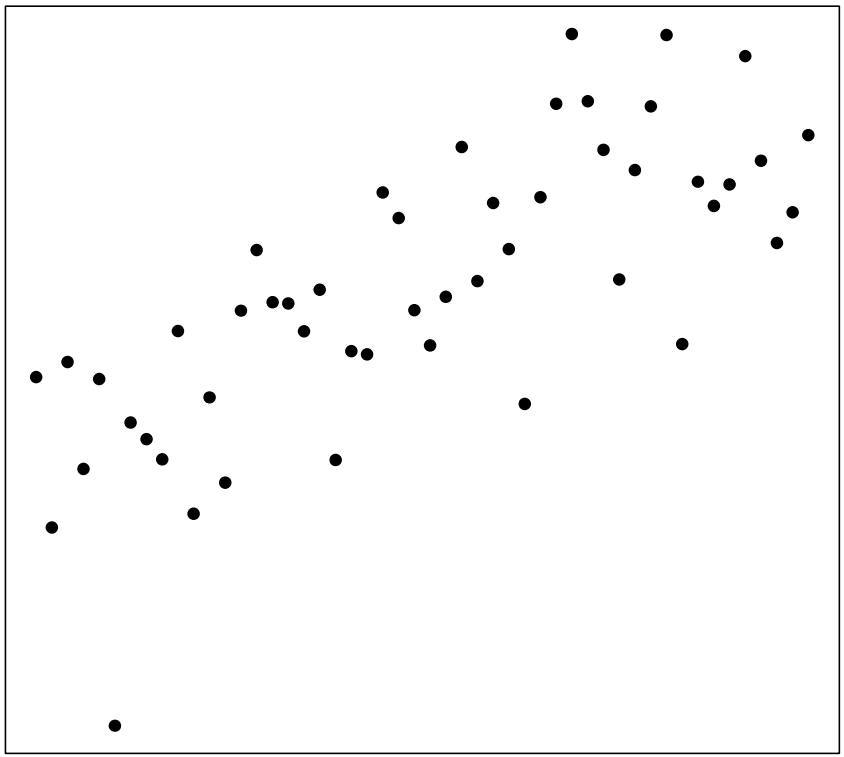
r = 0.81



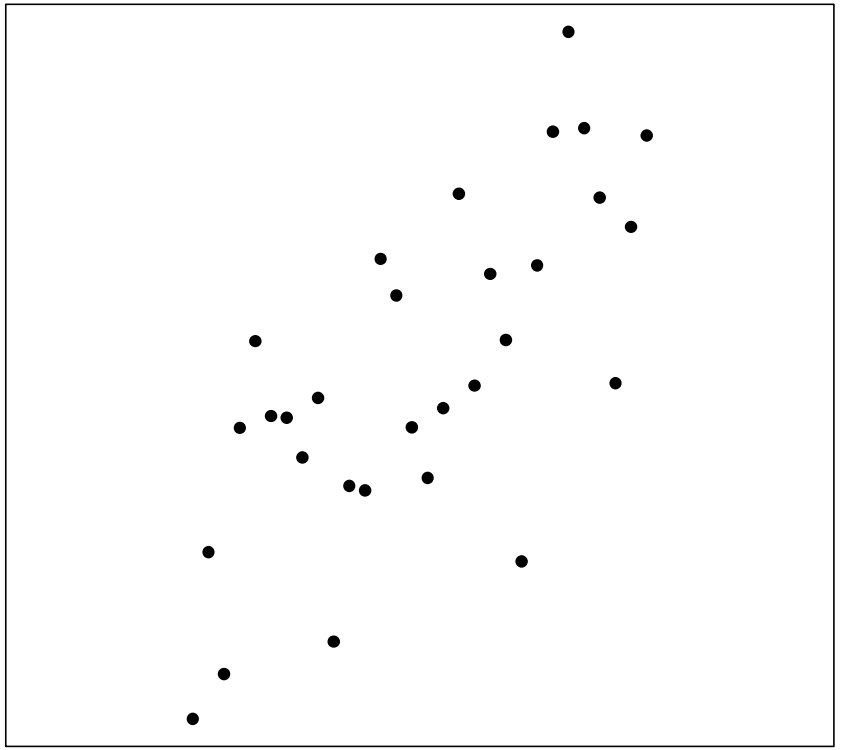
R^2: Stratification

- R^2 takes different values when different values of X are observed.

r = 0.75



r = 0.72



R^2: Regression through the origin

- R^2 is not invariant under location changes like Fahrenheit to Celsius when we fit a line through the origin (no intercept).

$$R^2 = 1 - \frac{SSreg}{\sum y_i^2}$$

Uncorrected SS

R^2: Transformations

- R^2 is not invariant under transformations
- Example 1:

(0, 0.5), (1, 4), (2, 6), (3, 7), (16, 12), (20, 22)

SLR has $R^2 = 0.88$; using log(Y), $R^2 = 0.56$, but the fit is approximately equivalent

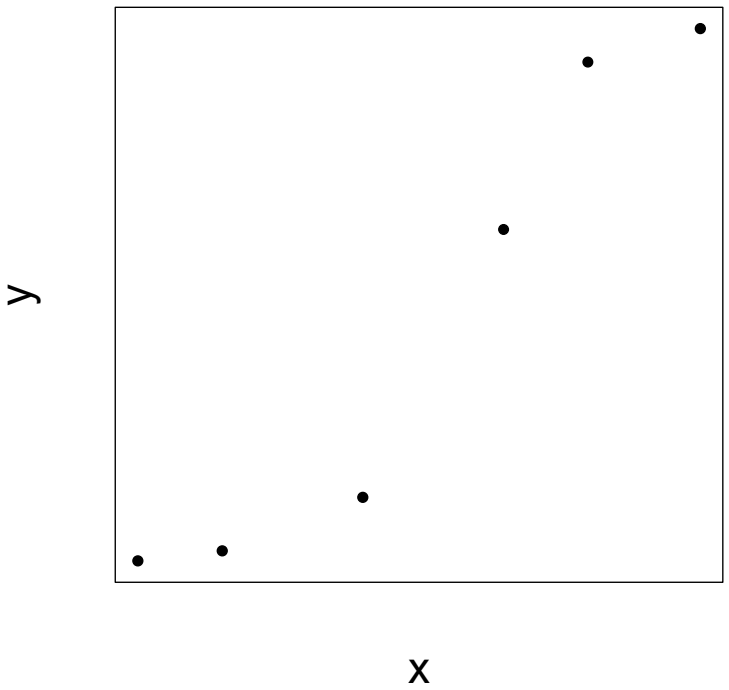
Scott & Wild, 1991. "Transformations and R^2."

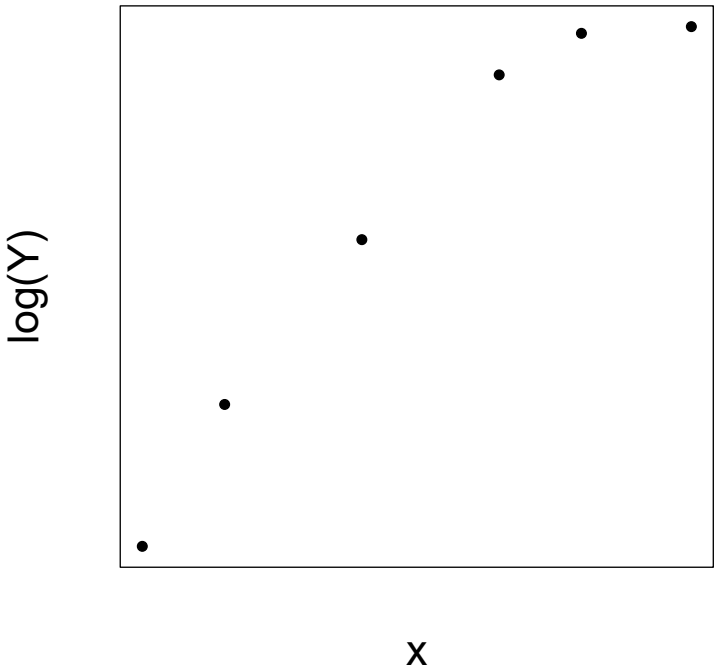
R^2: Transformations

- R^2 is not invariant under transformations
- Example 2:

(0, 0.1), (3, 0.4), (8, 2), (13, 10), (16, 15), (20, 16)

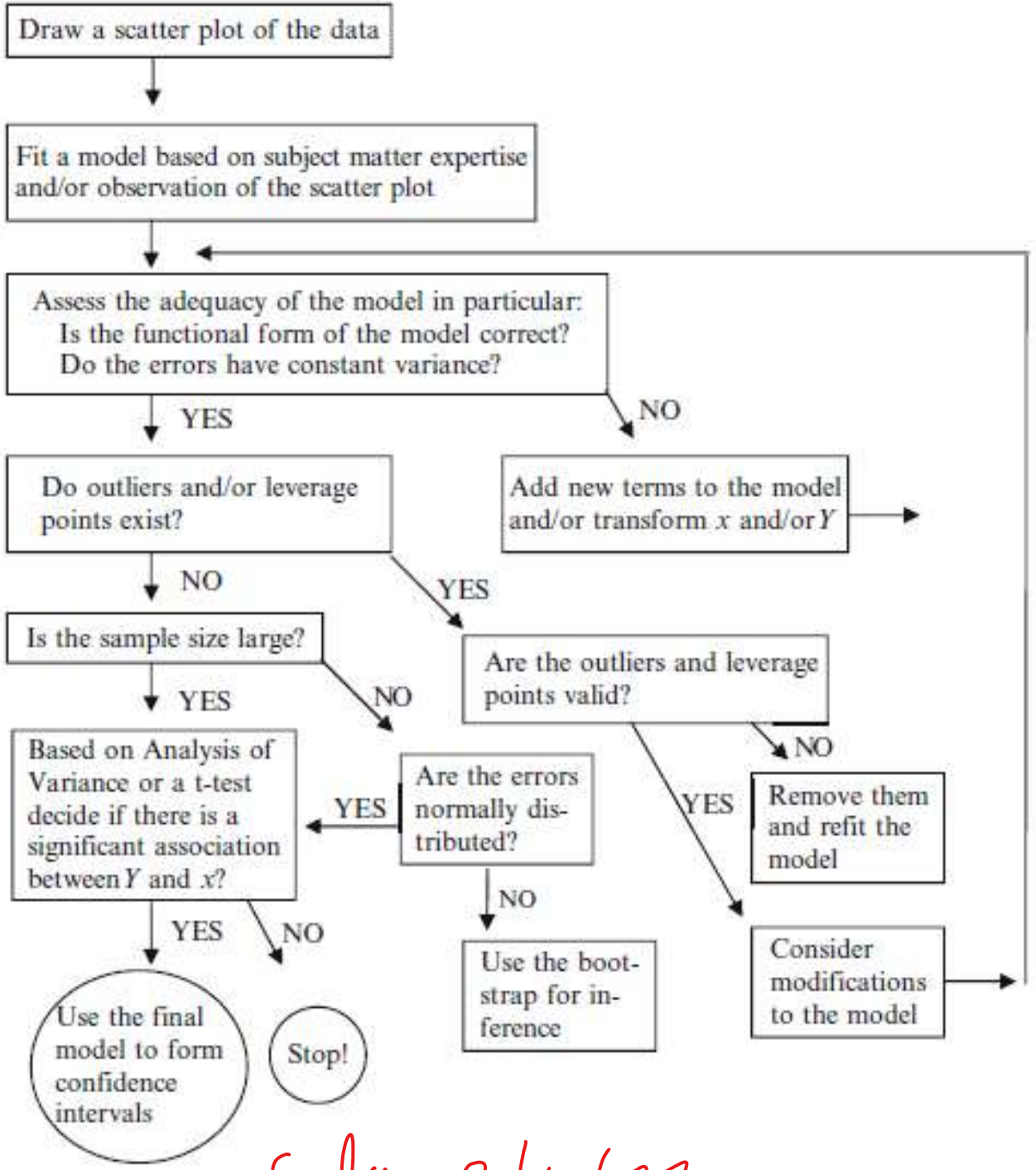
SLR has $R^2 = 0.92$; using log(Y), $R^2 = 0.94$, but the second model is arguably poorer.





If we can't use R^2 to compare models, how about lowest standard error?

- Minimizing the standard error is the same thing as maximizing R^2:



Finished friday 2/11/22