Regression III

Linearity II

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Diagnosing Non-Linearity

Diagnosing non-linearity in relationships between continuous predictors is a bit more tricky.

We will use an analysis of the residuals to diagnose whether the relationship between ${f X}$ and y is well-characterized by a line.

We will also need to figure out a flexible way to model the dependencies between ${f X}$ and the residuals.

• To do this, we will need to learn something about non-parametric regression

Goals for Today

- Develop local polynomial regression as a tool for modeling bivariate relationships. + Use C+R Plots to diagnose unmodeled non-linearity.
- Discuss non-linear transformations for fixing simple, monotone non-linearity.
- Discuss polynomial regression for fixing non-linear relationships that are not simple and monotone.

Parametric vs. Non-parametric

Our goal is to trace the dependence of y on x. Specifically, we usually want to get something like:

$$y_i|x_i=f(x_i)+e_i$$

We usually define $f(\cdot)$ to be "smooth".

ullet The linear functional form - $f(x_i)=lpha+eta x_i$ - is the "smoothest" of smooth function.

The above model is parametric, because we are estimating parameters that describe relationship between y and x.

It is possible to characterize the relationship without estimating global parameters (i.e., parameters that apply to all of the observations equally) - what we call *non-parametric* models.

Global vs. Local Parametric Models

All of the models we will talk about below are *locally* parametric.

- They fit a parametric model to a relatively small subset of the data.
- The sum total of these many local parametric fits is a non-parametric fit one that does not impose the same functional form for all of the data.

Because these models remain locally parametric, we can usually use information from the many local models to derive standard errors for the fit. (More on this later)

Local Polynomial Regression

To estimate the local polynomial regression between y and x, start with the smallest unique value of x, call it x_0 , and you would estimate:

$$y_iw_i=eta_0+eta_1x_iw_i+eta_2x_i^2w_i+arepsilon_iw_i$$

for the span imes 100% of the observations closest to x_0 . Let's say for the sake or argument that the span = 0.5.

- ullet Find the 50% of the points closes to x_0 by calculating $d_i=|x_i-x_0|$ and then taking the 50% smallest values of d_i .
- For the observations in the subsample, calculate the scaled distance such that $\tilde{d}_i = \frac{d_i}{max(d_i)}$. This makes the largest distance in the subsample equal to 1.

Local Polynomial Regression II

• Calculate the weights for the subset using the tricube weight function.

$$w_i = \left(1 - { ilde d}^3
ight)^3$$

 w_i for observations outside the subset will be 0.

Robustness Weighting in LPR

- ullet Fit the local regressions using weights w_i
- ullet Calculate the residuals $\hat{arepsilon}_i = y_i \hat{y}_i$
- ullet Determine the median of the absolute values of the residuals $\hat{q}_{.5}$
- Find the robustness weights (with the Bisquare weight function):

$$r_i = B\left(rac{\hat{arepsilon}_i}{6\hat{q}_{.5}}
ight)$$

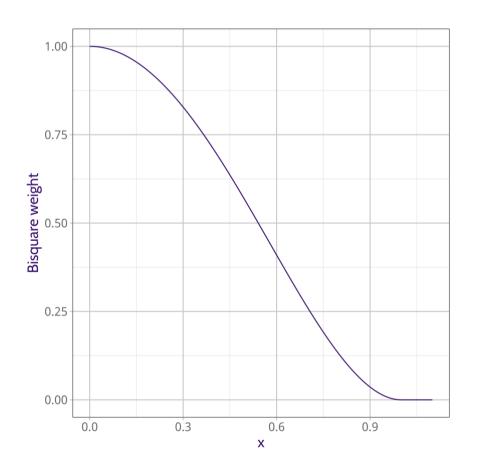
where:

$$B(u) = egin{cases} (1-u^2)^2, & ext{if } |u| < 1; \ 0, & ext{otherwise.} \end{cases}$$

- ullet Repeat the loess procedure using weights $r_i w_i$
- Repeat steps 2-5 until the loess model converges.

Bisquare Weighting Function

What does the bisquare weight function look like?



Choosing the Span

The choice of *span* (i.e., the number of points included in each local model) - this encapsulates the bias-variance tradeoff.

- A bigger span can induce bias which results in a non-parametric estimate that is not faithful to the local patterns in the data
- A smaller span can exhibit considerable variability while sticking very closely to the local pattern in the data. Overfitting is a potential problem here.

Overfitting is not necessarily a problem if we *only* care about the relationship in this sample. However, if we are (either explicitly or implicitly) trying to say something about a population with the sample, then overfitting can be a real problem.

Choosing Polynomial Degree and Weight Function

Polynomial Degree:

- Higher degree polynomials are more likely to overfit the data.
- The most common advice is to set the polynomial degree to 2 and adjust the span to generate the required smoothness of fit.

Weight Function:

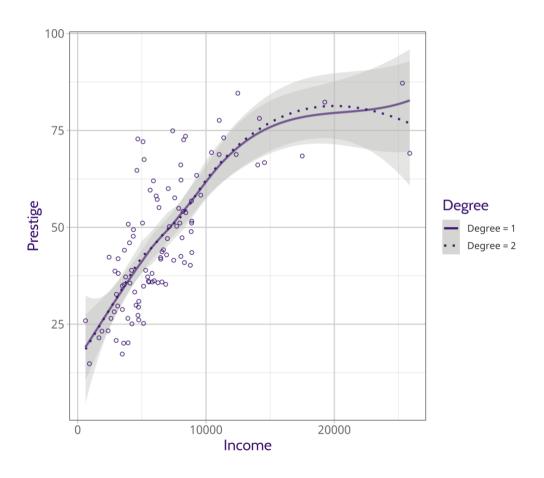
- The default in R is the *tricube* weight function.
- There is little reason to change this as it generally has a relatively small effect on the overall estimate.

LPR in R

There are two different versions of this type of regression: Loess and Lowess.

- In R, The important difference between these two is that Loess can take multiple predictors (i.e., multiple nonparametric regression) whereas Lowess only takes 1. Further, the user has much more control over loess than lowess, so we spend time on the former.
 - Both loess and lowess are in the stats package that comes with every distribution of R.
 - The robustness weighting is done by specifying family = symmetric in the loess command. Otherwise, if family = gaussian, no robustness weighting (only distance weighting) will be done.

Loess Graph

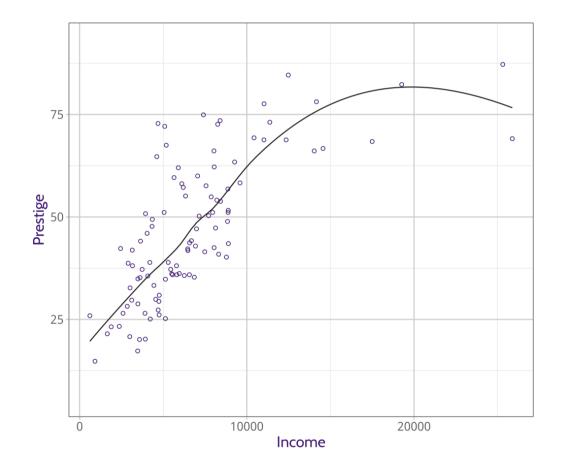


Interpretation of Non-Parametric Fits

Often, we are tempted to impose some meaning on small bumps and dips in the local fit. As Keele (2007) suggests - "it is a temptation analysis should resist."

• It is often useful to consider the overall general pattern in the data and if there appears to be a pattern that can be modeled parametrically - impose that fit and assess the difference between the parametric and non-parametric models (more on this later).

Plotting the LOESS curve



Non-linearity

The assumption that the average error E(arepsilon) is everywhere zero implies that the regression surface accurately reflects the dependency of Y on the X's

- We can see this as linearity in the broad sense
- i.e., non-linearity refers to a partial relationship between two variables that is not summarized by a straight line, but it could also refer to situations when two variables specified to have additive effects actually interact.
 - \circ Violating this assumption implies that the model fails to account for a systematic pattern between Y and the X's
 - Often models characterized by this violation will still provide a useful approximation of the pattern in the data, but they can also be misleading

It is impossible to directly view the regression surface when more than two predictors are specified, but we can employ *partial residual plots* to assess non-linearity.

Partial-Residual Plots (C+R plots)

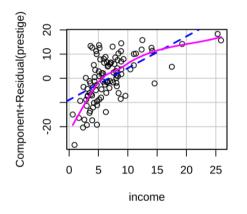
The partial residual for the j^{th} explanatory variable from a multiple regression is

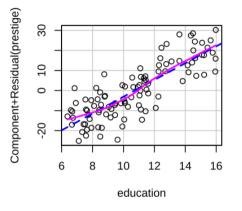
$$E_i^{(j)} = E_i + B_j X_{ij} \, .$$

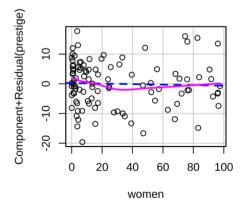
- ullet This simply adds the linear component of the partial regression between Y and X_j (which may be characterized by a non-linear component) to the least squares residuals
- ullet The "partial residuals" $E^{(j)}$ are plotted versus X_j , meaning that B_j is the slope of the multiple simple regression of $E^{(j)}$ on X_j
- ullet A non-parametric smooth helps assess whether the linear trend adequately captures the partial relationship between Y and X.

Example: The Canadian Prestige Data

```
data(Prestige)
Prestige$income <- Prestige$income/1000
Prestige.model<-lm(prestige ~
  income + education +
    women, data=Prestige)
crPlot(Prestige.model, "income")
crPlot(Prestige.model, "education")
crPlot(Prestige.model, "women")</pre>
```







Testing Non-linearity with CR Plots

While this is not a substitute for looking at the graphs, I have written a couple of functions that will allow you to use an F-test to evaluate significant departures from linearity.

```
library(DAMisc)
crTest(Prestige.model, adjust.method="holm")

## RSSp RSSnp DFnum DFdenom F p
## income 6033.57 5107.50 2.356 97.644 7.514 0.001
## education 6033.57 5740.21 1.235 98.765 4.088 0.075
## women 6033.57 5909.90 1.366 98.634 1.511 0.227
```

There is an option to use automatic span selection through wither AICc or GCV - both of which we'll talk about next lecture.

Inference for Nonparametric Models

In the example above, we are testing the local polynomial regression against the straight line in the CR Plot. The main issue is figuring out the degrees of freedom for the LPR.

We know in OLS:

- ullet $\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$ and $df_{\mathrm{model}} = tr(\mathbf{H})$
- ullet $oldsymbol{H}$ is symmetric and idempotent so $tr(oldsymbol{H})=tr(oldsymbol{H}oldsymbol{H}')$
- Residual variance is $\frac{\mathbf{e}'\mathbf{e}}{tr[(\mathbf{I}-\mathbf{H})'(\mathbf{I}-\mathbf{H})]}$ where the denominator is the residual degrees of freedom.

Degrees of Freedom II

In LPR, y = Sy, we have three different degrees of freedom estimates based on the OLS properties from above:

- $tr(\mathbf{S})$ (df model)
- tr(SS') (df model)
- $tr[(\mathbf{I}-\mathbf{S})'(\mathbf{I}-\mathbf{S})]=n-tr(2\mathbf{S}+\mathbf{SS}')$ (df residual), so $tr(2\mathbf{S}-\mathbf{SS}')$ would be the model df.

Each provides a potentially different number with none being particularly preferred over the other.

F-Tests and Nonparametric Models

We can perform an incremental F-tests for a local polynomial model versus a linear model with:

$$F = rac{rac{RSS_{linear} - RSS_{loess}}{tr(S) - 2}}{rac{RSS_{loess}}{n - tr(S)}}$$

• This statistic follows and F distribution with tr(S)-2 numerator and n-tr(S) denominator degrees of freedom.

Example

```
linmod <- lm(prestige ~ income, data=Prestige)
lomod <- loess(prestige ~ income, data=Prestige, span = .5)
testLoess(linmod, lomod)</pre>
## F = 3.6
```

Two Dimensions of Nonlinearity

Simple vs. Complex

- Simple means the curvature of the function relating x to y does not change direction (i.e., there is no inflection point).
- Complex means that there is an inflection point.

Monotone vs Non-monotone

• Monotone means that as x increases the function relating x to y never decreases or x increases the function relating x to y never increases, depending on the nature of the function.

Handling Non-linearity: Common Strategies

Simple, monotone

ullet Transformations of Y and/or X

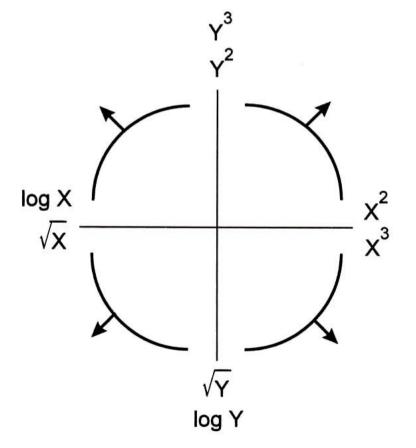
Complicated Non-linearity

- Polynomial Regression
- If pattern has too many turns, polynomials tend to oversmooth peaks
- Regression Splines
- More complicated non-parametric models.

Transformable Non-linearity: Bulging rule

- ullet The direction of the bulge indicates the appropriate type of power transformation for Y and/or X
- ullet A bulge to the top left of the scatterplot suggests transforming Y up the ladder of powers and/or X down the ladder of powers will straighten the relationship

Figure 4.6 from Fox (1997)



Maximum Likelihood Transformation Methods

Although the *ad hoc* methods for assessing non-linearity are usually effective, there are more sophisticated techniques based on maximum likelihood estimation

- These techniques embed the usual multiple-regression model in a more general non-linear model that contains (a) parameter(s) for the transformation(s)
- The transformation parameter λ is estimated simultaneously with the usual regression parameters by maximizing the likelihood and this obtaining MLEs: $\mathcal{L}(\lambda, \alpha, \beta_1, \dots, \beta_k, \sigma_{\varepsilon}^2)$
- If $\lambda=\lambda_0$ (i.e., there is no transformation), a likelihood ratio test, Wald test, or score test of $H_0:\lambda=\lambda_0$ can assess whether the transformation is required
- If several variables need to be transformed, several such parameters need to be included

Box-Tidwell Transformation of the X's (1)

- ullet Maximum likelihood can also be used to find an appropriate linearizing transformation for the X variables
- ullet The Box-Tidwell model is a non-linear model that estimates transformation parameters for the X's simultaneously with the regular parameters

$$Y_i = lpha + eta_1 X_{i1}^{\gamma_1} + \dots + eta_k X_{ik}^{\gamma_k} + arepsilon_i$$

where the errors are iid: $arepsilon \sim \mathcal{N}(0,\sigma_arepsilon^2\mathbf{I}_n)$ and the X_{ij} are positive

- ullet Explicit in this model is a power transformation of each of the X's
- Of course, we would not want to transform dummy variables and the like, so we should not attempt to estimate transformation parameters for them

Box-Tidwell Transformation of the X's (2)

The Box and Tidwell procedure yields a constructed variable diagnostic in the following way:

- Regress Y on the X's and obtain A, B_1, \ldots, B_k .
- Regress Y on the X's and the constructed variables $X_1\log_e X_1,\ldots,X_k\log_e X_k$ to obtain $A',B'_1,\ldots,B'_k,D_1,\ldots,D_k$
- The constructed variables are used to assess the need for a transformation of X_j by testing the null hypothesis $H_0:\delta_j=0$ where $D_j=\hat{\delta}_j$
- A preliminary estimate of the transformation parameter γ_i is given by

$$ilde{\gamma}_j = 1 + rac{D_j}{B_j}$$

where B_j is the coefficient on X_j from the original equation in step 1

Steps 1,2, and 4 are iterated until the transformation parameters converge

Box-Tidwell transformation Example: Prestige Data

- The statistically significant score test indicates that a transformation is needed for income
- The MLE of Power suggests that income should be transformed by a power of -0.037 (suggesting the log might work well)

Testing the Transformations

If you wanted to test whether the transformations were "close enough", you could just rerun the Box-Tidwell function on the new model with the transformed variables.

• If the transformations you provided (e.g., the log instead of -0.03) were good enough, then the transformation powers on the new data should be insignificant.

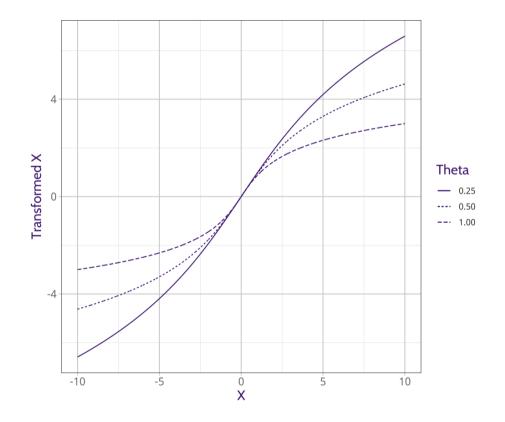
Notice that the p-value is >0.05

iterations = 5

Inverse Hyperbolic Sine Transformation

Sometimes, the log transform is not the most useful because a variable has lots of zeros and you don't want to add a constant to all counts. The IHS transformation is a good alternative.

$$ext{IHS}(x) = rac{\sinh^{-1}(heta x)}{ heta} \ = rac{log\left(heta x + log(heta x^2 + 1)^{\left(rac{1}{2}
ight)}
ight)}{ heta}$$



Using the IHS Transform

```
IHS <- function(x,theta = 1){asinh(theta*x)/theta}</pre>
trans.mod2 <- lm(prestige ~ IHS(income) + education+</pre>
women, data=Prestige)
summary(trans.mod2)
##
## Call:
## lm(formula = prestige ~ IHS(income) + education + women, data = Prestige)
## Residuals:
      Min
               1Q Median
## -17.364 -4.429 -0.101 4.316 19.179
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
                         16.1459 -7.450 3.72e-11 ***
## (Intercept) -120.2805
## IHS(income) 13.4382 1.9138
                                   7.022 2.90e-10 ***
## education 3.7305 0.3544 10.527 < 2e-16 ***
             0.0469
## women
                           0.0299
                                   1.568
                                              0.12
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 7.093 on 98 degrees of freedom
## Multiple R-squared: 0.8351, Adjusted R-squared: 0.83
## F-statistic: 165.4 on 3 and 98 DF, p-value: < 2.2e-16
```

The IHS transform will also work with the effects and ggeffects packages.

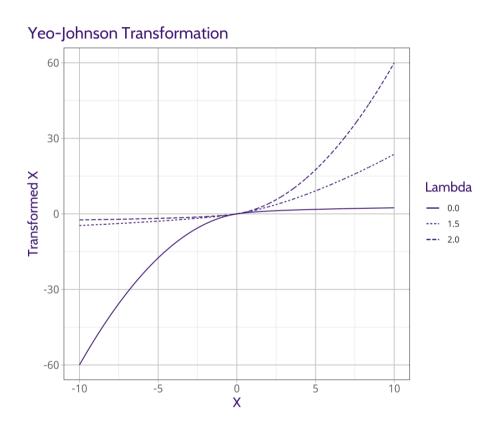
ggeffect plot

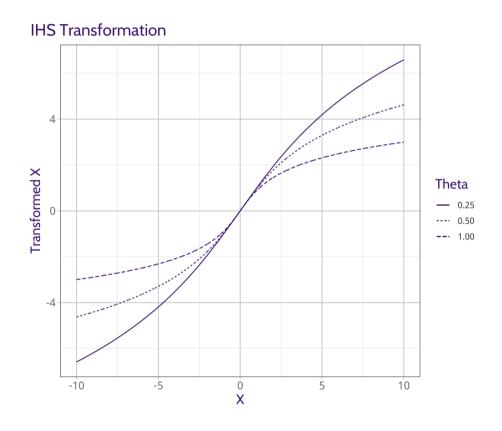
Yeo-Johnson Transformation

The Y-J transform is also an alternative when the variable of interest has negative or zero values. The transformation (with the parameter $\lambda=[0,2]$) is as follows:

$$y_i^{(\lambda)} = egin{cases} ((y_i+1)^{\lambda}-1)/\lambda & ext{if } \lambda
eq 0, y \geq 0 \ \log(y_i+1) & ext{if } \lambda = 0, y \geq 0 \ -[(-y_i+1)^{(2-\lambda)}-1]/(2-\lambda) & ext{if } \lambda
eq 2, y < 0 \ -\log(-y_i+1) & ext{if } \lambda = 2, y < 0 \end{cases}$$

Y-J vs IHS





Finding Optimal Values of λ

```
summary(vi trans(prestige ~ income + education +
women + type, data=Prestige,
trans.vars=c("income"), round.digits=3))
##
## Call:
## lm(formula = form, data = data)
## Residuals:
       Min
                10 Median
## -13.8760 -4.0575 0.5504 4.2132 16.6404
## Coefficients:
                          Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                        -115.69605 18.80605 -6.152 1.96e-08 ***
## yeo.johnson(income, 0) 14.65764 2.31198 6.340 8.43e-09 ***
## education
                           2.97382 0.60206 4.939 3.49e-06 ***
                           0.08381
## women
                                     0.03223
                                               2.601 0.0108 *
## typeprof
                                     3.55588
                                               1.488
                       5.29196
                                                      0.1401
## typewc
                        -3.21579
                                    2.40657 -1.336 0.1848
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '* 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.44 on 92 degrees of freedom
    (4 observations deleted due to missingness)
## Multiple R-squared: 0.8654, Adjusted R-squared: 0.8581
## F-statistic: 118.3 on 5 and 92 DF, p-value: < 2.2e-16
```

Box-Cox Transformation of Y

- ullet The Box-Cox transformation of Y functions to normalize the error distribution, stabilize the error variance and straighten the relationship of Y to the X's
- The general Box-Cox model is:

$$Y_i^{\lambda} = \alpha + \beta_1 X_{i1} + \dots + \beta_k X_{ik} + \varepsilon_i$$

where $arepsilon_i \sim \mathcal{N}(0, \sigma_arepsilon^2)$ and

$$Y_i^\lambda = egin{cases} rac{Y_i^{\lambda}-1}{\lambda}, & ext{for } \lambda
eq 0 \ \log_e Y_i, & ext{for } \lambda = 0 \end{cases}$$

- If λ =1, no transformation is necessary
- Note that all of the Y_i must be positive

Box-Cox Transformation Example: Ornstein Data (1)

```
library(car)
data(Ornstein)
optpwr <- powerTransform(I(interlocks + 1) ~ log(assets) +</pre>
                            sector + nation, data=Ornstein)
summary(optpwr)
## bcPower Transformation to Normality
      Est Power Rounded Pwr Wald Lwr Bnd Wald Upr Bnd
## Y1
        0.2227
                       0.22
                                   0.126
                                                0.3193
## Likelihood ratio test that transformation parameter is equal to 0
   (log transformation)
##
                              LRT df
                                            pval
## LR test, lambda = (0) 19.75696  1 8.7941e-06
```

Likelihood ratio test that no transformation is needed

LR test, lambda = (1) 243.4049 1 < 2.22e-16

IRT df

pval

Model

You can then run the model with the optimized λ parameter from the previous slide:

```
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -2.17047
                           0.58490 -3.711 0.000258 ***
## log(assets) 0.73699
                           0.08089
                                     9.112 < 2e-16 ***
                           0.61547
## sectorBNK
               -0.26138
                                    -0.425 0.671461
              -0.59772
## sectorCON
                           0.64389
                                    -0.928 0.354213
               0.05439
                           0.40505
                                     0.134 0.893293
  sectorFIN
## sectorHLD
              -0.45594
                           0.54763
                                   -0.833 0.405935
               -0.02196
                           0.28093
                                    -0.078 0.937775
## sectorMAN
                           0.36024
                                     0.353 0.724542
## sectorMER
                0.12710
                0.38246
                           0.29021
## sectorMIN
                                     1.318 0.188843
## sectorTRN
                0.43596
                           0.39201
                                    1.112 0.267232
## sectorWOD
               0.63923
                           0.36788
                                    1.738 0.083600 .
## nationOTH
              -0.31476
                           0.36648
                                    -0.859 0.391292
              -0.51269
## nationUK
                           0.36460
                                    -1.406 0.161007
## nationUS
               -1.17941
                           0.20387
                                    -5.785 2.31e-08 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '* 0.05 '.' 0.1 ' ' 1
## Residual standard deviation: 1.337 on 234 degrees of freedom
## Multiple R-squared: 0.5051
## F-statistic: 18.37 on 13 and 234 DF, p-value: < 2.2e-16
     ATC.
## 863.49 916.20
```

Other Transformations

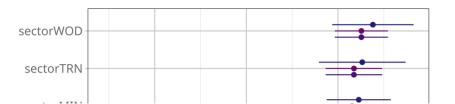
We talked about the IHS and Y-J transforms above, both of which permit negative values. Hawkins and Weisberg (2017) developed a new version of the Box-Cox transform that allows negative values. This distribution has two parameters λ and γ .

$$BCN(x_i) = egin{cases} \log(.5(x_i + s_i)) & ext{if } \lambda pprox 0 \ rac{(0.5(x_i + s_i))^\lambda}{\lambda} & ext{if } |\lambda| > 0 \end{cases}$$

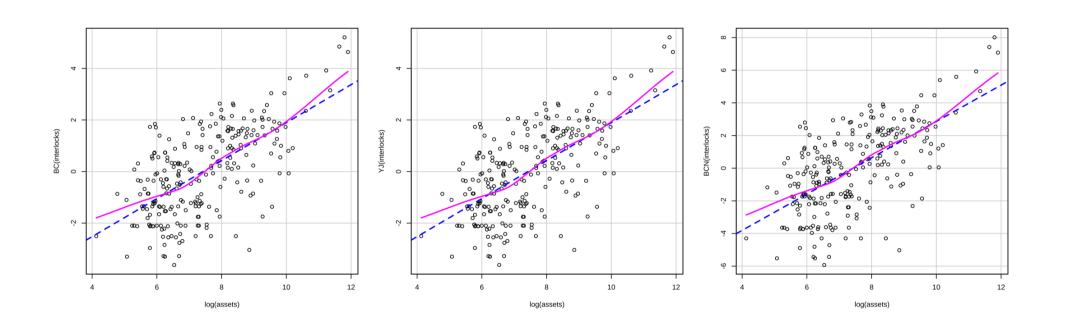
where
$$s_i = \sqrt{x_i^2 + \gamma^2}$$

Example of Other Power Transforms

Figure



CR Plots



Polynomial Regression

Two or more regressors of ascending power (i.e., linear, quadratic and cubic terms) are used to capture the effects of a single variable

- For every bend in the curve, we add another term to the model, going up in power each time
- Polynomial models are linear in the parameters even though they are non-linear in the variables

| Order | Equation |
|--------|--|
| First | $Y = \alpha + \beta_1 X$ |
| Second | $Y = \alpha + \beta_1 X + \beta_2 X^2$ |
| Third | $Y = \alpha + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$ |

Polynomial equations: How to choose the order

It is initially useful to look at the bends in a smooth of the scatterplot or partial residual plot

- If there is only one, a second order polynomial should be tried. For each extra bulge, we go up one in order
- A good strategy is to start with one more than you think the model needs and drop the term if it is not statistically significant
- ullet Incremental F-tests can be used to help pick the "right" order to use in the equation
 - If the term is not statistically significant, it is usually advisable to delete the term from the model - we want as few order terms as possible
- For orthogonal polynomials, t-tests can be used

If the order is too high, however, the results will not be easy to interpret (higher than third order is rarely used)

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Orthogonal Polynomials: Prestige

One can fit a polynomial regression by calculating the regressors individually and adding them to the regression equation - i.e., calculate and add a quadratic term X^2 and a cubic term X^3 manually.

- Orthogonal Polynomials can be added in a much more simple and better way in R, however, by specifying a poly function of the variable.
- Non-orthogonal polynomials can be specified with the raw=T argument to poly.
- The order of the polynomial is specified after the variable name: eg poly(income, 3)

Note, in R, the poly() function doesn't allow missing values.

Orthogonalizing Regressors

It is possible to orghotonalize the power regressors before fitting the model, below is an example for a 3^{rd} degree polynomial.

- Create $(p_1, p_2, p_3) = (X, X^2, X^3)$
- Use p_1 as the value for the first-degree term.
- ullet Regress the p_2 and p_3 on p_1 and create residuals $e_2^{(1)}$ and $e_3^{(1)}$, respectively. Use $e_2^{(1)}$ as the value for the second-degree term
- Regress $e_3^{(1)}$ on p_1 and $e_2^{(1)}$ and use the residuals from that equation (call them $e_3^{(2)}$) as the third degree term.

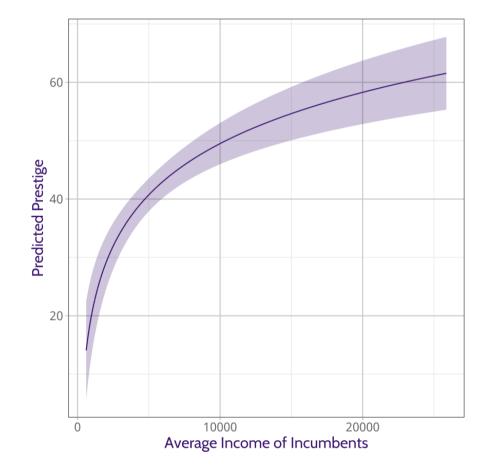
This is not exactly what poly in R does, but the idea is similar. poly() also does some other normalization, so results using the above method, while equivalent in model fit terms will generate different coefficient estimates.

Regression Output

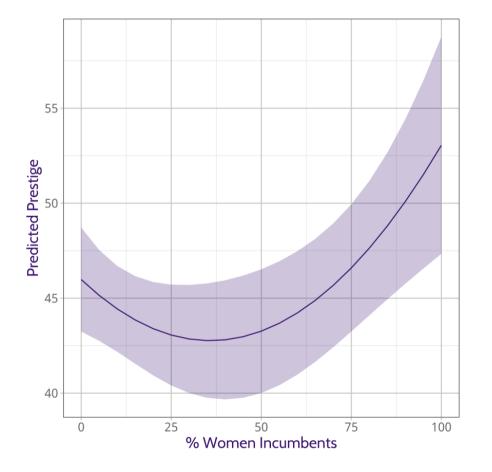
```
## Coefficients:
                      Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                       -62.910
                                    15.916 -3.953 0.000149 ***
## log(income)
                        12.672
                                    1.836
                                            6.901 5.74e-10 ***
## poly(education, 3)1 106.494
                                    9.284 11.471 < 2e-16 ***
## poly(education, 3)2
                        15.045
                                    6.977
                                            2.156 0.033577 *
## poly(education, 3)3
                       -13.348
                                    6.984 -1.911 0.058972 .
## poly(women, 2)1
                                           1.276 0.204893
                        11.978
                                     9.384
## poly(women, 2)2
                                    6.828
                                            2.704 0.008110 **
                        18,465
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Residual standard deviation: 6.721 on 95 degrees of freedom
## Multiple R-squared: 0.8564
## F-statistic: 94.46 on 6 and 95 DF, p-value: < 2.2e-16
     ATC.
## 686.89 707.89
```

- After evaluating the 3rd degree polynomial in education, it appears only two of those terms are needed.
 The third degree term is significant at the 0.1 level, so you might leave it in, but it would be a judgment call.
- Since the 2^{nd} degree term for women is significant we would have to leave in the first degree term as well. The inclusion of the first degree term allows the function to be non-monotonic.

Effect Display for Income



Effect Display for Women



Effect Display for Education

