Precept 8: Regression Diagnostics & Solutions

Soc 400: Applied Social Statistics

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[1]Based on slides from Shay O'Brien, Alex Kindel, Simone Zhang, and Matt Blackwell.

Today's Agenda

- What can go wrong & how to fix it
  - Reviewing marginal effects
  - Non-normality
  - Extreme Values
  - Non-linearity
- RStudio
  - Practicing `dplyr` for data cleaning and manipulation
  - Diagnostics & Solutions

Marginal "effects"

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What is the variance of the marginal effect?

$$Var\left(\frac{\partial Y}{\partial X}\right) = Var(\hat{\beta}_1 + Z\hat{\beta}_3)$$

$$= Var(\hat{\beta}_1) + Z^2 Var(\hat{\beta}_3) + 2ZCov(\hat{\beta}_1, \hat{\beta}_3)$$

If this model is fit using the `lm()` function, we can use `vcov(fit)` to extract the variance covariance matrix that has these variance and covariance elements.

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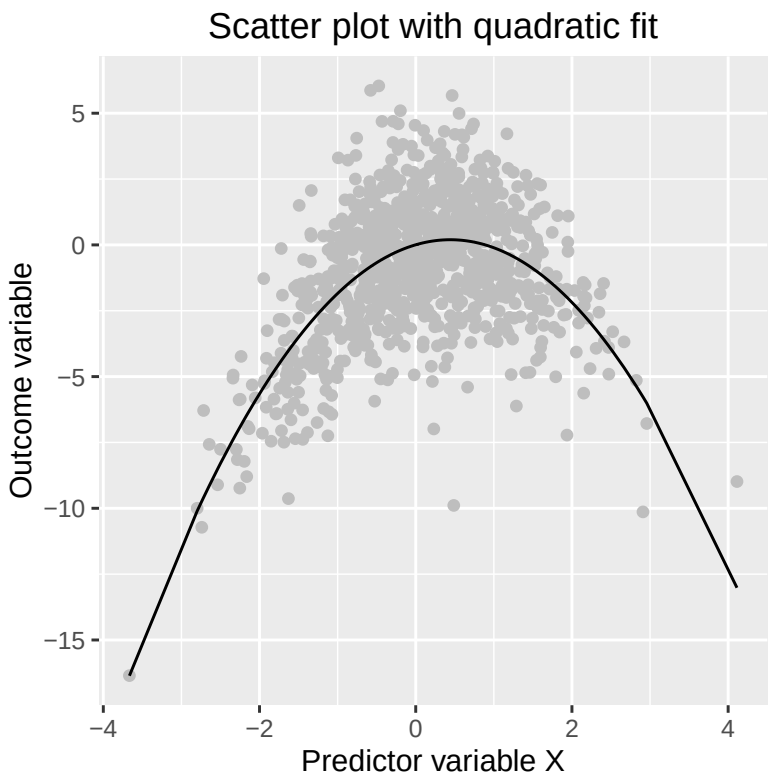
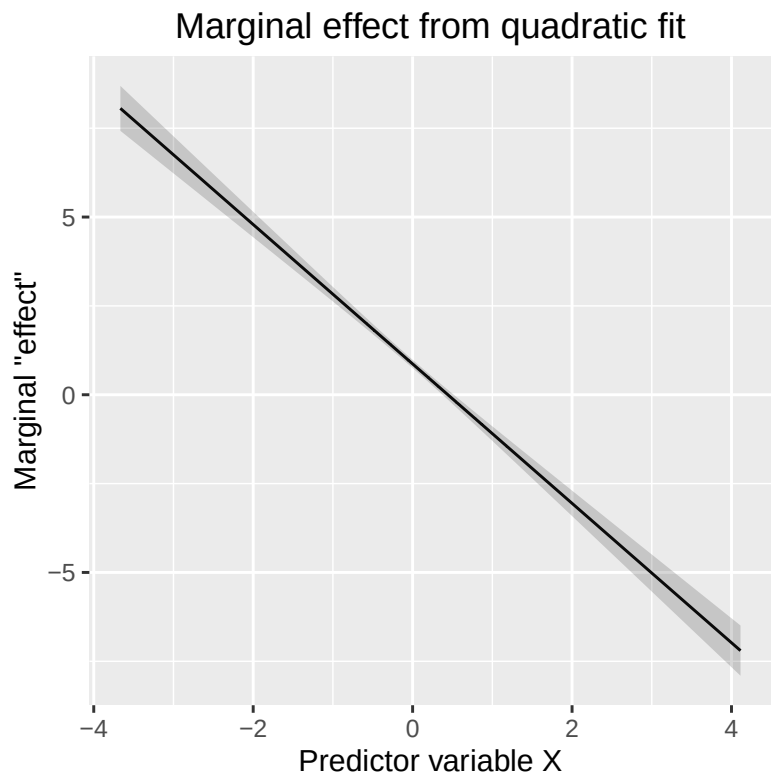
$$\frac{\partial Y}{\partial X} = \beta_1 + 2X\beta_2$$

$$\begin{aligned} Var\left(\frac{\partial Y}{\partial X}\right) &= Var(\hat{\beta}_1 + 2X\hat{\beta}_2) \\ &= Var(\hat{\beta}_1) + (2X)^2 Var(\hat{\beta}_2) + 2 * 2X * Cov(\hat{\beta}_1, \hat{\beta}_2) \end{aligned}$$

Plotting marginal effects

Given estimated coefficients, we could plot the marginal effect of X on Y as a function of X





Learning about distribution of errors through residuals

- Assumption is about **unobserved** $\mathbf{u} = \mathbf{y} - \mathbf{X}\boldsymbol{\beta}$
- We can only **observe** residuals, $\widehat{\mathbf{u}} = \mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}$
- If **distribution of residuals** $\approx$ **distribution of errors**, we could check residuals
- But this is actually **not true**—the distribution of the residuals is complicated

To understand the relationship between residuals and errors, we need to derive the distribution of the residuals.

Hat matrix

- Define matrix $\mathbf{H} = \mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'$

$$\begin{aligned}\widehat{\mathbf{u}} &= \mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}} \\ &= \mathbf{y} - \mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y} \\ &\equiv \mathbf{y} - \mathbf{H}\mathbf{y} \\ &= (\mathbf{I} - \mathbf{H})\mathbf{y}\end{aligned}$$

- $\mathbf{H}$ is the **hat matrix** because it puts the "hat" on $\mathbf{y}$:

$$\widehat{\mathbf{y}} = \mathbf{H}\mathbf{y}$$

  - $\mathbf{H}$ is an $n \times n$ symmetric matrix

Relating the residuals to the errors

$$
\begin{aligned}
\widehat{\mathbf{u}} &= (\mathbf{I} - \mathbf{H})(y) \\
&= (\mathbf{I} - \mathbf{H})(\mathbf{X}\boldsymbol{\beta} + \mathbf{u}) \\
&= (\mathbf{I} - \mathbf{H})\mathbf{X}\boldsymbol{\beta} + (\mathbf{I} - \mathbf{H})\mathbf{u} \\
&= \mathbf{I}\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{I} - \mathbf{H})\mathbf{u} \\
&= \mathbf{X}\boldsymbol{\beta} - \mathbf{X}\boldsymbol{\beta} + (\mathbf{I} - \mathbf{H})\mathbf{u} \\
&= (\mathbf{I} - \mathbf{H})\mathbf{u}
\end{aligned}
$$

- Residuals $\widehat{\mathbf{u}}$ are a linear function of the errors, $\mathbf{u}$
- For instance,

$$\widehat{u_1} = (1 - h_{11})u_1 - \sum_{i=2}^{n} h_{1i}u_i$$

- Note that the residual is a function of all of the errors

Distribution of the residuals

$$\mathbb{E}[\widehat{\mathbf{u}}] = (\mathbf{I} - \mathbf{H})\mathbb{E}[\mathbf{u}] = \mathbf{0}$$

$$\text{Var}[\hat{\mathbf{u}}] = \sigma_u^2(\mathbf{I} - \mathbf{H})$$

The variance of the ith residual $\hat{u}_i$ is $V[\hat{u}_i] = \sigma_u^2(1 - h_{ii})$, where h_{ii} is the ith diagonal element of the matrix $\mathbf{H}$ (called the **hat value**).

Distribution of the Residuals

Notice in contrast to the unobserved errors, the estimated residuals

1. are not independent (because they must satisfy the two constraints $\sum_{i=1}^{n} \widehat{u}_i = 0$ and $\sum_{i=1}^{n} \widehat{u}_i x_i = 0$)
2. do not have the same variance. The variance of the residuals varies across data points $V[\hat{u}_i] = \sigma^2(1 - h_{ii})$, even though the unobserved errors all have the same variance σ^2

These properties can obscure the true patterns in the error distribution, and thus are inconvenient for our diagnostics.

Standardized Residuals

Let's address the second problem (unequal variances) by standardizing $\hat{u}_i$, i.e., dividing by their estimated standard deviations.

This produces **standardized** (or "internally studentized") **residuals**:

$$\hat{u}'_i = \frac{\hat{u}_i}{\hat{\sigma}\sqrt{1 - h_{ii}}}$$

where $\hat{\sigma}^2$ is our usual estimate of the error variance.
The standardized residuals are still not ideal, since the numerator and denominator of $\hat{u}'_i$ are not independent. This makes the distribution of $\hat{u}'_i$ nonstandard.

Studentized residuals

If we remove observation i from the estimation of σ, then we can eliminate the dependence and the result will have a standard distribution.

- estimate residual variance without residual i:

$$\widehat{\sigma}^2_{-i} = \frac{\hat{u}'\hat{u} - \hat{u}_i^2/(1-h_{ii})}{n-k-2}$$

- Use this i-free estimate to standardize, which creates the **studentized residuals**:

$$\widehat{u}^*_i = \frac{\widehat{u}_i}{\widehat{\sigma}_{-i}\sqrt{1-h_{ii}}}$$

- If the errors are Normal, the studentized residuals follow a t distribution with $(n-k-2)$ degrees of freedom. (Q-Q plot)
- Deviations from $t \implies$ violation of Normality

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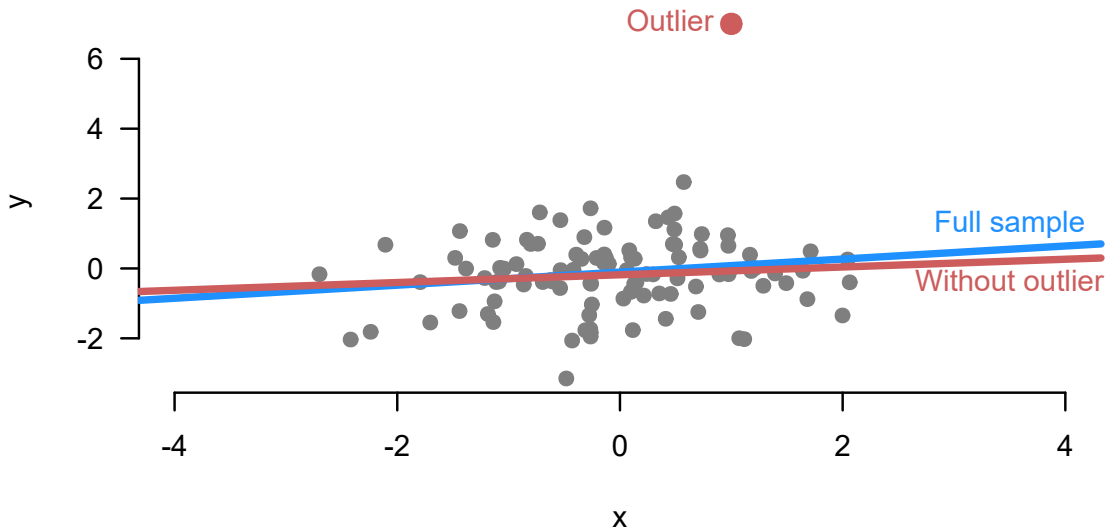
- Use estimators other than OLS that are robust to nonnormality (later this class)
- Consider other causes (next two classes)

Three types of extreme values

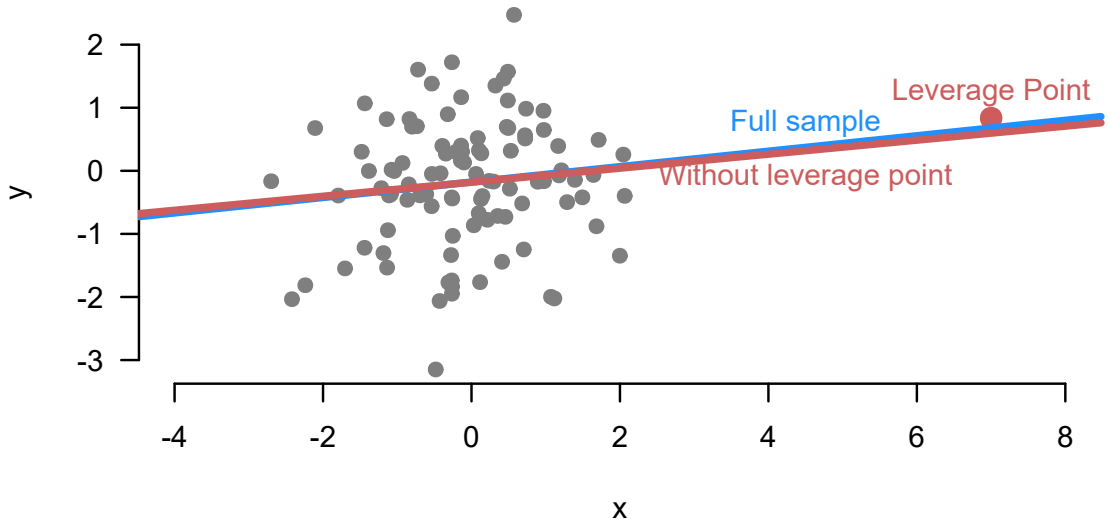
1. Outlier: extreme in the y direction
2. Leverage point: extreme in one x direction
3. Influence point: extreme in both directions

Outlier definition



-
- Very **distant** from the rest of the data **in the y-dimension**
- Increases estimated standard errors (by increasing $\widehat{\sigma}^2$)
- No bias if typical in the x's

Leverage point definition



- Values that are extreme in the x direction
- That is, values far from the center of the covariate distribution
- Decrease estimated SEs (more X variation)
- No bias if typical in y dimension

Leverage Points: Hat values

To measure leverage in multivariate data we will go back to the hat matrix **H**:

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

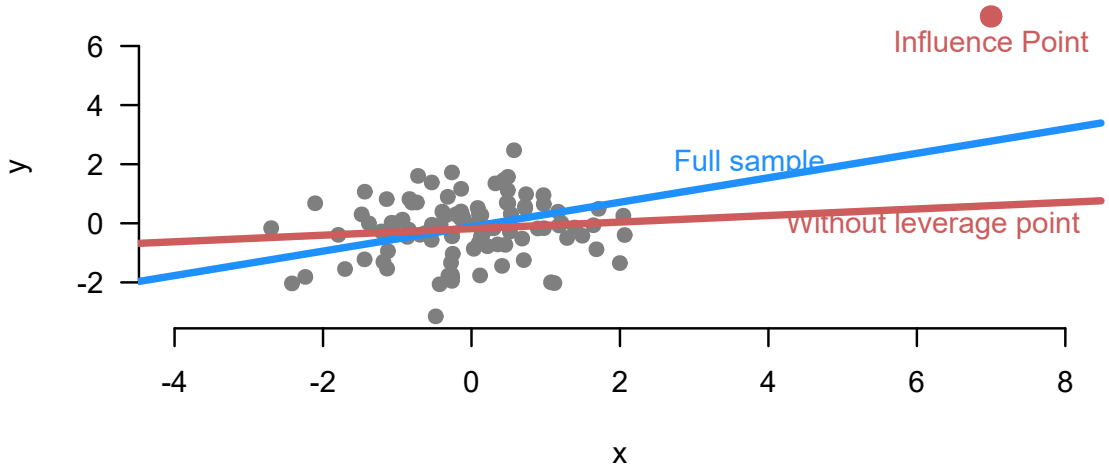
H is $n \times n$, symmetric, and idempotent. It generates fitted values as follows:

$$\hat{y}_i = \mathbf{h}_i'\mathbf{y} = \begin{bmatrix} h_{i,1} & h_{i,2} & \cdots & h_{i,n} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{j=1}^{n} h_{i,j} y_j$$

Therefore,

- h_{ij} dictates how important y_j is for the fitted value $\hat{y}_i$ (regardless of the actual value of y_j, since **H** depends only on **X**)
- The diagonal entries $h_{ii} = \sum_{j=1}^{n} h_{ij}^2$, so they summarize how important y_i is for all the fitted values. We call them the **hat values** or **leverages** and a single subscript notation is used: $h_i = h_{ii}$
- Intuitively, the hat values measure how far a unit's vector of characteristics $\mathbf{x}_i$ is from the vector of means of **X**
- **Rule of thumb**: examine hat values greater than $2(k+1)/n$

Influence points



- An **influence point** is one that is both an **outlier** (extreme in X) and a **leverage point** (extreme in Y).
- Causes the regression line to move toward it (bias?)

Detecting Influence Points/Bad Leverage Points

- **Influence Points**:
  Influence on coefficients = Leverage × Outlyingness

- More formally: Measure the change that occurs in the slope estimates when an observation is removed from the data set. Let

$$D_{ij} = \hat{\beta}_j - \hat{\beta}_{j(-i)}, \quad i = 1, \ldots, n, \quad j = 0, \ldots, k$$

  where $\hat{\beta}_{j(-i)}$ is the estimate of the jth coefficient from the same regression once observation i has been removed from the data set.

- D_{ij} is called the **DFbeta**, which measures the **influence** of observation i on the estimated coefficient for the jth explanatory variable.

Standardized Influence

To make comparisons across coefficients, it is helpful to scale D_{ij} by the estimated standard error of the coefficients:

$$D_{ij}^{*} = \frac{\hat{\beta}_j - \hat{\beta}_{j(-i)}}{\hat{SE}_{-i}(\hat{\beta}_j)}$$

where D_{ij}^{*} is called **DFbetaS**.

- $D_{ij}^{*} > 0$ implies that removing observation i decreases the estimate of $\beta_j \rightarrow$ obs i has a positive influence on β_j.
- $D_{ij}^{*} < 0$ implies that removing observation i increases the estimate of $\beta_j \rightarrow$ obs i has a negative influence on β_j.
- Values of $|D_{ij}^{*}| > 2/\sqrt{n}$ are an indication of high influence.
- In R: `dfbetas(model)`

Summarizing Influence across All Coefficients

- Leverage tells us how much one data point affects a **single coefficient**.
- A number of summary measures exist for influence of data points across all coefficients, all involving both leverage and outlyingness.
- A popular measure is **Cook's distance**:

$$D_i = \frac{\hat{u}_i'^2}{k+1} \times \frac{h_i}{1-h_i}$$

  where $\hat{u}_i'$ is the standardized residual and h_i is the hat value.
  - It can be shown that D_i is a weighted sum of $k+1$ DFbetaS's for observation i
  - In R, `cooks.distance(model)`
  - $D > 4/(n-k-1)$ is commonly considered large

- The **influence plot**: the studentized residuals plotted against the hat values, size of points proportional to Cook's distance.

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  - Use a method that is robust to outliers (robust regression)

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- We can apply this to regression fairly straightforwardly. In robust *M*-estimators we choose $\rho()$ so that observations with large residuals get less weight.
- One option of robust M-estimators (that Brandon recommends) is MM-estimator because it has:
  - very high breakdown point (the fraction of arbitrarily bad data that the estimator can tolerate without being affected to an arbitrarily large extent)
  - and good efficiency (low variance).

OLS Assumption I: Liearnity in Parameters

- Linearity in Parameters: the population regression model is linear in its parameters and correctly specified as:

$$Y = \beta_0 + \beta_1 X_1 + u$$

- Note that it can be nonlinear *in variables*
- β_0, β_1: Population **parameters** — fixed and unknown
- u: Unobserved random variable with $E[u] = 0$ — captures all other factors influencing Y other than X
- We assume this to be the structural model, i.e., the model describing the true process generating Y

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- If **homoskedasticity** is violated, the spread of the residuals *around that mean* will vary with the predicted values.
- These are **distinct** assumptions; though one plot tells you about both, they are not mechanically linked.

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- In general the idea is to do a linear regression of y on $\phi_1(x), \phi_2(x), \ldots, \phi_{m-1}(x)$ where ϕ_j are **basis functions**.

Model non-linearities with basis function

- We talked before about polynomials x^2, x^3, x^4 for modeling non-linearities, this is a **linear basis function model**.
- In general the idea is to do a linear regression of y on $\phi_1(x), \phi_2(x), \ldots, \phi_{m-1}(x)$ where ϕ_j are **basis functions**.
- The model is now:

$$y = f(x, \beta) + \epsilon$$

$$f(x, \beta) = \beta_0 + \sum_{j=1}^{m-1} \beta_j \phi_j(x) = \beta^T \phi(x)$$

Polynomial Basis Functions

We can look at OLS fits with polynomial basis functions of increasing order.

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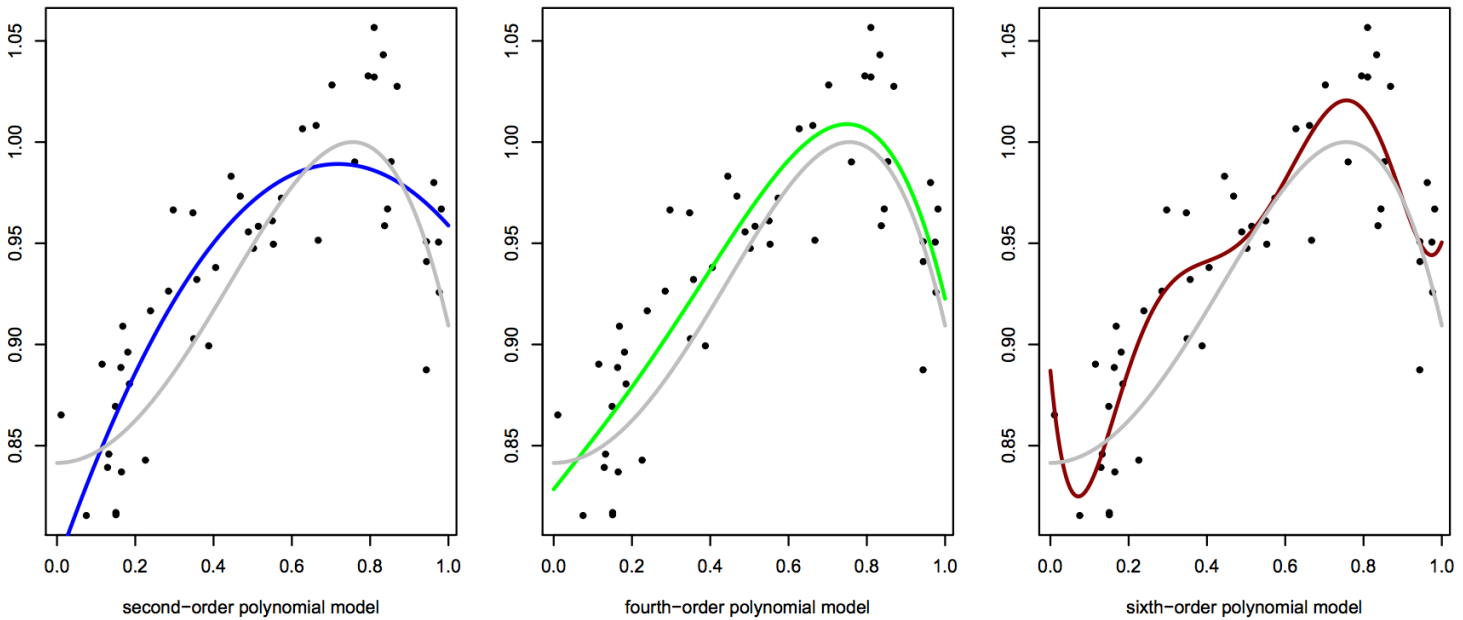

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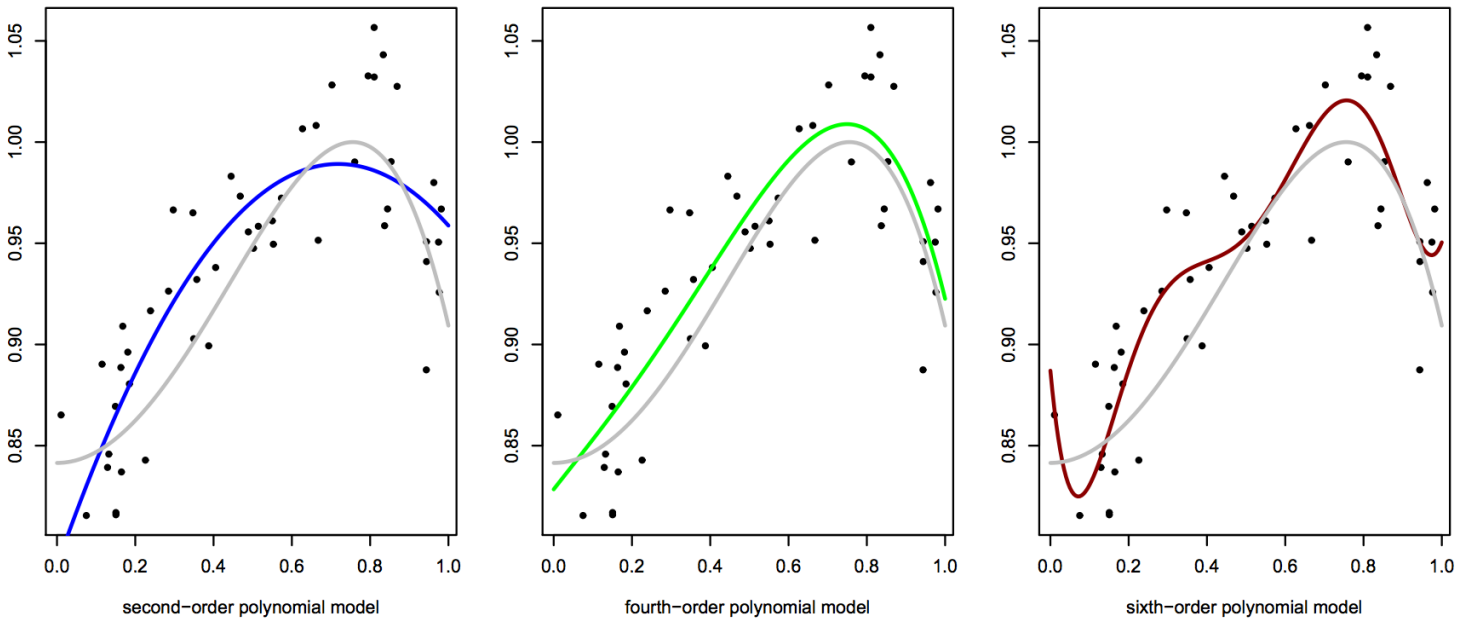

It appears that the last model is too complex and is overfitting a bit.

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- The penalty trades off some **bias** for an improvement in **variance**
- The trick in general is how to set λ

Generalized Additive Models (GAM)

Recall the linear model,

$$y_i = \beta_0 + x_{1i}\beta_1 + x_{2i}\beta_2 + x_{3i}\beta_3 + u_i$$

For GAMs, we maintain additivity, but instead of imposing linearity we allow flexible functional forms for each explanatory variable, where $s_1(\cdot), s_2(\cdot),$ and $s_3(\cdot)$ are smooth functions that are estimated from the data:

$$y_i = \beta_0 + s_1(x_{1i}) + s_2(x_{2i}) + s_3(x_{3i}) + u_i$$

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$$y_i = \beta_0 + s_1(x_{1i}) + s_2(x_{2i}) + s_3(x_{3i}) + u_i$$

- GAMS are semi-parametric, they strike a compromise between nonparametric methods and parametric regression
- $s_j(\cdot)$ are usually estimated with locally weighted regression smoothers or cubic smoothing splines (but many approaches are possible)
- They do NOT give you a set of regression parameters $\hat{\beta}$. Instead you get a graphical summary of how $E[Y|X, X_2, ..., X_k]$ varies with X_1 (estimates of $s_j(??)$ at every value of $X_{i,j}$)

Split-Apply-Combine[2]

Data analysis using Split-Apply-Combine strategy:

- break up large problem into smaller, more manageable pieces
  - ex: cleaning data, sub-group analysis
- operate on each piece independently
  - ex: summary statistics, model estimation
- put the pieces back togther
  - ex: plotting results, table of aggregate statistics,

`dplyr` and `ggplot()` are both based around the split-apply-combine concept.

[2]Wickham, Hadley. "The split-apply-combine strategy for data analysis." Journal of Statistical Software 40.1 (2011): 1-29.

Summary of problems & tools & solutions

- non-normality -> studenized residuals
- extreme values -> Cook's distance, removal, robust estimation
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- Questions?