Regression

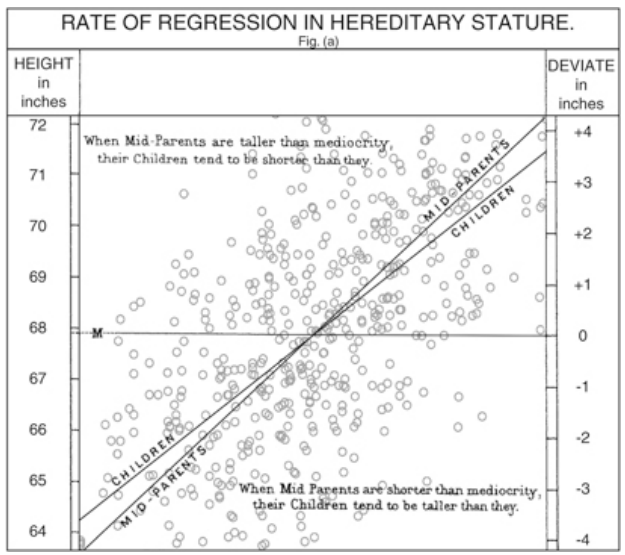
Schwartz

July 22, 2017

The Sophomore Slump

...or *sophomore jinx* or *sophomore jitters* refers to an instance in which a second, or sophomore, effort fails to live up to the standards of the first effort. It is commonly used to refer to the apathy of students (second year of high school, college or university), the performance of athletes (second season of play), singers/bands (second album), television shows (second seasons) and films (sequels/prequels). In the United Kingdom the *sophomore slump* is more commonly referred to as *second year blues*, particularly when describing university students. And in Australia it is known as *second year syndrome*, and is particularly common when referring to professional athletes who have a mediocre second season following a stellar debut. The phenomenon of a sophomore slump can be explained psychologically, where earlier success has a reducing effect on the subsequent effort, but it can also be explained statistically, as an effect of the regression towards the mean.

The concept of *regression* comes from genetics and was popularized by Sir Francis Galton's late 19th century publication of "Regression towards mediocrity in hereditary stature." Galton observed that extreme characteristics (e.g., height) in parents are not completely passed on to offspring, but rather the characteristics in the offspring "regress" towards a mediocre point. By measuring the heights of hundreds of people Galton was able to quantify this "regression" and in so doing invented linear regression analysis, thus laying the groundwork for much of modern statistical modeling. The term *regression* stuck.



Objectives

- Linear Model Regression
  - Terminology
  - Model Fitting (Least Squares)
  - Diagnostics (Evaluation and Critiquing)
- Multiple (not Multivariate) Linear Regression
  - Assumptions
  - Normal Distribution Theory
  - Model Selection
  - Coefficient Testing
- Alternatives to linear forms

Linear Models and Regression Terminology

- $Y_i = \beta_0 + x_i\beta_1 + \epsilon_i, \epsilon_i \overset{i.i.d.}{\sim} Normal(0, \sigma^2)$

Linear Models and Regression Terminology

Outcome / Response / Label / Dependent/Endogenous Var.

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  I don't like to call these *Predictors*...

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  Intercept

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Intercept Error/Noise

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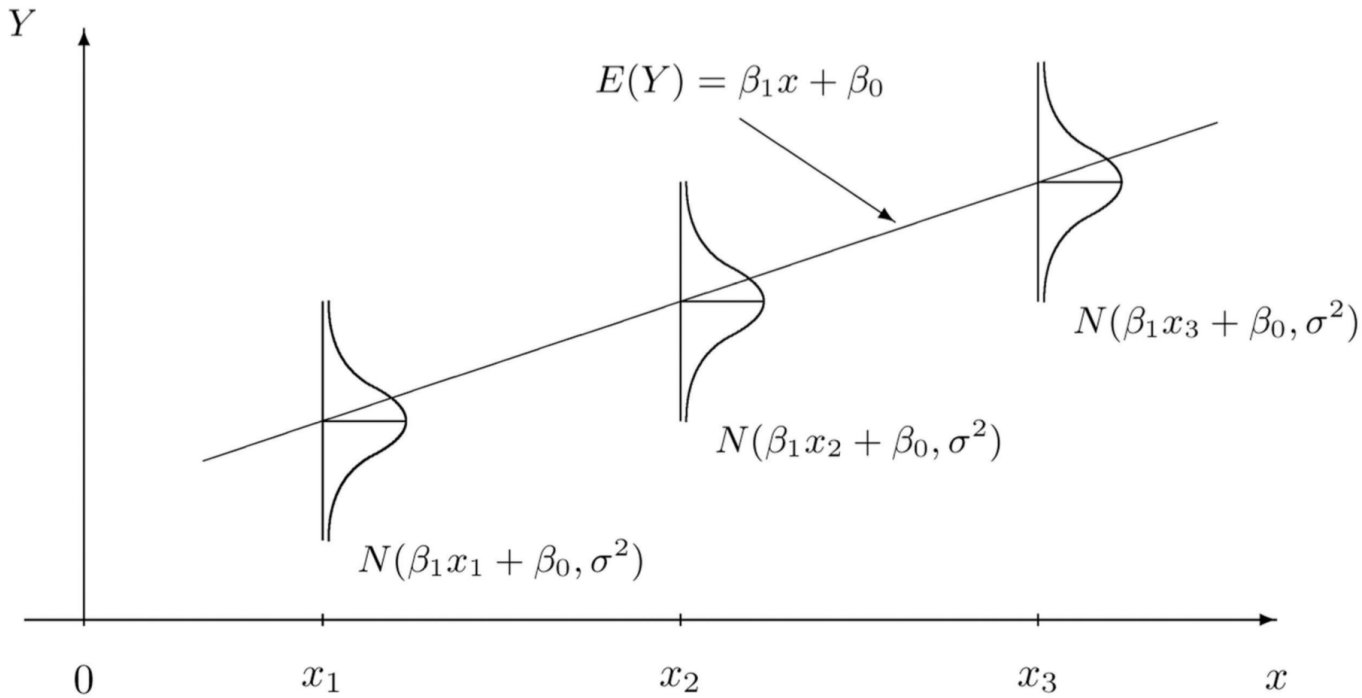

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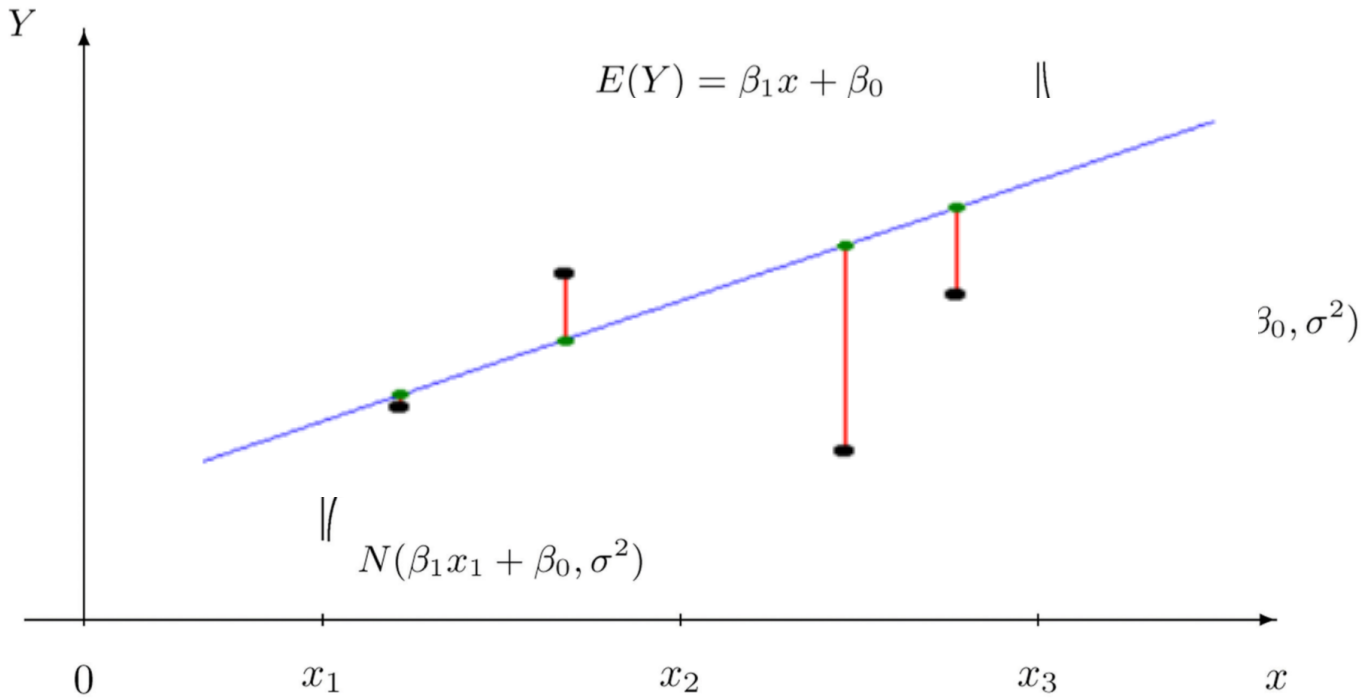

- $Y_i = \hat{\beta}_0 + x_i\hat{\beta}_1 + \hat{\epsilon}_i, \quad \hat{\sigma}^2 = \frac{\sum_{i=1}^{n} \hat{\epsilon}_i^2}{n-p-1} \quad (p = \#of\ coefficients)$

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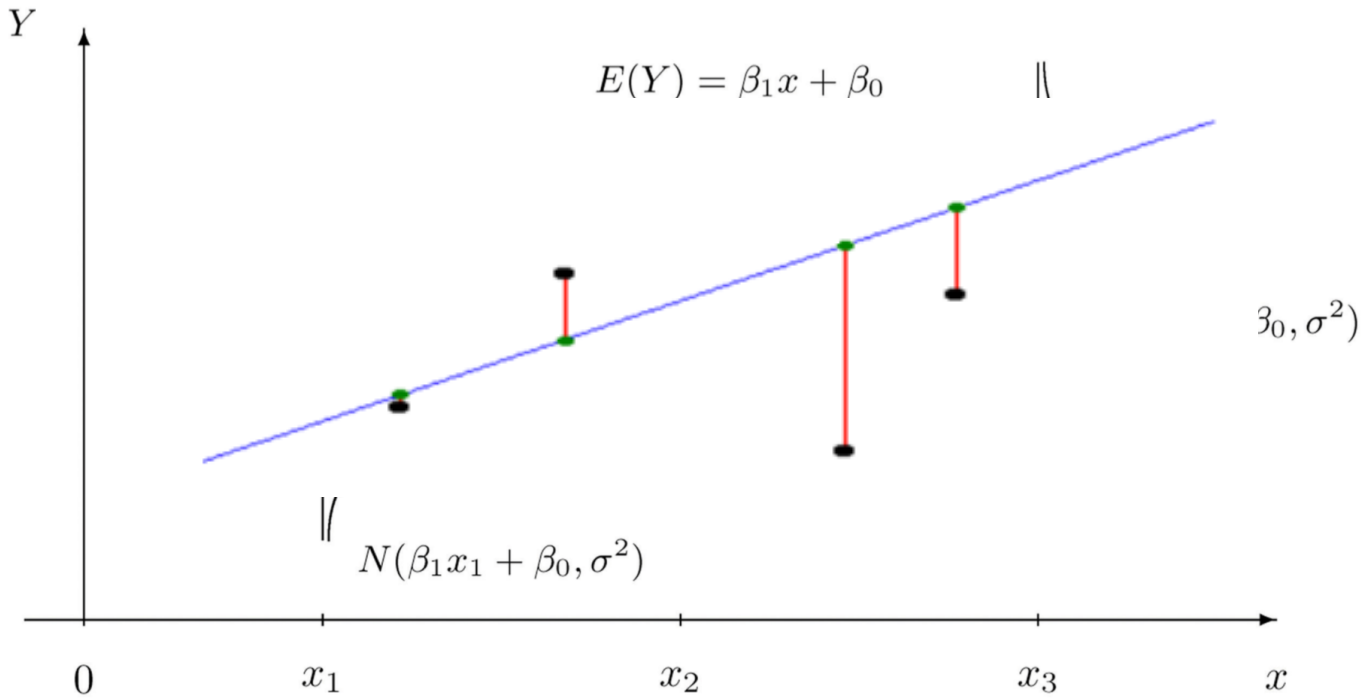

Fitted/Predicted value $\hat{Y}_i$

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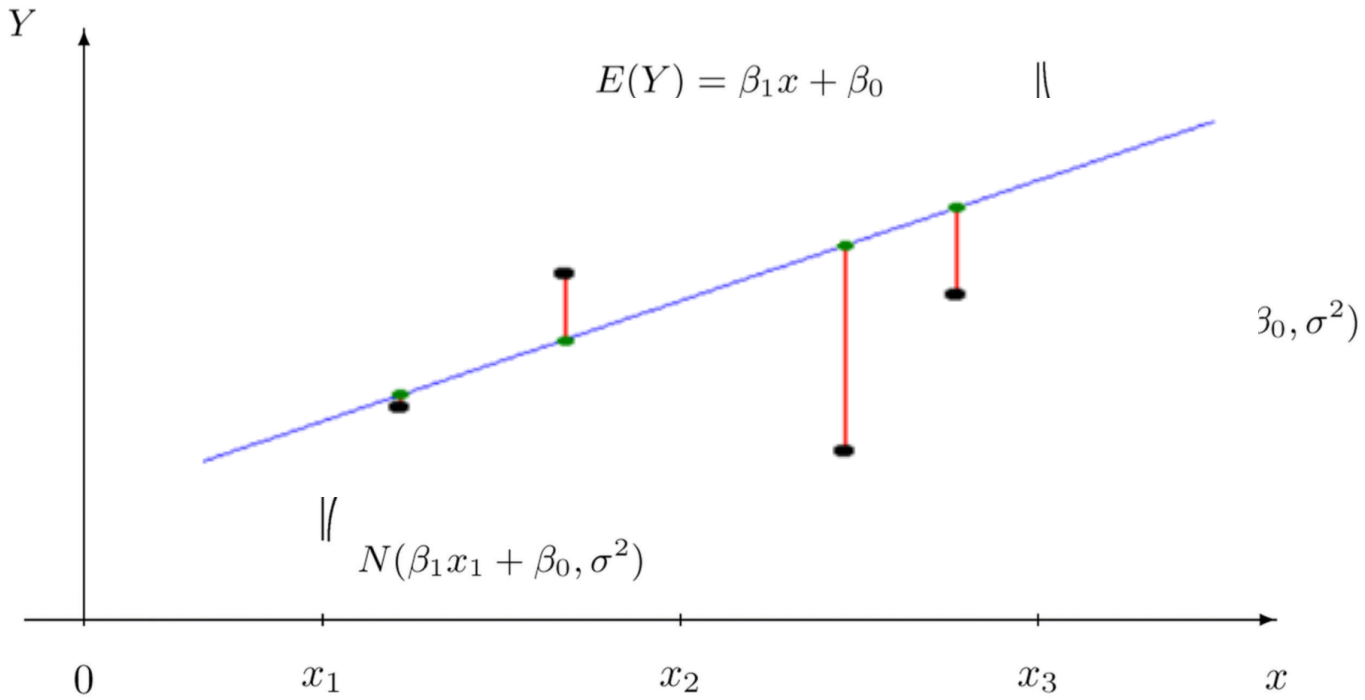

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Residual

Linear Models and Regression Terminology

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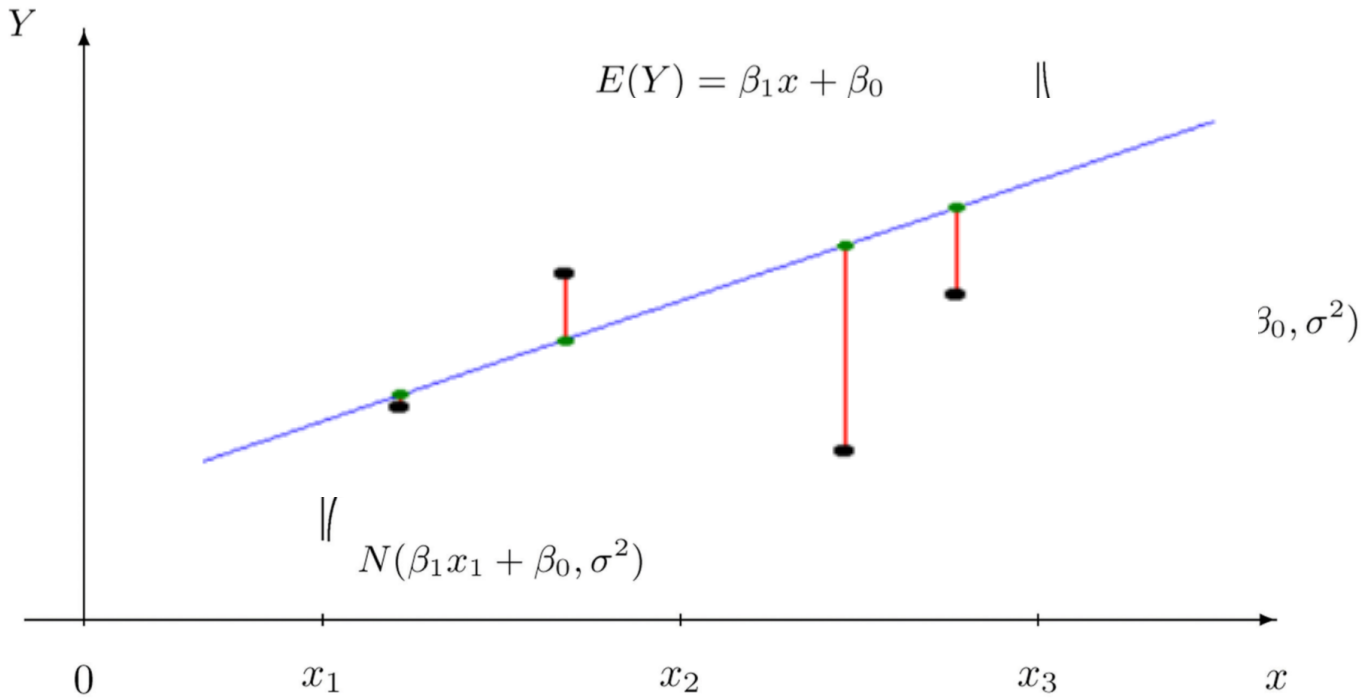

Fitted/Predicted value $\hat{Y}_i$ Residual Variance

- $Y_i = \hat{\beta}_0 + x_i\hat{\beta}_1 + \hat{\epsilon}_i, \quad \hat{\sigma}^2 = \frac{\sum_{i=1}^{n} \hat{\epsilon}_i^2}{n-p-1} \quad (p = \#of\ coefficients)$

Residual

Quiz: what are these things and their parts?

$$Y_i = \beta_0 + x_i\beta_1 + \epsilon_i$$

$$Y_i = \hat{\beta}_0 + x_i\hat{\beta}_1 + \hat{\epsilon}_i, \quad \hat{\sigma}^2 = \frac{\Sigma_{i=1}^{n}\hat{\epsilon}_i}{n-p-1}$$

$$\hat{Y}_i = \hat{\beta}_0 + x_i\hat{\beta}_1$$

Least Squares Fit

- $Y_i = \hat{\beta}_0 + x_i \hat{\beta}_1 + \hat{\epsilon}_i$

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where $\mathbf{x}_i^T = [1, x_i]$ and $\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$

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where $\mathbf{Y}^T = [Y_1, Y_2, \cdots, Y_n]$ and $\mathbf{x}^T = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{bmatrix}$

Least Squares Fit

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$$\nabla_\beta \beta^T(\mathbf{x}^T\mathbf{x})\beta - 2\mathbf{Y}^T\mathbf{x}\beta + \mathbf{Y}^T\mathbf{Y}$$

$$= 2(\mathbf{x}^T\mathbf{x})\beta - 2\mathbf{Y}^T\mathbf{x} \qquad \text{(set to } \mathbf{0} \text{ to minimize)}$$

$$\implies \hat{\beta} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{Y} \implies \text{fitted values } \hat{\mathbf{Y}} = \mathbf{x}\hat{\beta}$$

$$\hat{\mathbf{Y}} = \mathbf{x}(\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{Y}$$

Least Squares Fit *bonus*

1. Maximum likelihood estimation (MLE) $\iff$ to lease squares!

$$\underset{\beta}{argmax} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(Y_i - \mathbf{x}_i^T\beta)^2}$$

$$= \underset{\beta}{argmax} (2\pi\sigma^2)^{-\frac{n}{2}} e^{-\frac{1}{2\sigma^2}(\mathbf{Y}-\mathbf{x}\beta)^T(\mathbf{Y}-\mathbf{x}\beta)}$$

$$= \underset{\beta}{argmax} -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{Y}-\mathbf{x}\beta)^T(\mathbf{Y}-\mathbf{x}\beta)$$

$$= \underset{\beta}{argmin} (\mathbf{Y}-\mathbf{x}_i\beta)^T(\mathbf{Y}-\mathbf{x}\beta) \quad \text{[same as least squares!!]}$$

2. In simple linear regression the $\underset{\beta}{argmin}(\mathbf{Y}-\mathbf{x}\beta)^T(\mathbf{Y}-\mathbf{x}\beta)$ is

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1\bar{x}$$

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(x_i - \bar{x})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{R_{xY}S_Y}{S_x}$$

Assumptions of Linear Regression

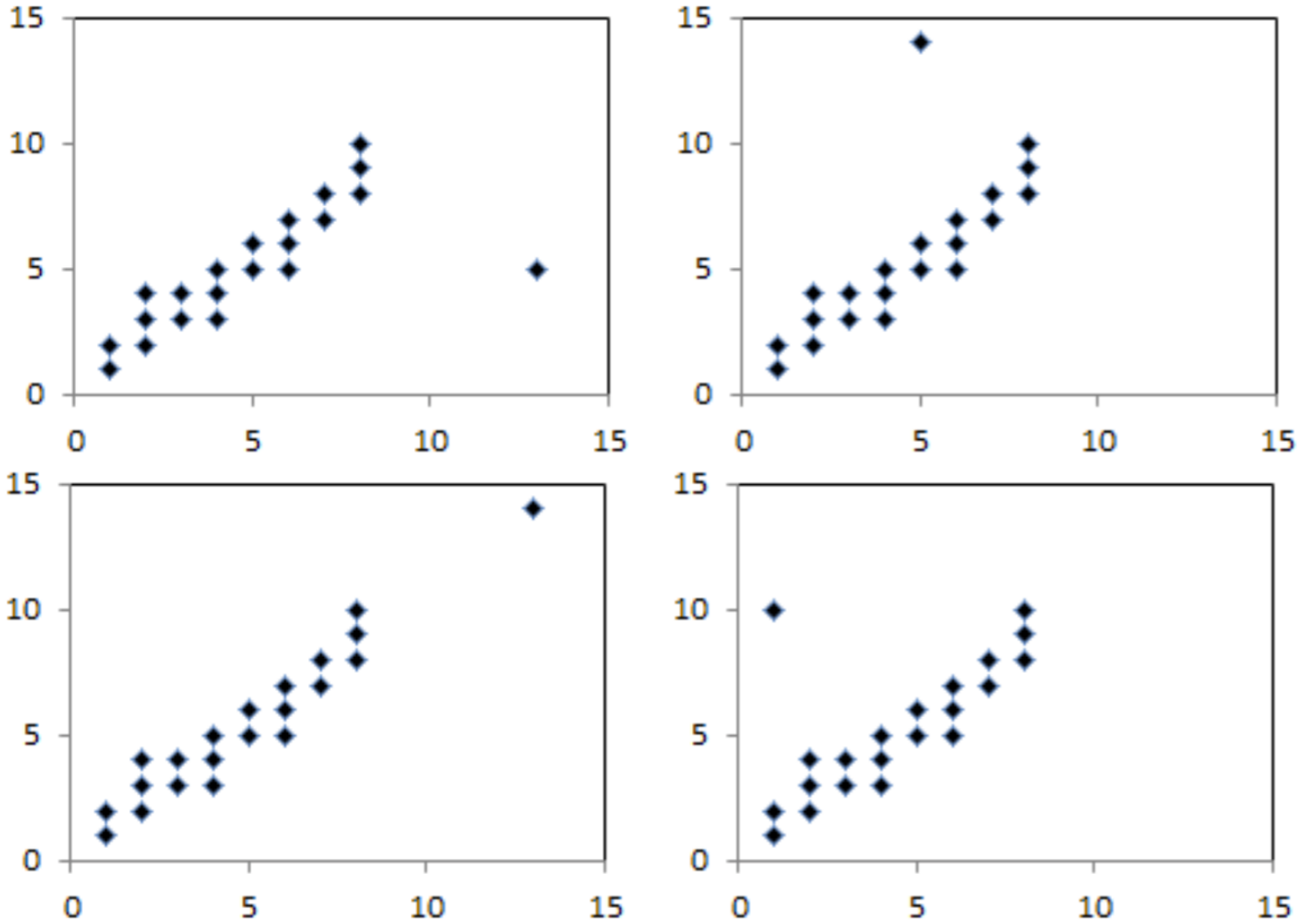
1. Sample data is representative of the population.
2. True relationship between *X* and *y* is linear.
3. Feature matrix *X* has full rank (rows and columns are linearly independent).
4. Residuals are independent.
5. Residuals are normally distributed.
6. Variance of the residuals is constant (homoscedastic).

Note: Linear regression does *not* assume anything about the distributions of *x* and *y*, it only makes assumptions about the distribution of the residuals, and this is all that's needed for the statistical tests to be valid.

Colinearity of the Feature Matrix

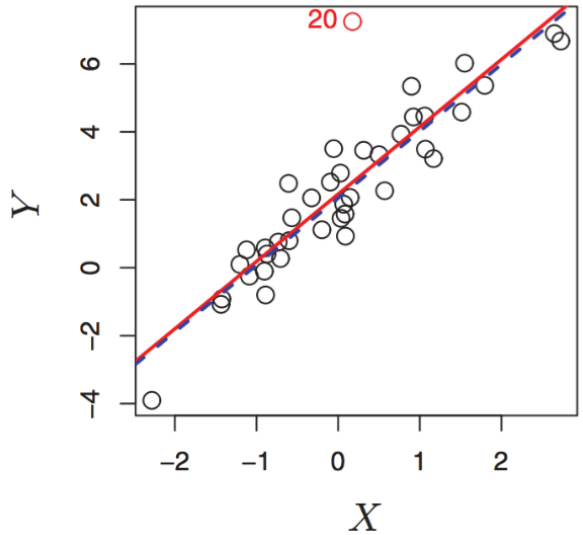
- Colinearity occurs in a dataset when two or more features (columns of X) are highly correlated. These features provide redundant information.
- *Perfect* colinearity violates the full-rank assumption, and the feature matrix becomes singular or degenerate.
- Signs of colinearity include:
  - Opposing signs for the coefficients of the effected variables, when it's expected that both would have the same sign.
  - Standard errors of the regression coefficients of the effected variables tend to be large.
  - Large changes to the regression coefficients when a feature is added or deleted (unstable solution).
  - Rule of thumb: a variance inflation factor (VIF) > 5 indicates a multicollinearity problem.
    - $VIF = 1 / (1 - R_j^2)$
    - R_j^2 is the coefficient of determination of a regression of feature j on all the other features.
- Remedies to colinearity include:
  - Regularization (Ridge and Lasso -- tomorrow)
  - Principal component analysis (PCA − next week)
  - Engineering a feature that combines the affected features (ahem first case study)
  - Simply dropping one of the features (lazy, but viable, option)

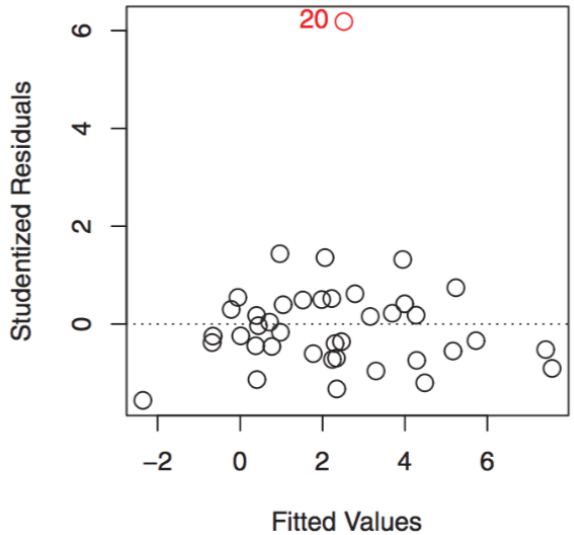
What makes these data points “unusual”?



Regression Diagnostics

Outliers





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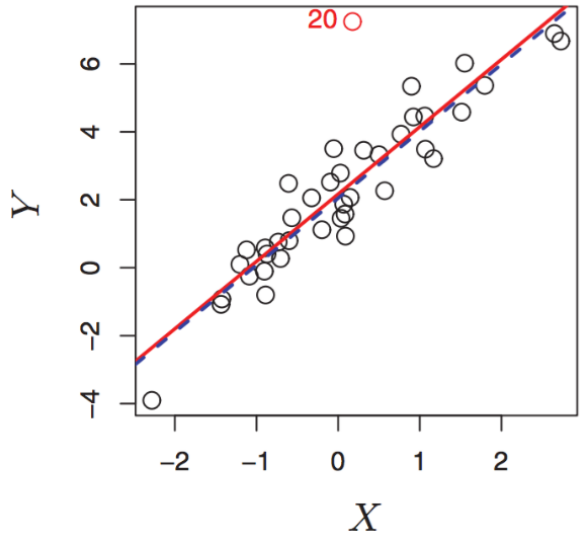
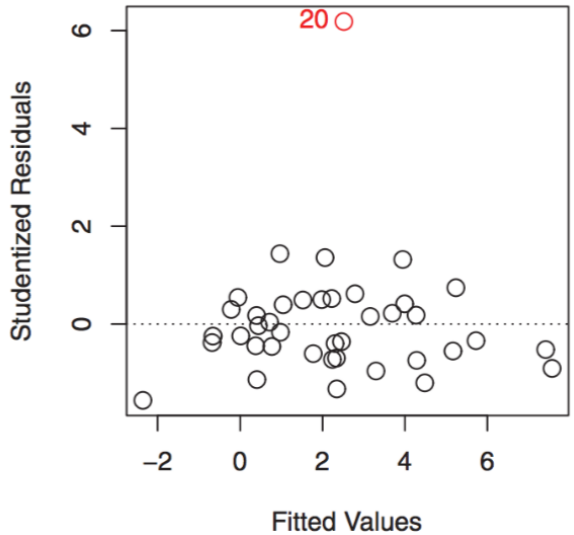
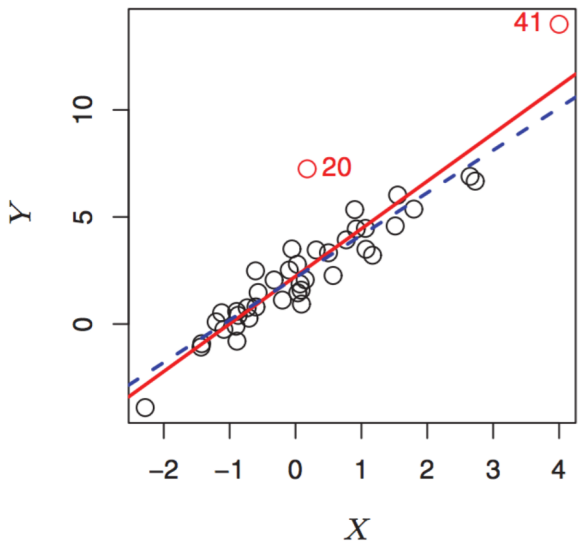
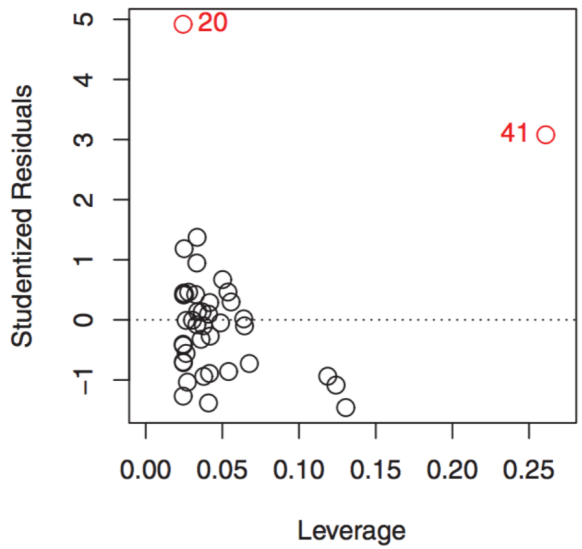




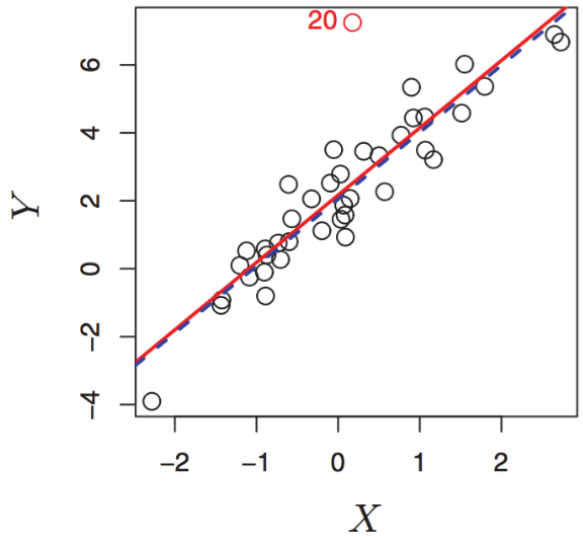
High Leverage Points

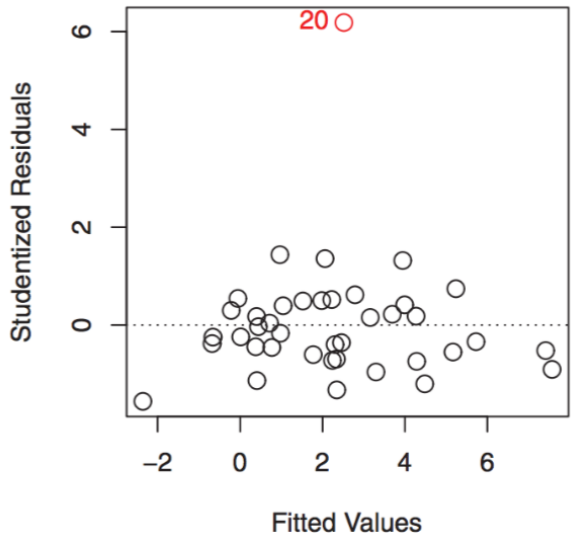




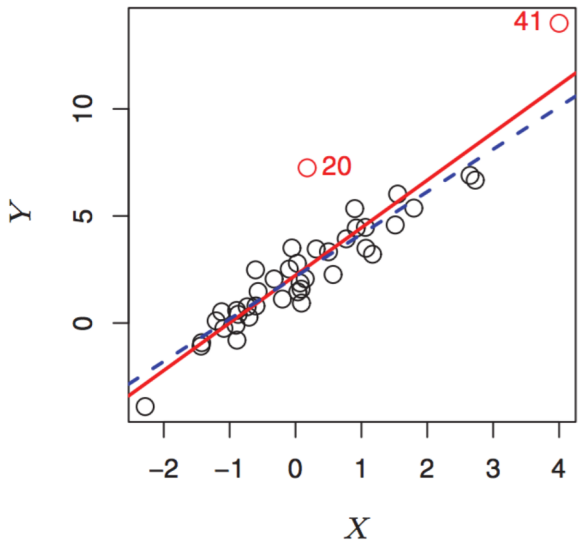
Regression Diagnostics

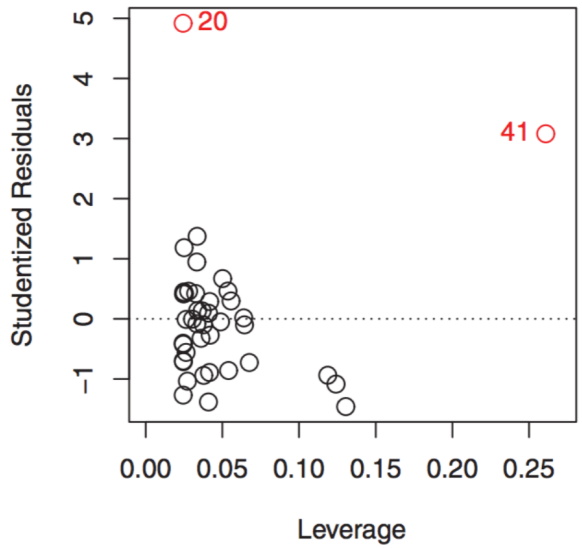
Outliers impact residual variance estimates



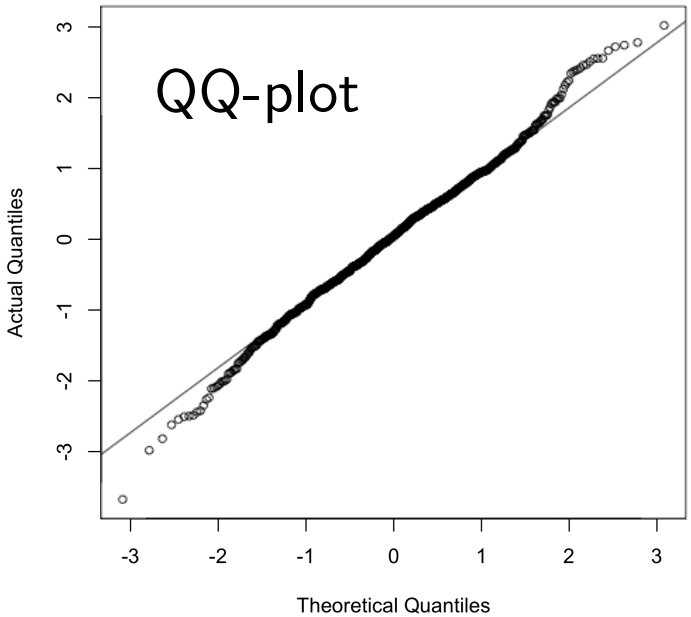


High Leverage Points impact prediction estimates





Regression Diagnostics (with residuals)



- What's wrong with the residual distribution?

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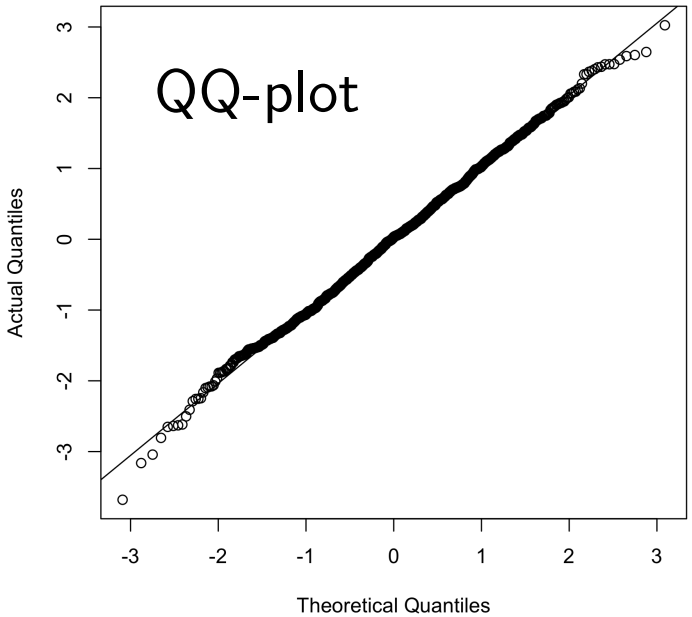

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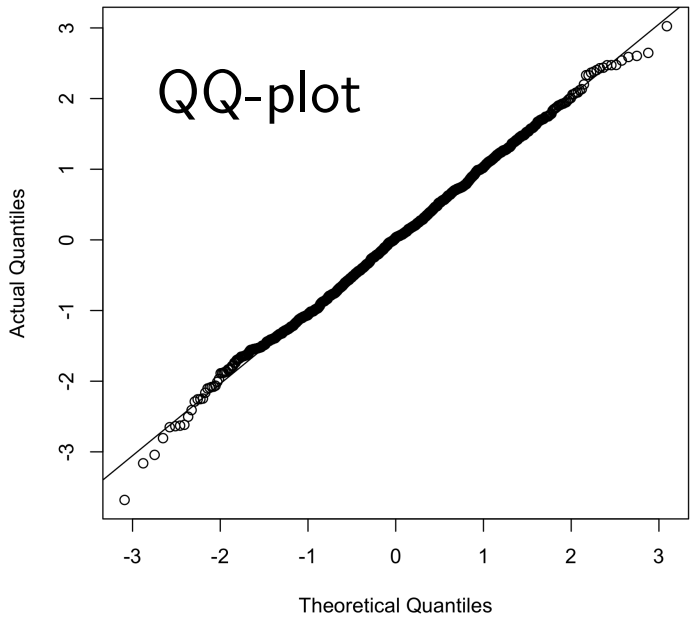
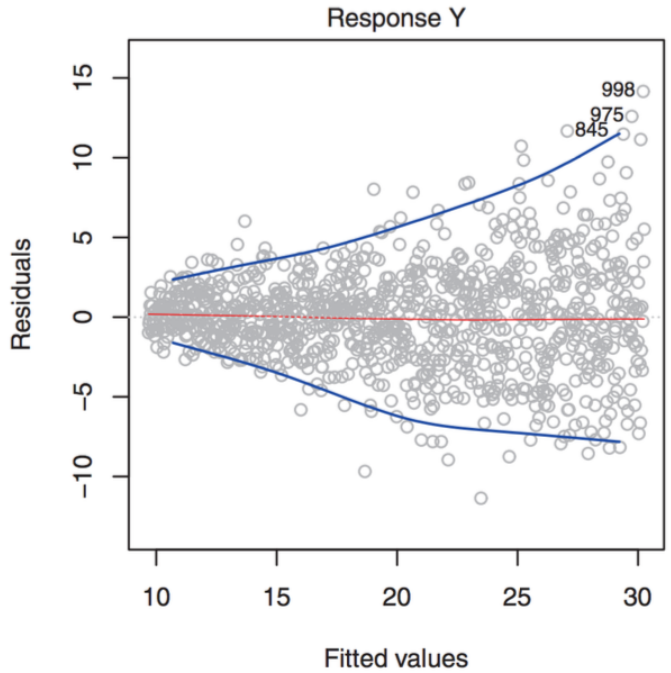
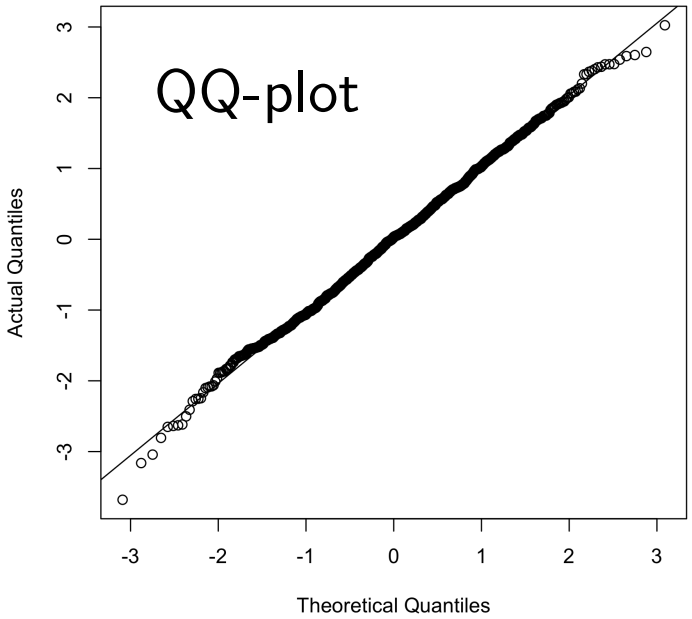
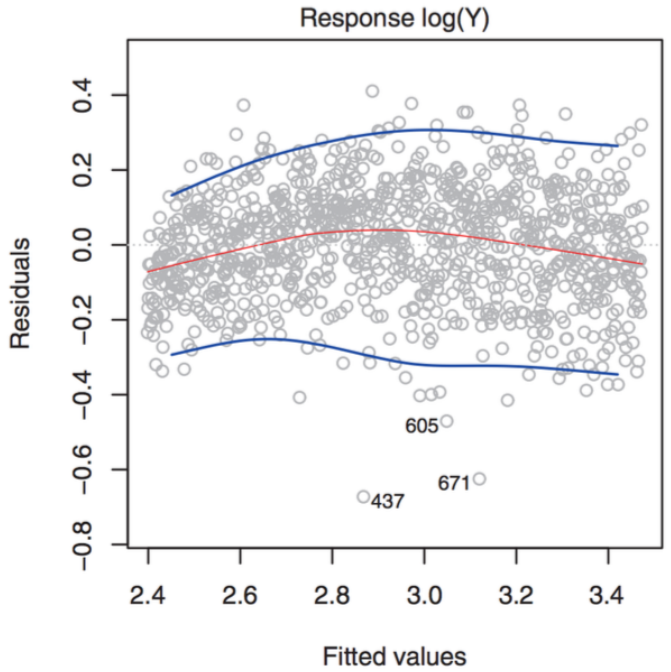




- What's wrong with the residual distribution?
- What's wrong with the residual variance?

Regression Diagnostics (with residuals)





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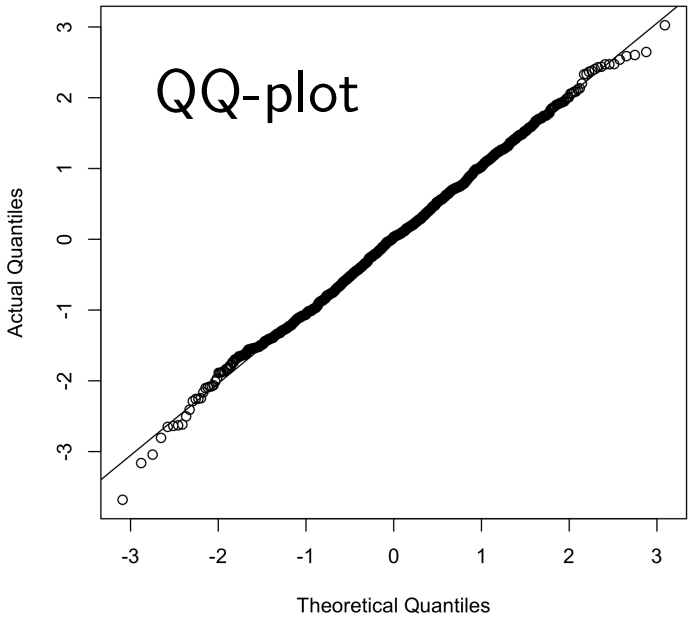
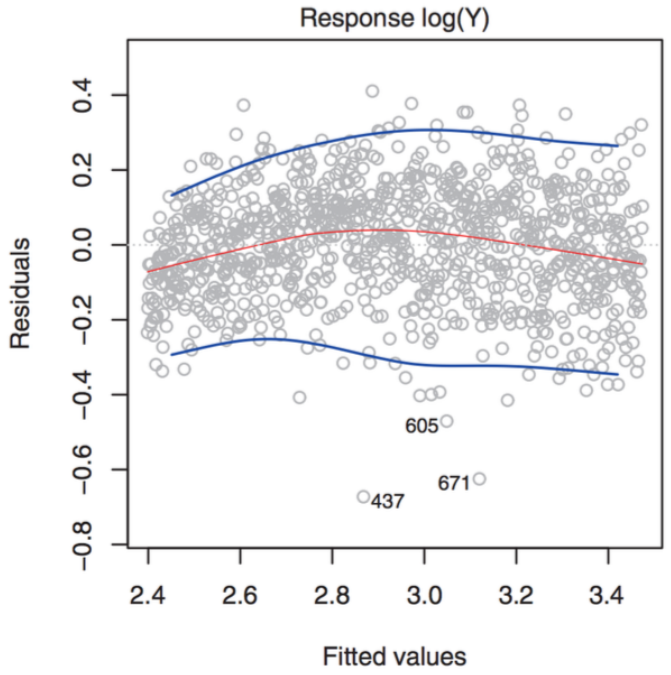
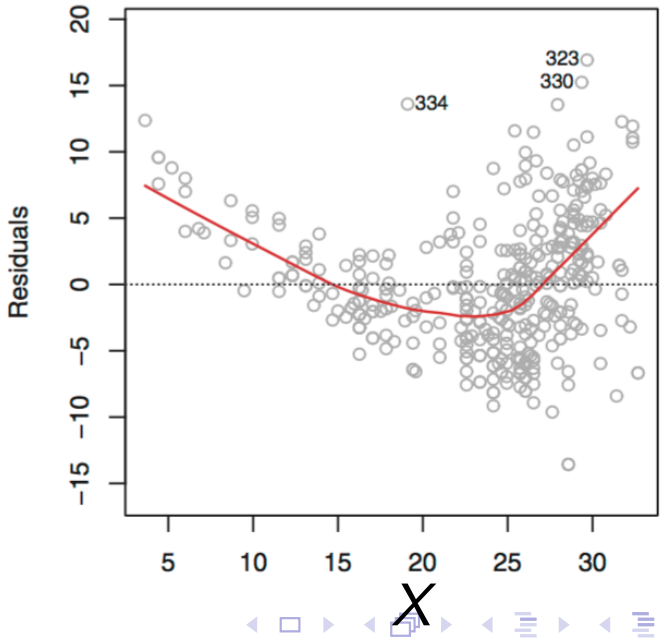
Regression Diagnostics (with residuals)





- What's wrong with the residual distribution?
- What's wrong with the residual variance?
- What's wrong with this feature/outcome relationship?



Leverage

The *hat* matrix H *"puts the hat on"* $\boldsymbol{Y}$ projecting $\boldsymbol{Y}$ onto the (least squares) closest vector to $\boldsymbol{Y}$ in the column space of $\boldsymbol{x}$, $\hat{\boldsymbol{Y}} \in \mathcal{R}(\boldsymbol{x})$

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\begin{aligned}
H &= \mathbf{x}(\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T \\
\hat{\boldsymbol{Y}} &= \mathbf{x}(\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{Y} \\
&= H\mathbf{Y}
\end{aligned}
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\end{aligned}
$$

- Diagonal element $H_{ii} \in [0, 1]$, and $\sum_{i=1}^{n} H_{ii} = rank(\mathbf{x})$
  H_{ii} is called the *leverage* of observation i

Leverage

The *hat* matrix H *"puts the hat on"* $\boldsymbol{Y}$ projecting $\boldsymbol{Y}$ onto the (least squares) closest vector to $\boldsymbol{Y}$ in the column space of $\boldsymbol{x}$, $\hat{\boldsymbol{Y}} \in \mathcal{R}(\boldsymbol{x})$

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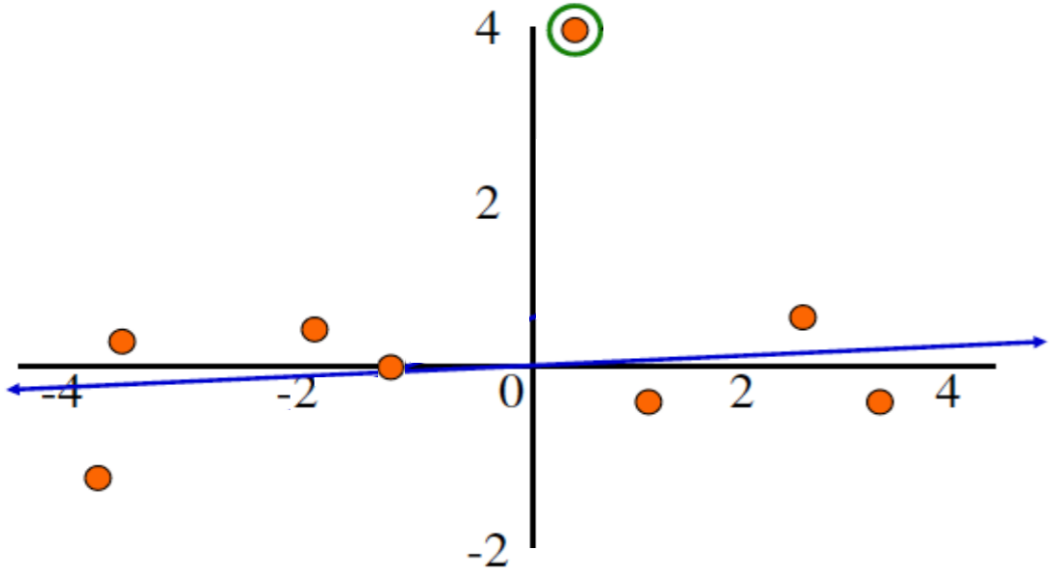

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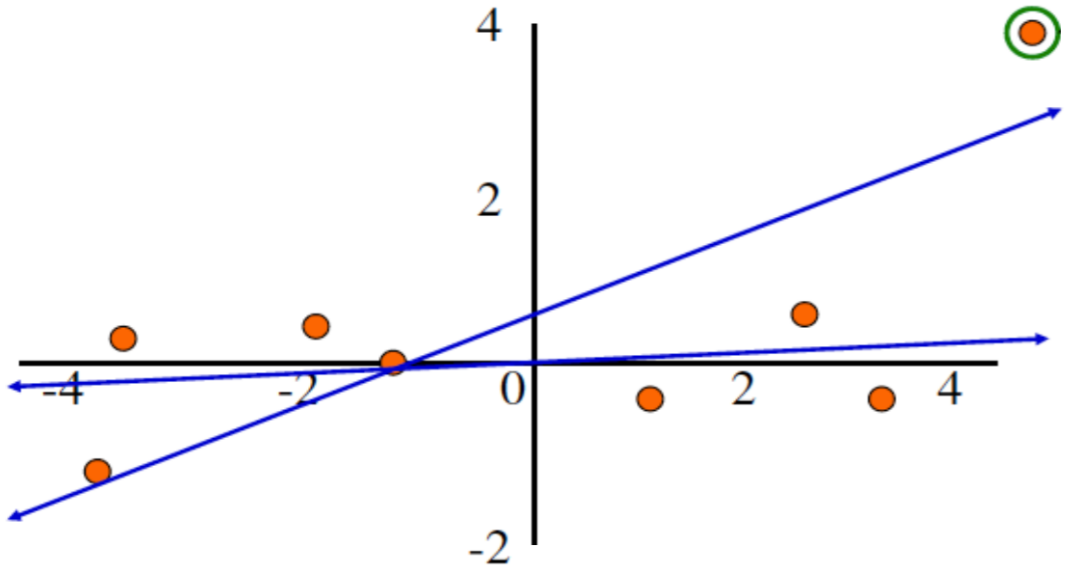

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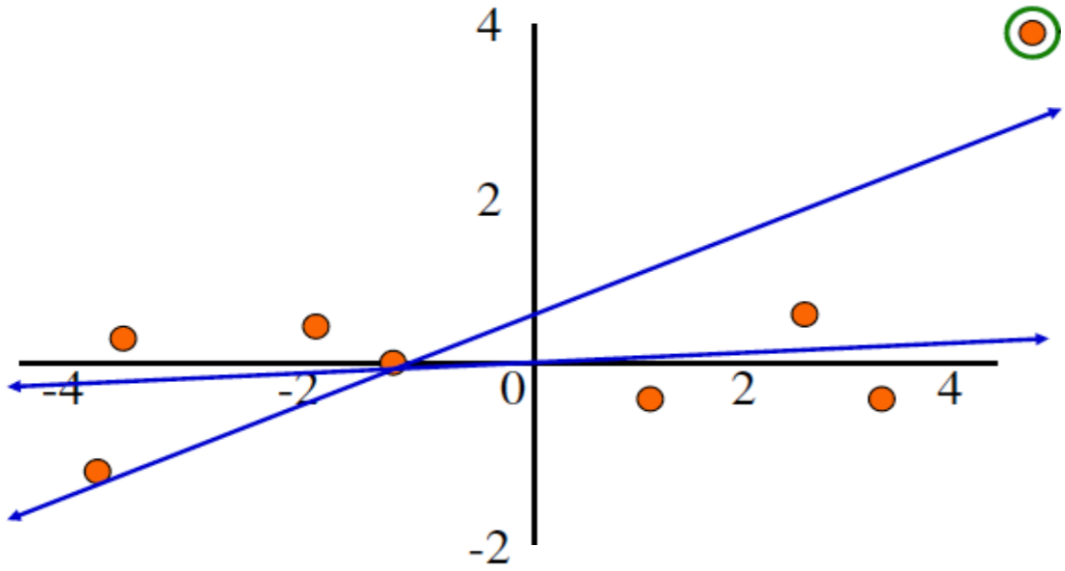

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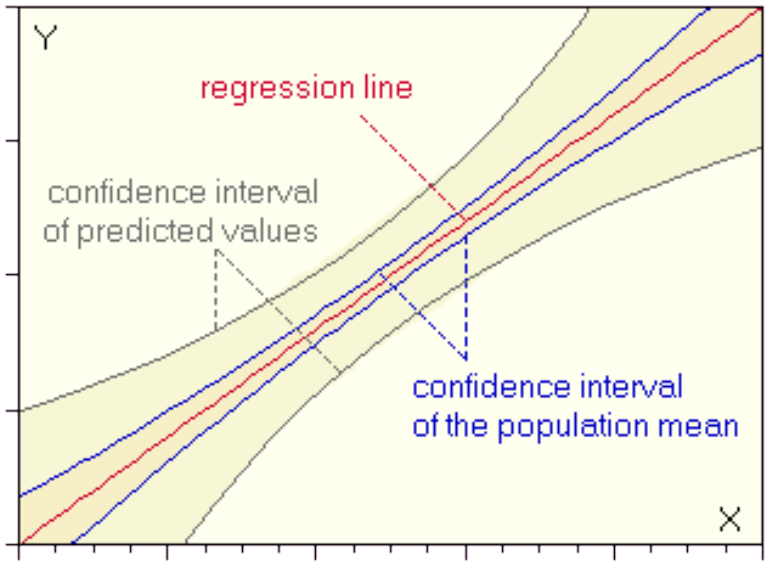
Influential Data Points

Studentized Residuals have a t-distribution...

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



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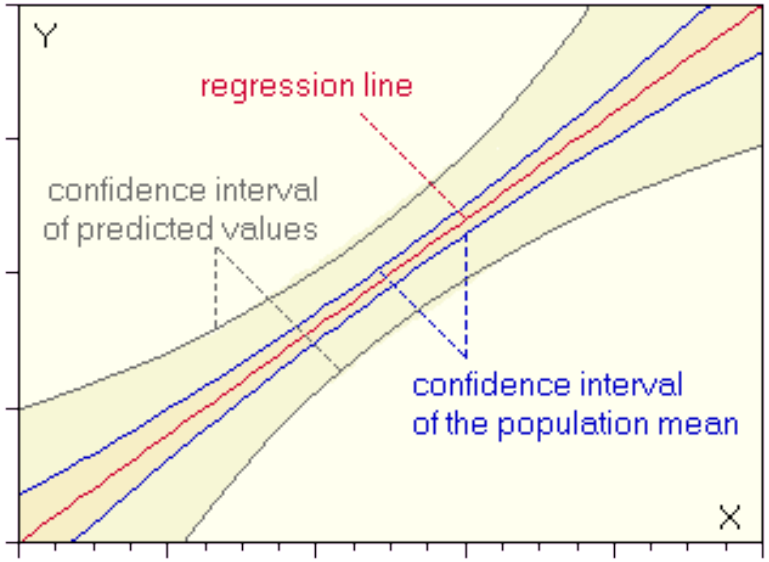
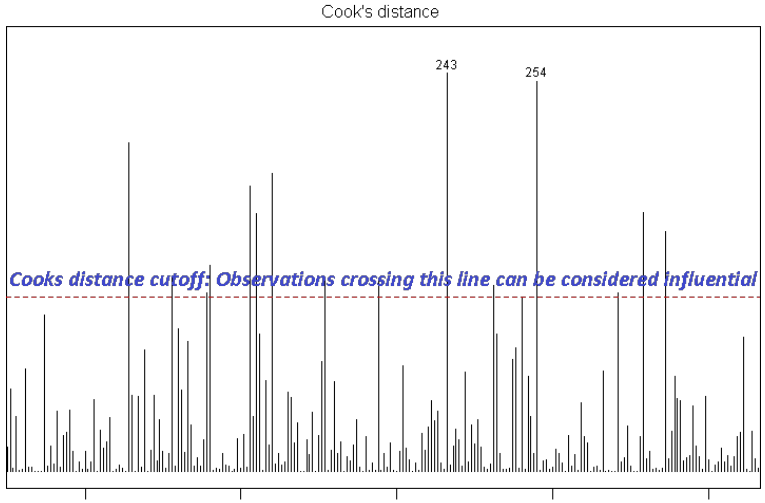


Cook's Distance is

$$D_i = \frac{\sum_{j=1}^{n}\left(\hat{y}_j - \hat{y}_{j(-i)}\right)^2}{\hat{\sigma}^2 p} = \frac{\hat{\epsilon}_i}{\hat{\sigma}^2 p}\frac{h_{ii}}{(1-h_{ii})^2}$$



Influential data point i may have $D_i > \{3 \times \bar{D}, 1, 4/n, F_{p,n-p}^{1-\alpha}\}$

Assumptions, violations, and remedial measures

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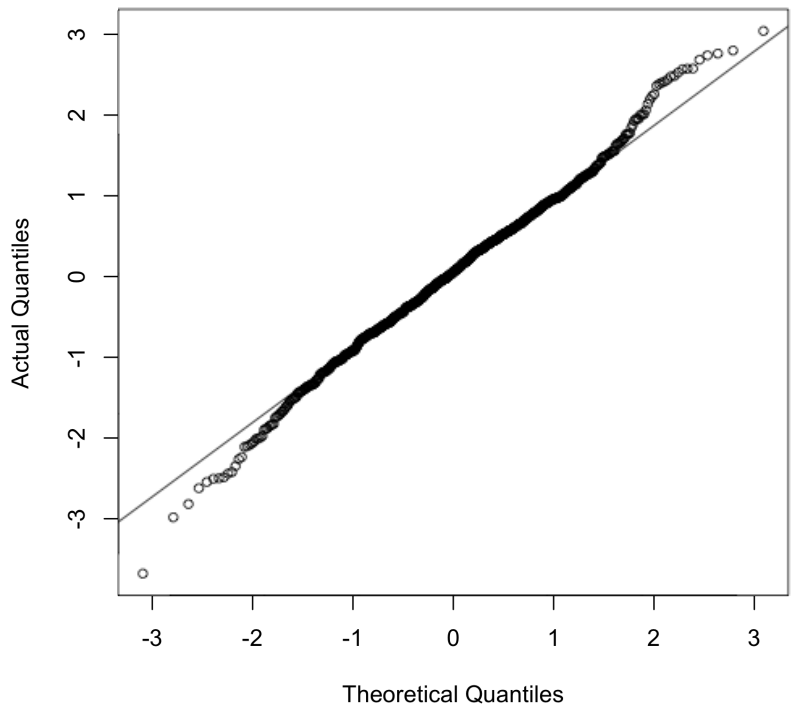

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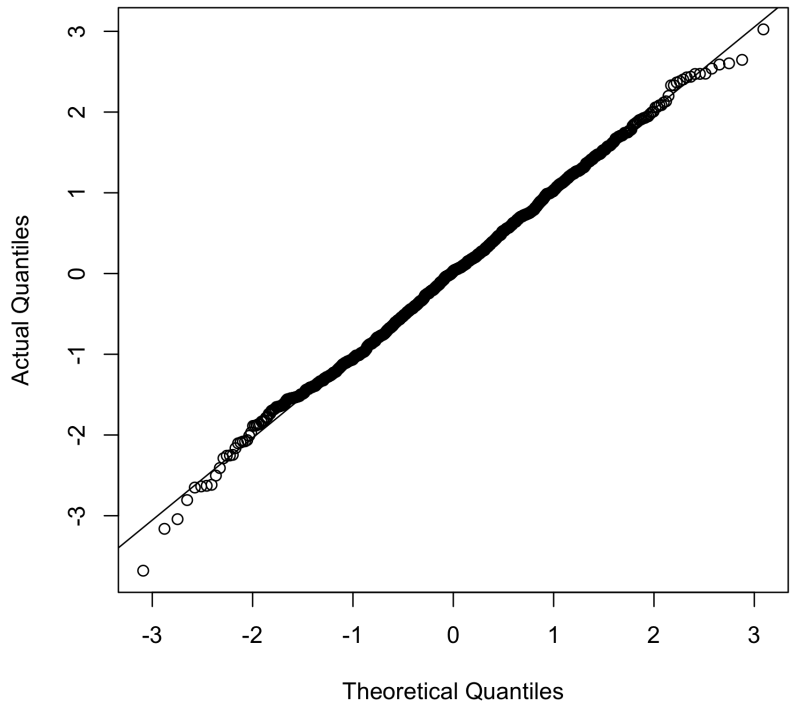

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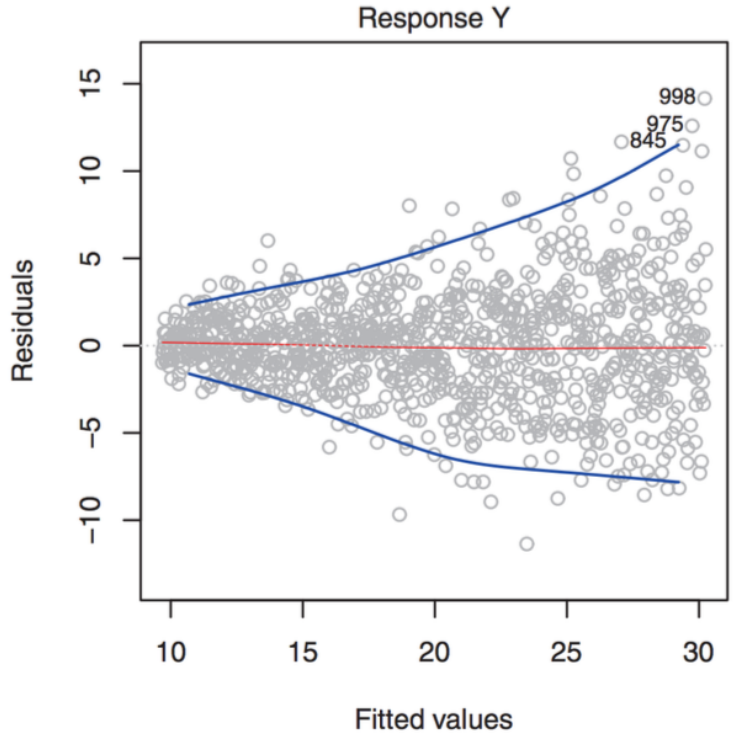

Residuals versus Fitted Values

Box-Cox transformations $\frac{Y^\lambda - 1}{\lambda}$ can help

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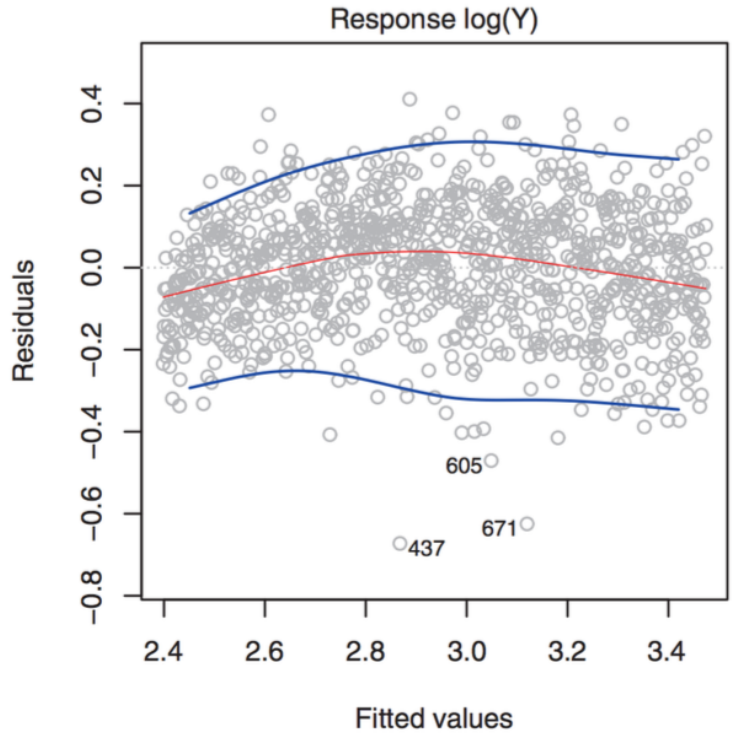

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- Independence

$$\mathrm{Cov}[\boldsymbol{Y} - \boldsymbol{X}\beta] \approx \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix}$$

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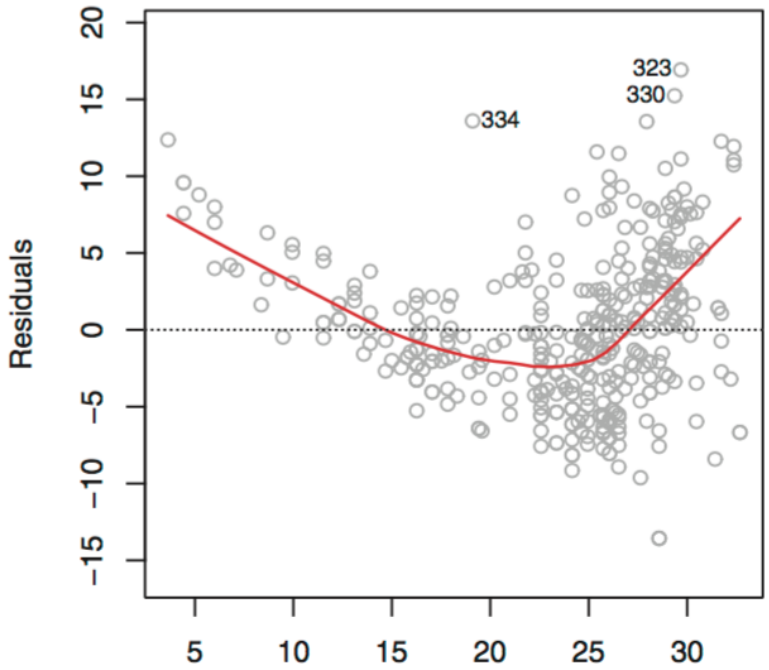

Residuals versus Feature Values

"All models are wrong, some are useful"
– George Box

Assumptions, violations, and remedial measures

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- Normality
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- Independence
- Linear form
- Fixed x's

$$\boldsymbol{Y} \sim \mathrm{MVN}(\mathbf{x}\boldsymbol{\beta}, \sigma^2 I)$$

Quiz: assumptions?

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1.
2.
3.
4.
5.

Half time

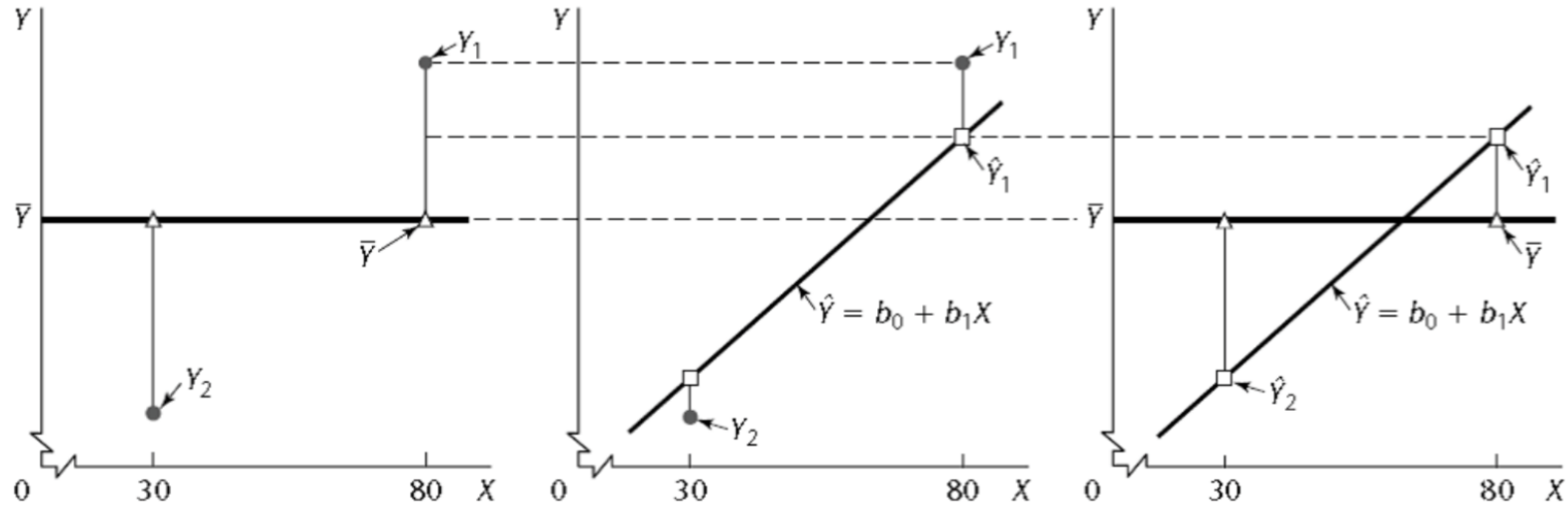
Assessing Model Fit **(more Machine Learning-ish)**

Residual Sum of Squares	Total Sum of Squares
$RSS = \sum(Y_i - \hat{Y}_i)^2 = \sum \hat{\epsilon}_i^2$	$TSS = \sum(Y_i - \bar{Y})^2 = \sum(\hat{Y}_i - \bar{Y})^2 + RSS$
Residual Standard Deviation	**Proportion of Variance Explained**
$\hat{\sigma} = \sqrt{\frac{1}{n-p-1} RSS} = \sqrt{\frac{\sum(Y_i - \hat{Y}_i)^2}{n-p-1}}$	$R^2 = \frac{TSS-RSS}{TSS} = 1 - \frac{RSS}{TSS}$

F-statistic

$$F = \frac{(TSS-RSS)/p}{RSS/(n-p-1)} = \frac{\sum(\hat{Y}_i - \bar{Y})^2/p}{\sum(Y_i - \hat{Y})^2/(n-p-1)}$$

Decomposition of Total Variation



$$
\begin{aligned}
TSS &= \sum (Y_i - \bar{Y})^2 = \sum (Y_i - \hat{Y}_i + \hat{Y}_i - \bar{Y})^2 \\
&= \sum (Y_i - \hat{Y}_i)^2 + 2\sum (Y_i - \hat{Y}_i)(\hat{Y}_i - \bar{Y}) + \sum (\hat{Y}_i - \bar{Y})^2 \\
&= \sum (Y_i - \hat{Y}_i)^2 + 2\sum \hat{\epsilon}_i (\hat{Y}_i - \bar{Y}) + \sum (\hat{Y}_i - \bar{Y})^2 \\
&\qquad \sum \hat{\epsilon}_i = 0 \uparrow \quad \uparrow \sum \hat{\epsilon}_i \hat{Y}_i = 0 \\
&= \sum (Y_i - \hat{Y}_i)^2 + \sum (\hat{Y}_i - \bar{Y})^2 = RSS + \sum (\hat{Y}_i - \bar{Y})^2
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- R^2 (model fit) is insufficient – more features means larger R^2

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- Classical Statistics Approaches:
  Model Selection Criterion (choose smallest)

Mallow's C_p	$\frac{1}{n}(RSS + 2p\hat{\sigma}^2)$	
AIC	$-2\log L + 2p$	$D_M = -2\log f(Y\|\hat{\theta}^{M_p}) + 2\log f(Y\|Y)$
BIC	$-2\log L + p\log n$	$D_M \overset{approx.}{\sim} \chi^2_{n-p-1}$
Adjusted R^2	$1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$	

Akaike Information Criterion (AIC) as a Method of Model Selection

Akaike (1973):

# of parameters

$$AIC = -2 \ln f(y \mid \hat{\theta}) + 2k$$

Goodness of fit (ML) + **Model Complexity**

The model that minimizes AIC should be preferred

Bayesian Information Criterion (BIC)

Schwarz (1978):

$$BIC = -2 \ln f(y \mid \hat{\theta}) + k \ln n$$

Goodness of fit (ML) + **Model Complexity**

Assessing Parameter Uncertainty **(definitely Statistics)**

For $\hat{\beta} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{Y}$, since (under H_0)

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$$\hat{\sigma}^2 = \frac{(\mathbf{Y} - \mathbf{x}\hat{\boldsymbol{\beta}})^T(\mathbf{Y} - \mathbf{x}\hat{\boldsymbol{\beta}})}{n - p - 1} = \frac{\sum_{i=1}^{n} \hat{\epsilon}_i^2}{n - p - 1}$$

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$$\frac{\hat{\beta}_i - \beta_i}{\widehat{\mathrm{SD}}(\hat{\beta}_i)} \sim t_{n-p-1}$$

And this works for any number of feature variables...

Hypothesis Testing for Feature Selection

$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)} = \frac{\sum(\hat{Y}_i - \bar{Y})^2/p}{\sum(Y_i - \hat{Y})/(n-p-1)}$$

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OLS Regression Results

Dep. Variable:	y	R-squared:	0.933
Model:	OLS	Adj. R-squared:	0.928
Method:	Least Squares	F-statistic:	211.8
Date:	Mon, 03 Nov 2014	Prob (F-statistic):	6.30e-27 ←
Time:	14:45:06	Log-Likelihood:	-34.438
No. Observations:	50	AIC:	76.88
Df Residuals:	46	BIC:	84.52
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[95.0% Conf.	Int.]
x1	0.4687	0.026	17.751	0.000	0.416	0.522
x2	0.4836	0.104	4.659	0.000	0.275	0.693
x3	-0.0174	0.002	-7.507	0.000	-0.022	-0.013
const	5.2058	0.171	30.405	0.000	4.861	5.550

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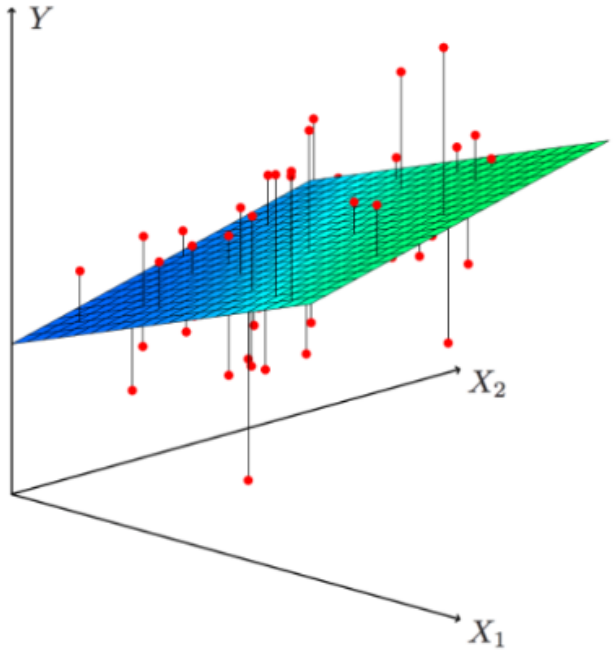

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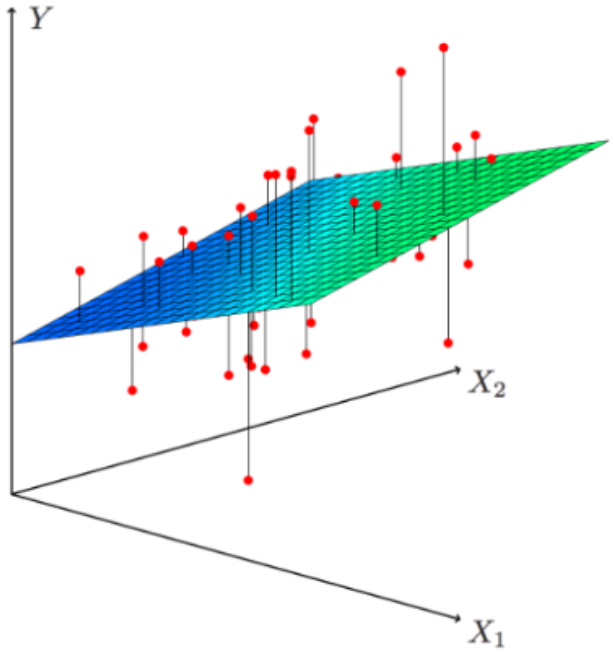

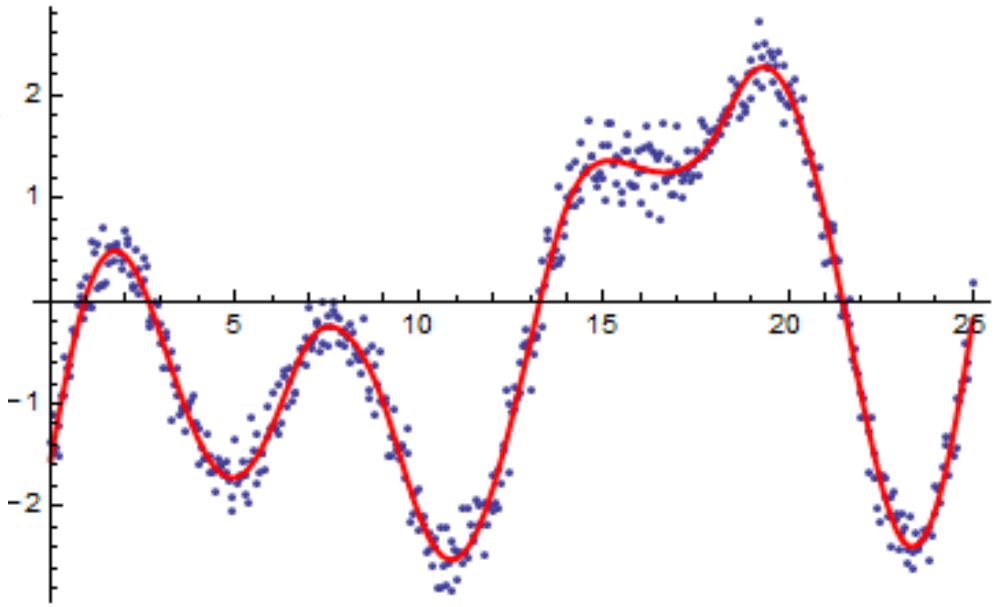

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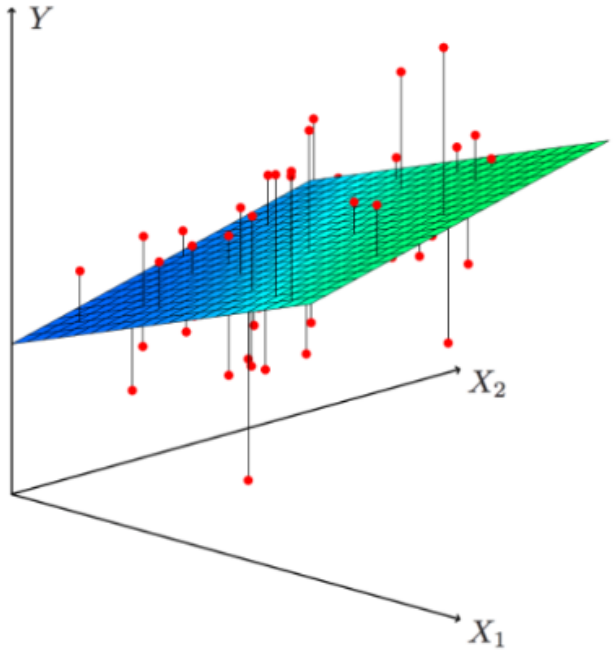

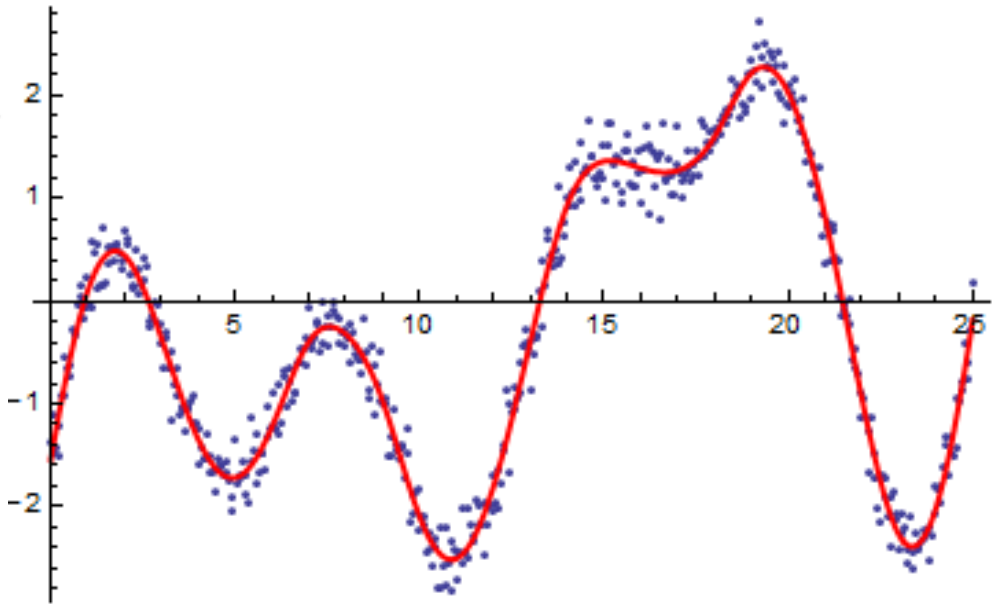

- "Linear" models are only linear in the coefficients

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i$$

- The x's can be pretty wild...

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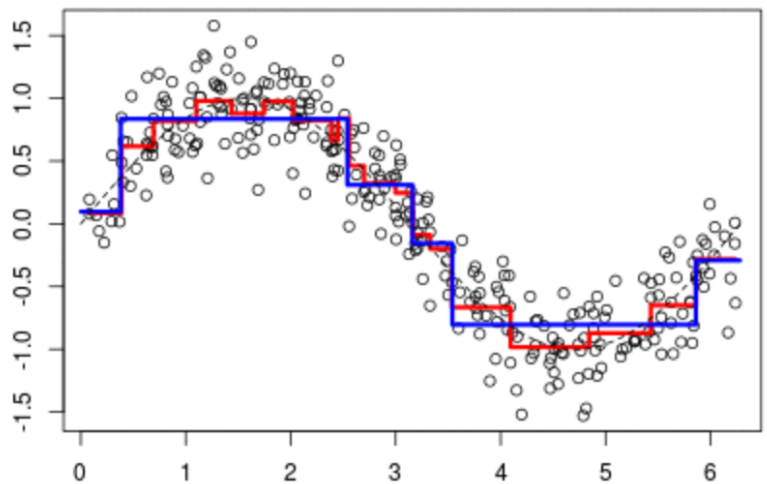
- Step functions

$$Y_i = \beta_j : \textit{if } a_j \leq X_i < b_j$$



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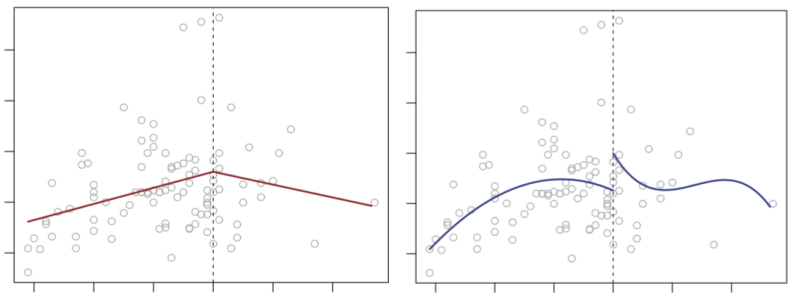

$$Y_i = \begin{cases} \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \epsilon_i : if\ X_i \leq c \\ \beta_0^* + \beta_1 X_i + \beta_2^* X_i^2 + \epsilon_i : if\ X_i > c \end{cases}$$

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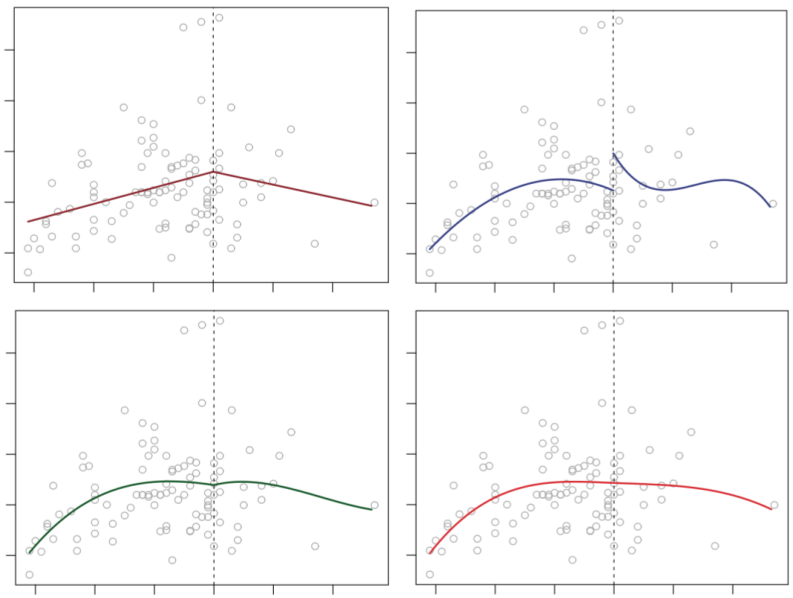
$$h(X_i, \xi) = \begin{cases} (x - \xi)^3 & : if\ X_i > \xi \\ 0 & : if\ X_i \leq \xi \end{cases}$$

basis functions & knots

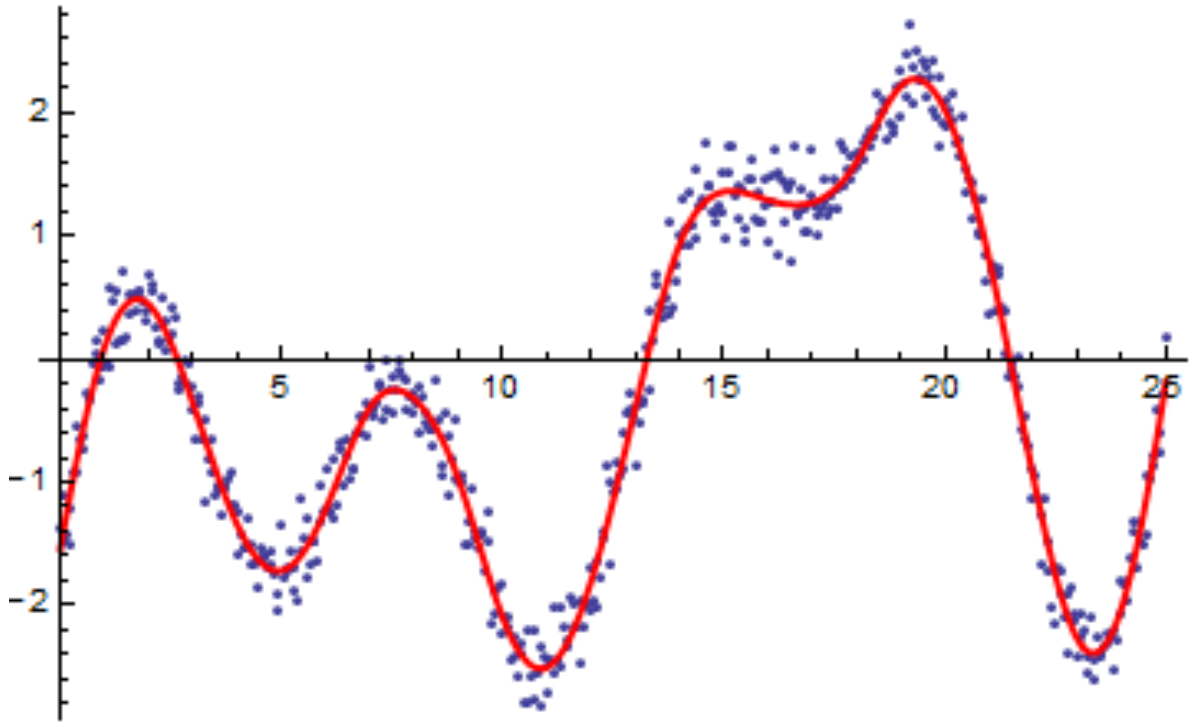
$$Y_i = \begin{array}{l} \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 \\ + \beta_{s1} h(X_i, \xi_1) + \cdots + \epsilon_i \end{array}$$



Linear models aren't really so "linear"

Other ways to get "non linear regressions"

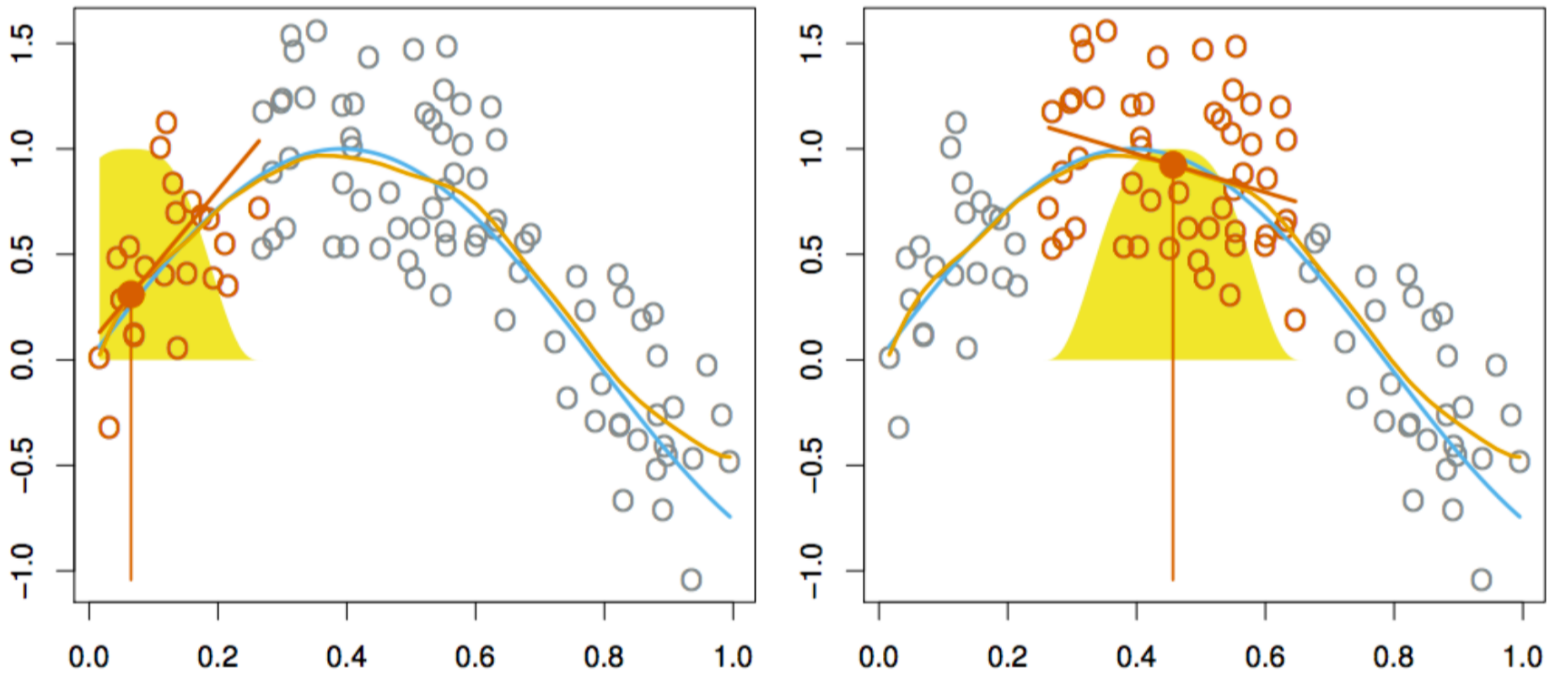
- Smoothing Splines



$$\min_g \sum_{i=1}^{n} (Y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

Other ways to get “non linear regressions”

- Local Regression (LOESS)



Other ways to get "non linear regressions"

- Generalized Additive Models

$$y_i = \beta_0 + f_1(x_{i1}) + f_2(x_{i2}) + \cdots + f_p(x_{ip}) + \epsilon_i.$$