

Regression

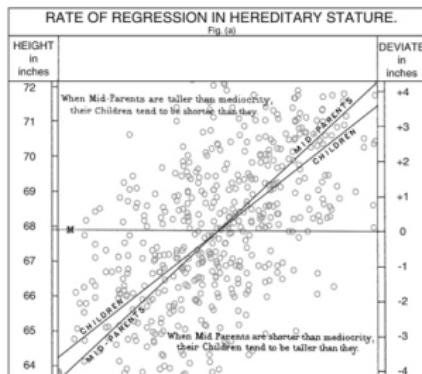
Schwartz

September 30, 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

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

Linear Models and Regression Terminology

Outcome / Response / Label / Dependent/Endogenous Var.

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

Linear Models and Regression Terminology

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Intercept

Linear Models and Regression Terminology

Coefficient

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Linear Models and Regression Terminology

Coefficient

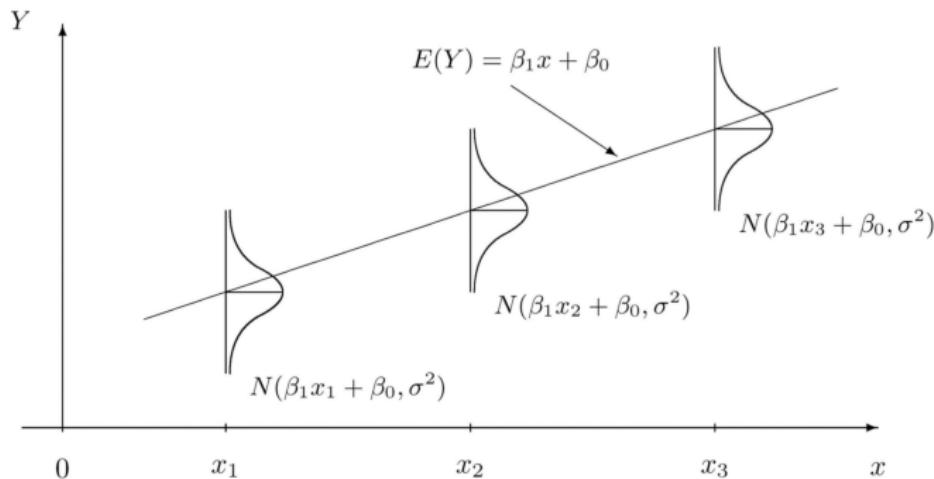
- $Y_i = \beta_0 + x_i \beta_1 + \epsilon_i, \epsilon_i \stackrel{i.i.d.}{\sim} Normal(0, \sigma^2)$
Intercept Error/Noise

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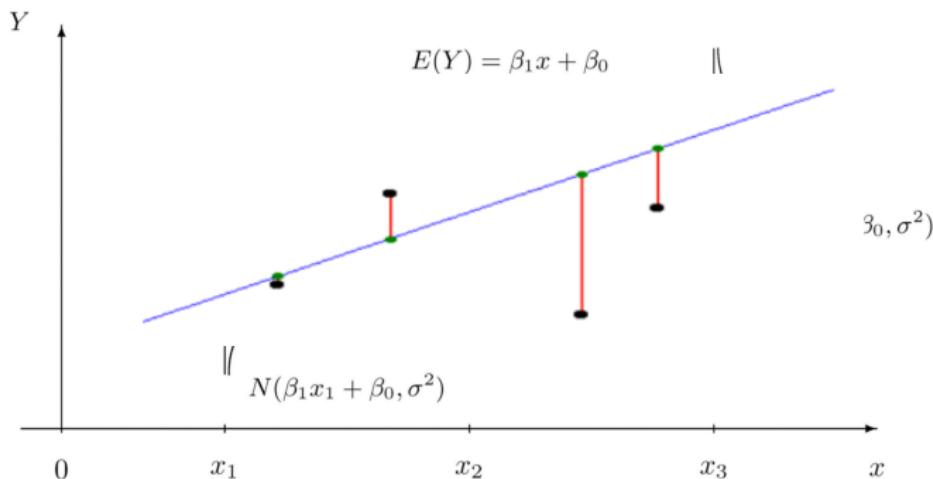


Linear Models and Regression Terminology

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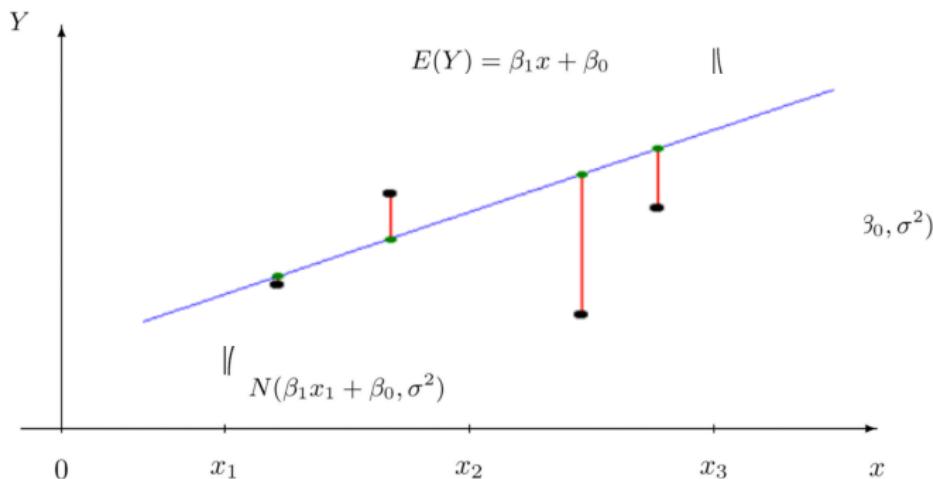
$$\blacktriangleright Y_i = \hat{\beta}_0 + x_i \hat{\beta}_1 + \hat{\epsilon}_i, \quad \hat{\sigma}^2 = \frac{\sum_{i=1}^n \hat{\epsilon}_i^2}{n-p-1} \quad (p = \# \text{of coefficients})$$

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Fitted/Predicted value \hat{Y}_i

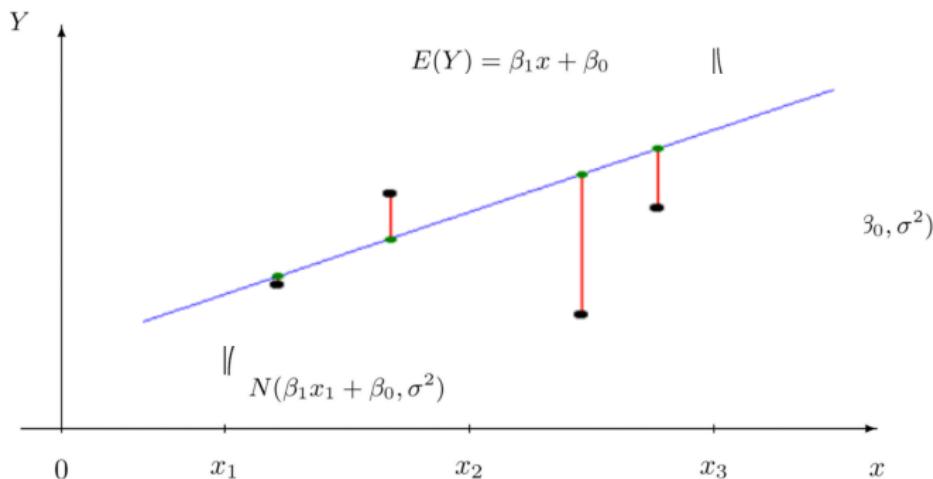
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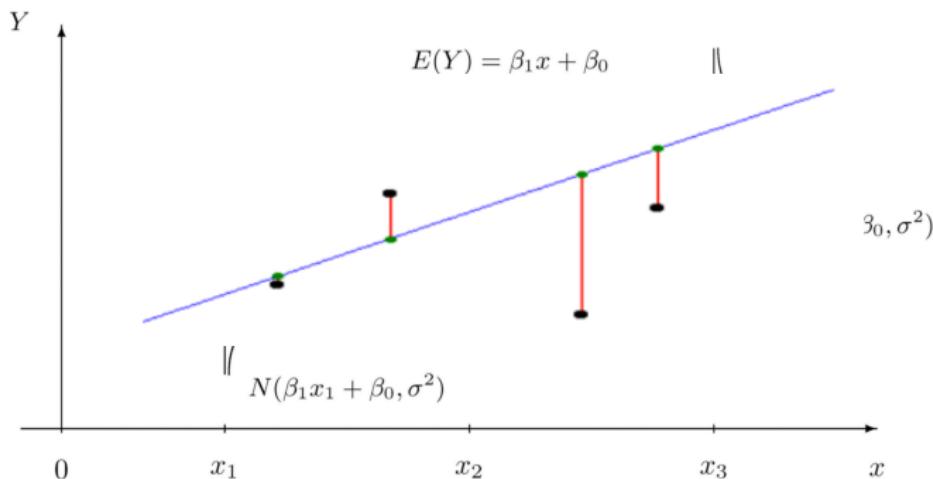
Residual

Linear Models and Regression Terminology

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

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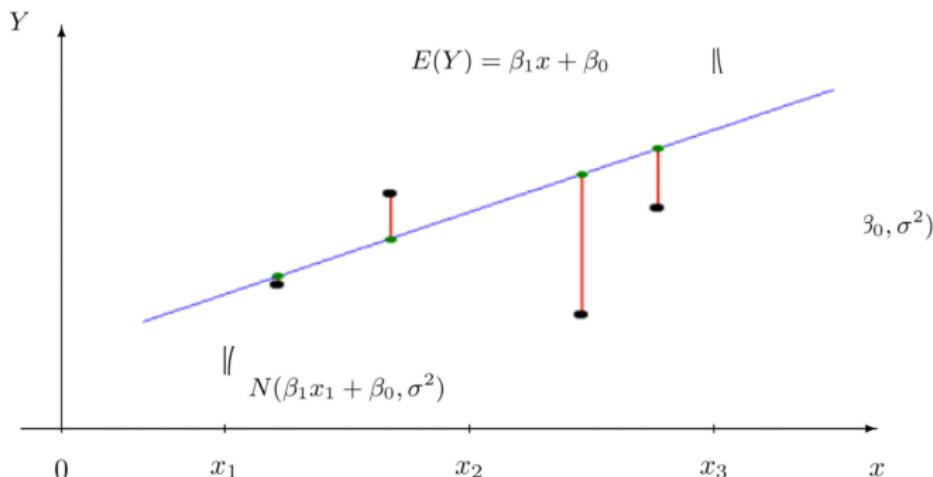
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Residual

Quiz: what are these things and their parts?

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

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

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

Least Squares Fit

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

Least Squares Fit

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

$$[\hat{\beta}_0, \hat{\beta}_1] = \underset{[\beta_0, \beta_1]}{\operatorname{argmin}} \sum_{i=1}^n \hat{\epsilon}_i^2 = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^n (Y_i - \mathbf{x}_i^T \beta)^2$$

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

Least Squares Fit

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$$\sum_{i=1}^n (Y_i - \mathbf{x}_i^T \beta)^2 = (\mathbf{Y} - \mathbf{x}\beta)^T (\mathbf{Y} - \mathbf{x}\beta)$$

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

Least Squares Fit

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

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

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

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

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

Least Squares Fit *bonus*

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

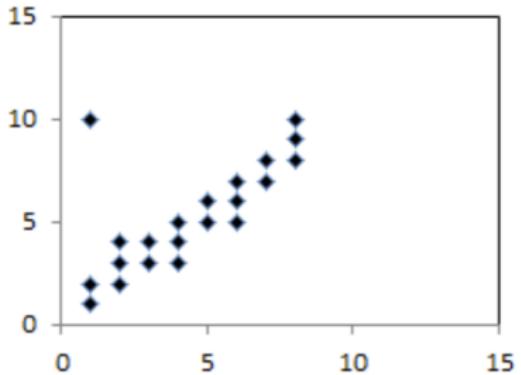
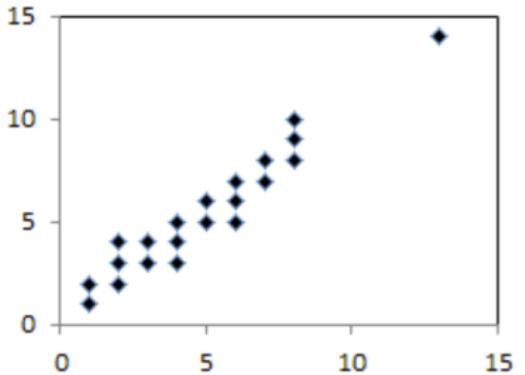
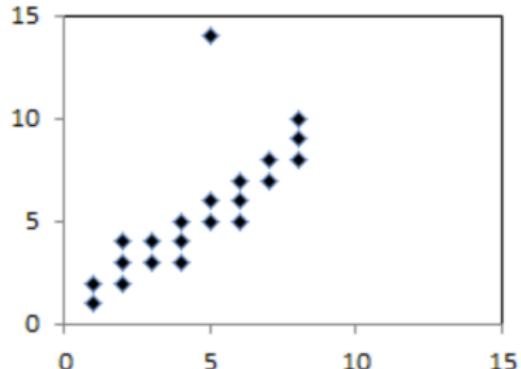
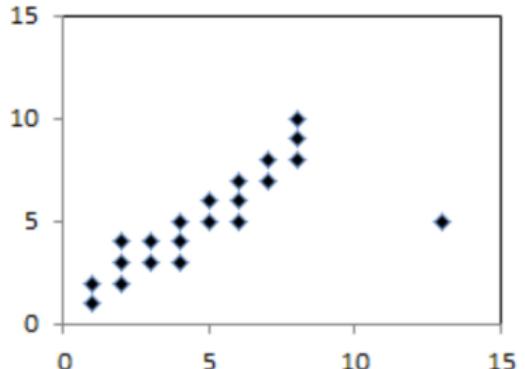
$$\begin{aligned} & \underset{\beta}{\operatorname{argmax}} \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(Y_i - \mathbf{x}_i^T \beta)^2} \\ &= \underset{\beta}{\operatorname{argmax}} (2\pi\sigma^2)^{-\frac{n}{2}} e^{-\frac{1}{2\sigma^2}(\mathbf{Y} - \mathbf{x}\beta)^T(\mathbf{Y} - \mathbf{x}\beta)} \\ &= \underset{\beta}{\operatorname{argmax}} -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\mathbf{Y} - \mathbf{x}\beta)^T(\mathbf{Y} - \mathbf{x}\beta) \\ &= \underset{\beta}{\operatorname{argmin}} (\mathbf{Y} - \mathbf{x}\beta)^T(\mathbf{Y} - \mathbf{x}\beta) \quad [\text{same as least squares!!}] \end{aligned}$$

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

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

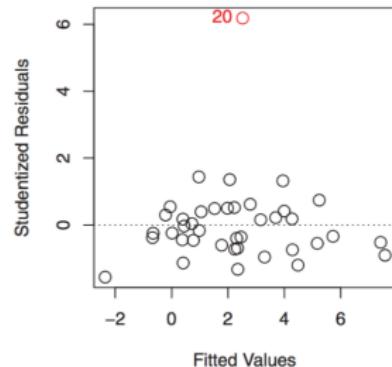
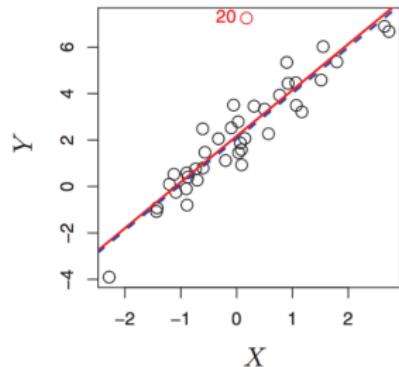
$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (Y_i - \bar{Y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{R_{xY} S_Y}{S_x}$$

What makes these data points “unusual”?



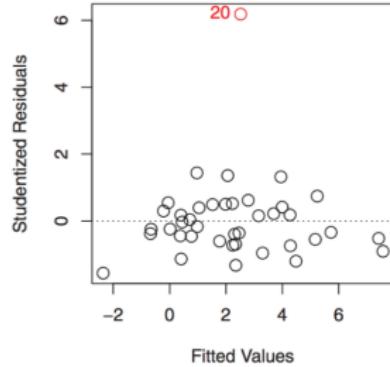
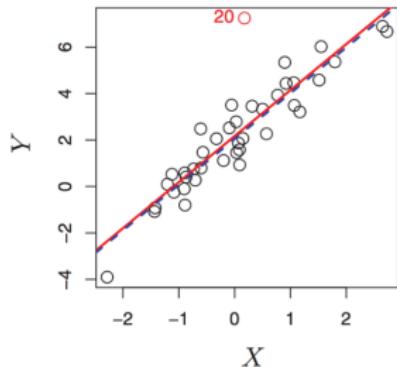
Regression Diagnostics

Outliers

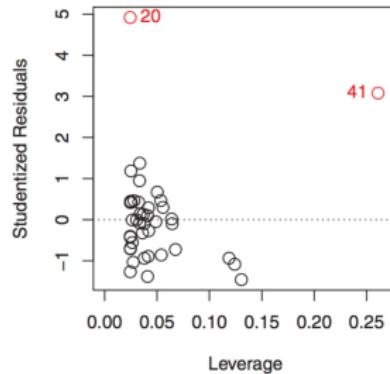
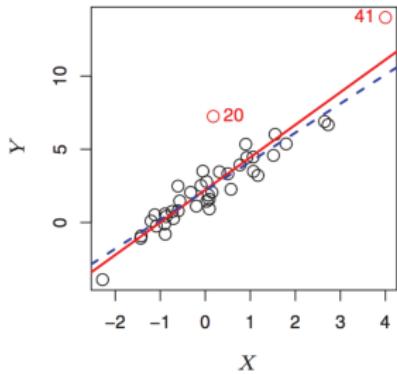


Regression Diagnostics

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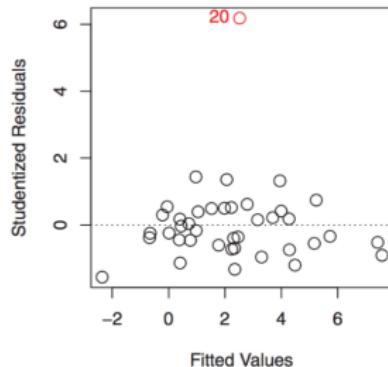
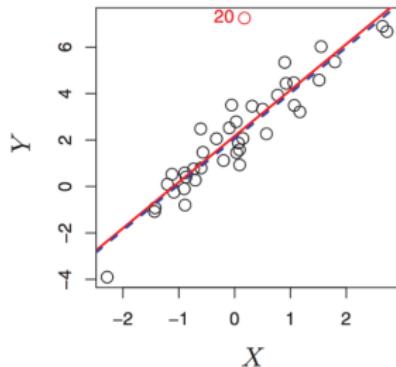


High Leverage Points

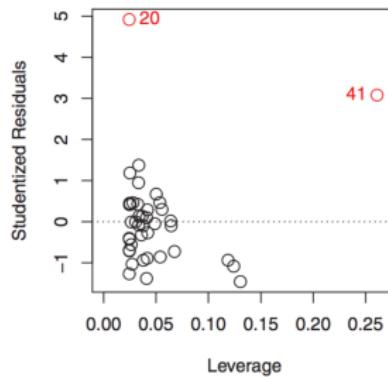
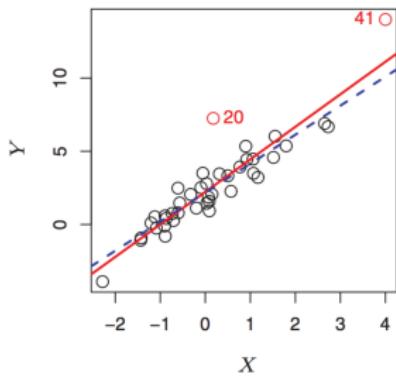


Regression Diagnostics

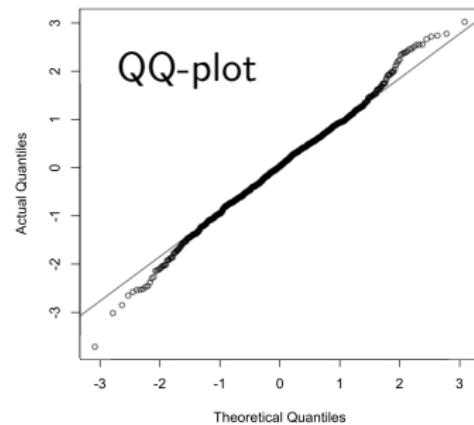
Outliers impact residual variance estimates



High Leverage Points impact prediction estimates

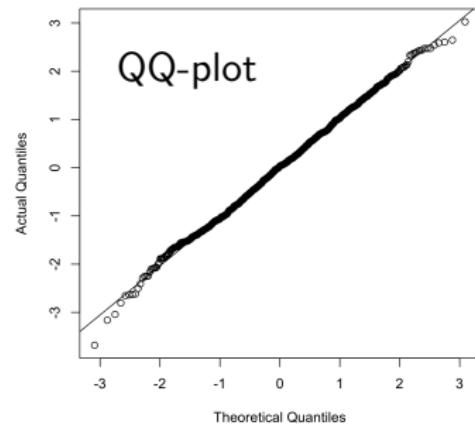


Regression Diagnostics (with residuals)



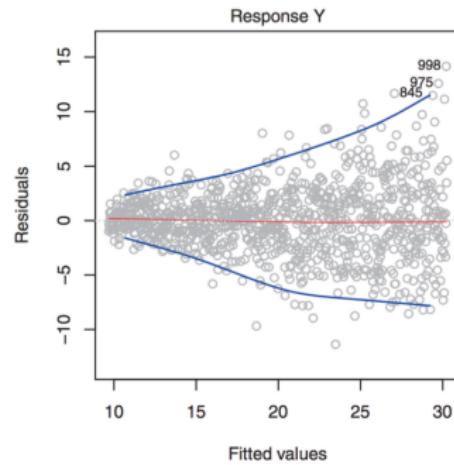
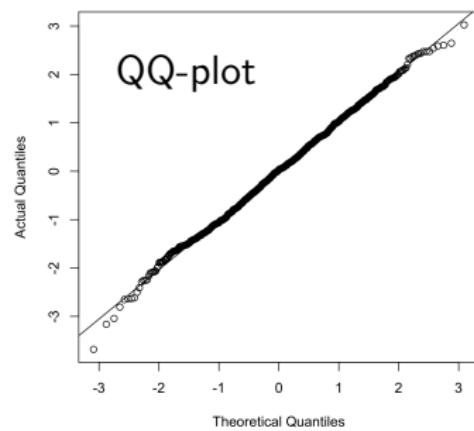
- ▶ What's wrong with the residual distribution?

Regression Diagnostics (with residuals)



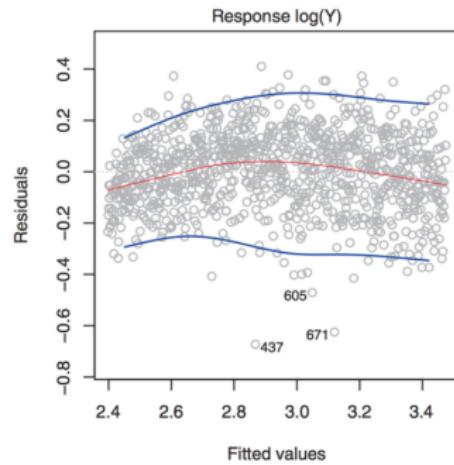
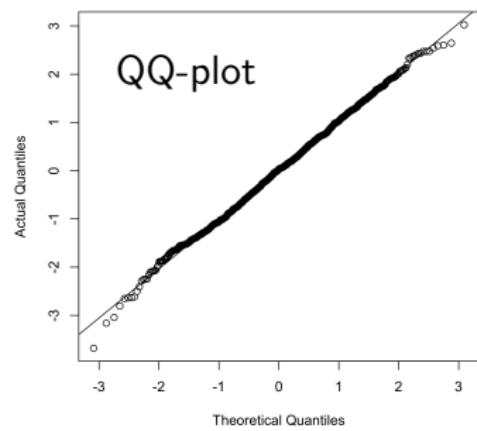
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Regression Diagnostics (with residuals)



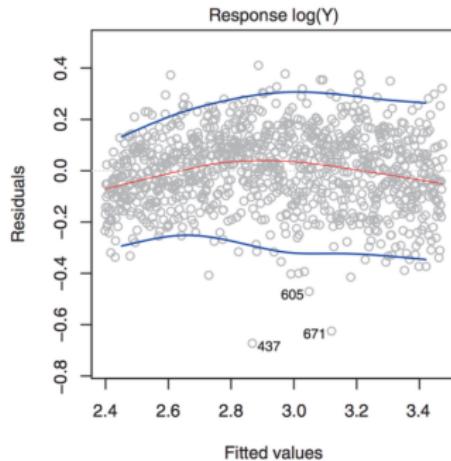
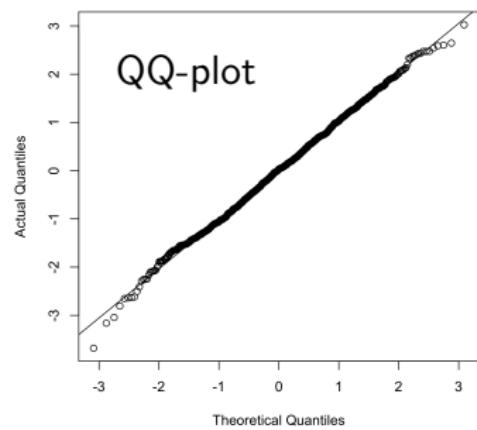
- ▶ What's wrong with the residual distribution?
- ▶ What's wrong with the residual variance?

Regression Diagnostics (with residuals)

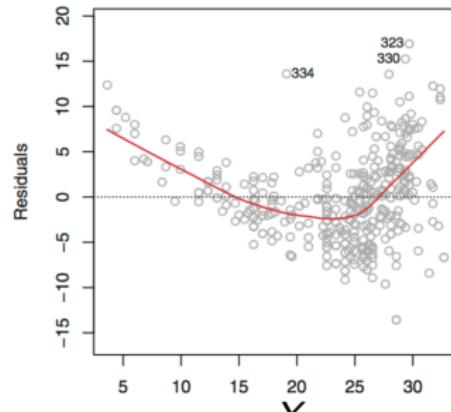


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- ▶ What's wrong with the residual variance?

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*” \mathbf{Y} projecting \mathbf{Y} onto the (least squares) closest vector to \mathbf{Y} in the column space of \mathbf{x} , $\hat{\mathbf{Y}} \in \mathcal{R}(\mathbf{x})$

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

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

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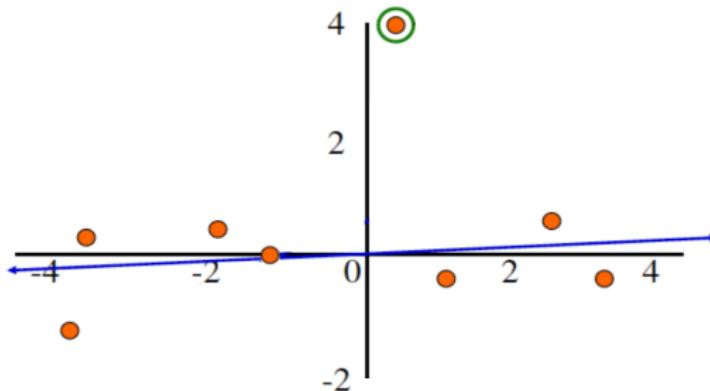
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- ▶ Diagonal element $H_{ii} \in [0, 1]$, and $\sum_{i=1}^n H_{ii} = \text{rank}(\mathbf{x})$
 H_{ii} is called the *leverage* of observation i

Leverage: So high or low leverage?

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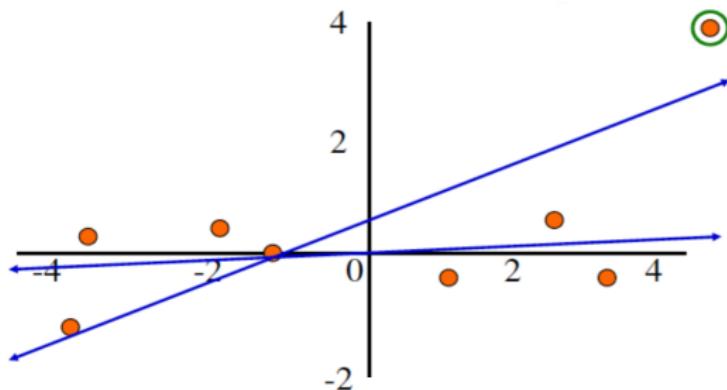


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- ▶ H_{ii} shows much \hat{Y}_i depends on Y_i
which depends on the “extremeness” of x_i

Leverage: And now high or low leverage?

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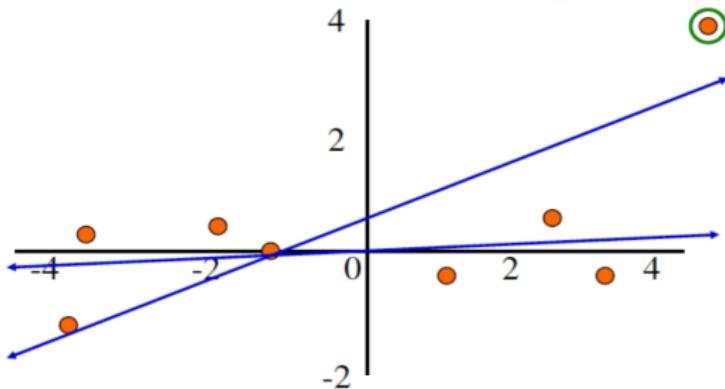


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Leverage

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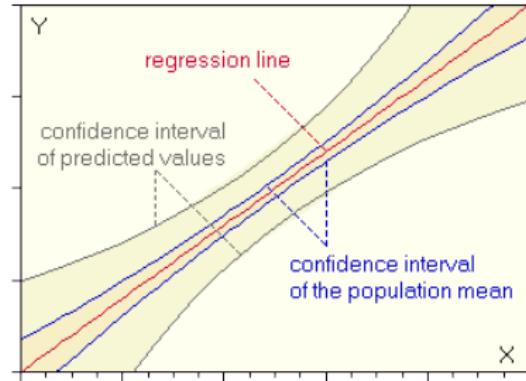


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- ▶ H_{ii} shows much \hat{Y}_i depends on Y_i
which depends on the “extremeness” of x_i
- ▶ Relative comparison of H_{ii} 's id.'s “high leverage observations”

Influential Data Points

Studentized Residuals
have a t-distribution...

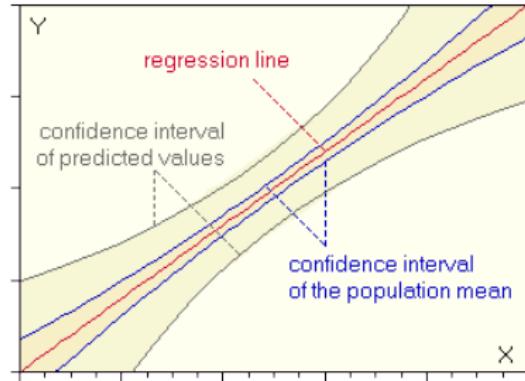
$$r_i = \frac{\hat{\epsilon}_i}{\hat{\sigma} \sqrt{1 - h_{ii}}}$$



Influential Data Points

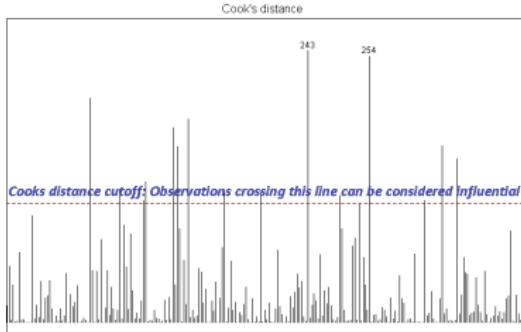
Studentized Residuals
have a t-distribution...

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



Cook's Distance is

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



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

Multivariate Regression

$$Y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i, \quad \epsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$$

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

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ \vdots \\ Y_n \end{bmatrix} = MVN \left(\begin{bmatrix} 1 & x_{11} \\ 1 & x_{12} \\ 1 & x_{13} \\ \vdots & \vdots \\ 1 & x_{1n} \end{bmatrix}, \begin{bmatrix} \beta_0 \\ \beta_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} \right)$$

- ▶ Regression is a (multivariate) normal distribution with a *linear model* component for the mean

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- ▶ Regression is a (multivariate) normal distribution with a *linear model* component for the mean
- ▶ Interpret: “vary one X and hold all others constant”?

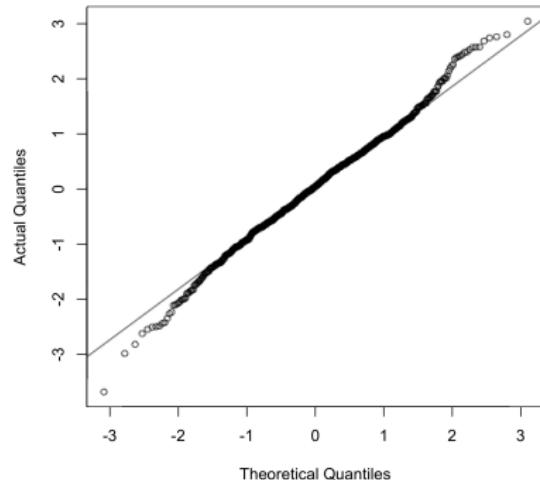
Assumptions, violations, and remedial measures

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i, \quad \epsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$$

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- ▶ Normality



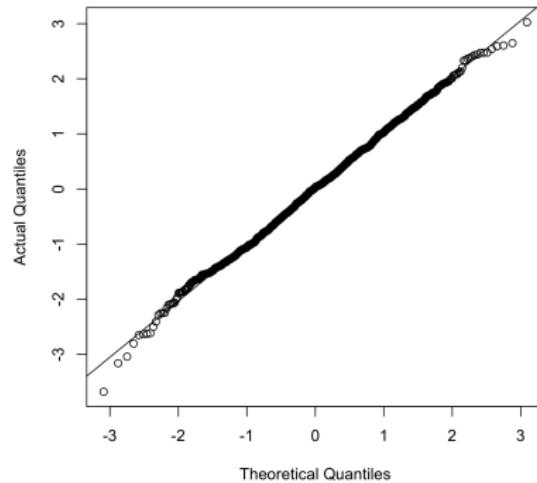
Q-Q Plot

Hypothesis testing depends on
distributional assumptions

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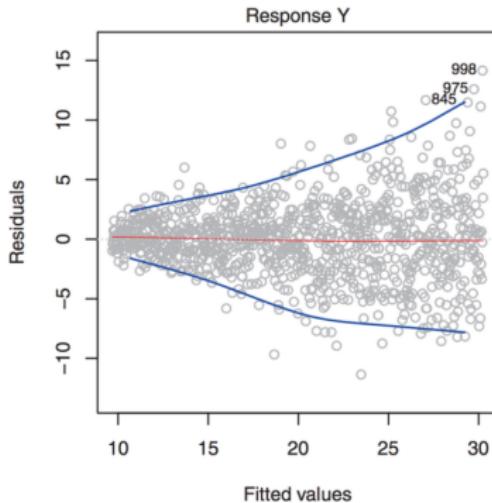
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- ▶ Normality
- ▶ Homoskedasticity



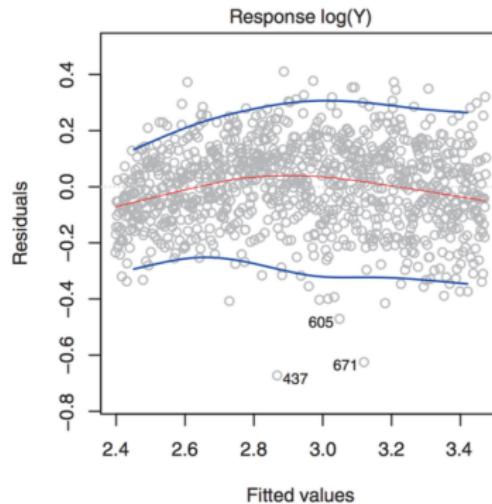
Residuals versus Fitted Values

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

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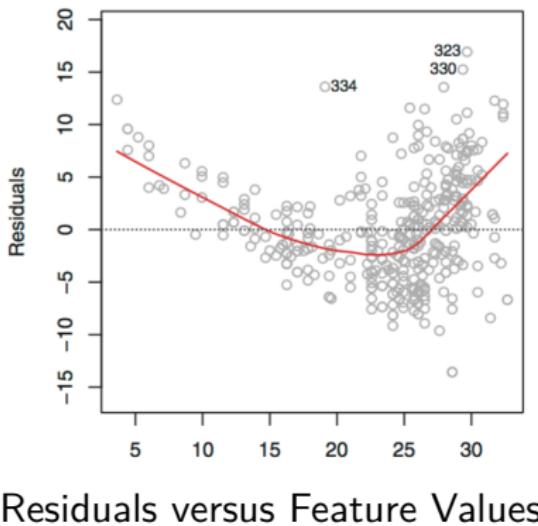
- ▶ Normality
- ▶ Homoskedasticity
- ▶ Independence

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

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- ▶ Normality
- ▶ Homoskedasticity
- ▶ Independence
- ▶ Linear form



“All models are wrong, some are useful”
– George Box

Assumptions, violations, and remedial measures

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i, \quad \epsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$$

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

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

Quiz: assumptions?

$$Y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i, \quad \epsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$$

- 1.
- 2.
- 3.
- 4.
- 5.

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but this is how **I want you to think about and remember and describe these assumptions**

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There are a number of ways these assumptions are characterized (i.e., differently in economics, e.g.)

but this is how **I want you to think about and remember and describe these assumptions**

so we just spent all this time looking at diagnostics and

Why care we so much this stuff??

Coefficients are Multivariate Normal (MVN)

$$\begin{aligned} f(\mathbf{Y}|\mathbf{x}, \boldsymbol{\beta}, \sigma^2) &= \prod_{i=1}^n f(Y_i|\mathbf{x}_i, \boldsymbol{\beta}, \sigma^2) \\ &= \prod_{i=1}^n N(\mathbf{x}_i^T \boldsymbol{\beta}, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(Y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2} \\ &= (2\pi\sigma^2)^{-\frac{n}{2}} e^{-\frac{1}{2\sigma^2}(\mathbf{Y} - \mathbf{x}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{x}\boldsymbol{\beta})} = MVN(\mathbf{x}\boldsymbol{\beta}, \sigma^2 I) \\ \\ \propto & e^{-\frac{1}{2\sigma^2}((\mathbf{x}^T \mathbf{x})^{-1} \mathbf{x}^T \mathbf{Y} - \boldsymbol{\beta})^T \mathbf{x}^T \mathbf{x} ((\mathbf{x}^T \mathbf{x})^{-1} \mathbf{x}^T \mathbf{Y} - \boldsymbol{\beta})} \\ &= e^{-\frac{1}{2\sigma^2}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \mathbf{x}^T \mathbf{x} (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})} \\ \implies & f(\hat{\boldsymbol{\beta}}|\mathbf{x}, \boldsymbol{\beta}, \sigma^2) = MVN\left(\boldsymbol{\beta}, \sigma^2(\mathbf{x}^T \mathbf{x})^{-1}\right) \end{aligned}$$

Multicollinearity and the Variance Inflation Factor (VIF)

And when you have any number of covariates (features)...

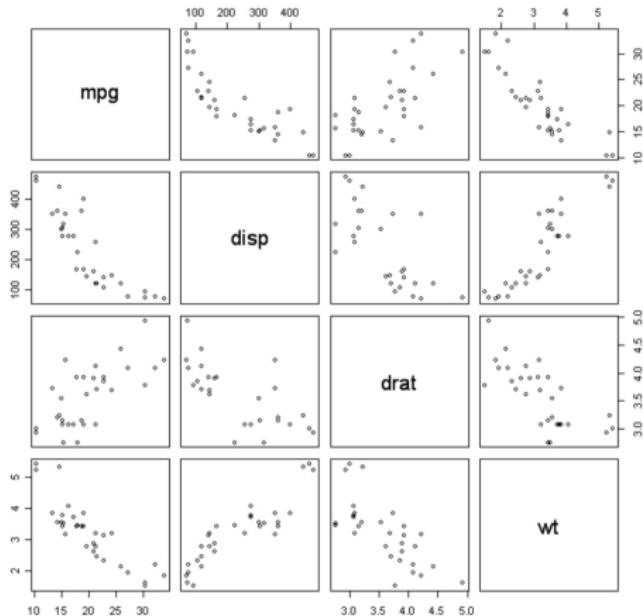
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Simple Scatterplot Matrix



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	DJIA	S&P 500	Nasdaq	Canada	Mexico	Brazil	Stoxx 50	FTSE 100	CAC 40	DAX	IBEX	Italy	Netherlands	Sweden	Switzerland	Nikkei	Hang Seng	Australia
DJIA		0.97	0.85	0.57	0.56	0.52	0.52	0.48	0.51	0.56	0.49	0.50	0.50	0.42	0.42	0.09	0.11	0.07
S&P 500	0.97		0.91	0.62	0.58	0.55	0.50	0.47	0.50	0.55	0.48	0.50	0.49	0.41	0.41	0.09	0.11	0.05
Nasdaq	0.85	0.91		0.58	0.56	0.52	0.48	0.43	0.48	0.54	0.47	0.48	0.48	0.42	0.38	0.14	0.16	0.07
Canada	0.57	0.62	0.58		0.53	0.53	0.42	0.45	0.41	0.41	0.42	0.42	0.39	0.37	0.35	0.17	0.22	0.17
Mexico	0.56	0.58	0.56	0.53		0.56	0.42	0.42	0.44	0.43	0.43	0.44	0.39	0.38	0.38	0.17	0.25	0.17
Brazil	0.52	0.55	0.52	0.53	0.56		0.33	0.35	0.32	0.34	0.34	0.34	0.29	0.30	0.28	0.17	0.22	0.15
Stoxx 50	0.52	0.50	0.48	0.42	0.42	0.33		0.92	0.94	0.89	0.87	0.88	0.92	0.78	0.86	0.26	0.30	0.24
FTSE 100	0.48	0.47	0.43	0.45	0.42	0.35	0.92		0.86	0.80	0.80	0.82	0.84	0.73	0.78	0.26	0.30	0.26
CAC 40	0.51	0.50	0.48	0.41	0.44	0.32	0.94	0.86		0.89	0.88	0.89	0.92	0.78	0.84	0.28	0.32	0.25
DAX	0.56	0.55	0.54	0.41	0.43	0.34	0.89	0.80	0.89		0.83	0.84	0.86	0.75	0.77	0.26	0.29	0.21
IBEX	0.49	0.48	0.47	0.42	0.43	0.34	0.87	0.80	0.88	0.83		0.84	0.83	0.75	0.77	0.27	0.32	0.26
Italy	0.50	0.50	0.48	0.42	0.44	0.34	0.88	0.82	0.89	0.84	0.84		0.85	0.74	0.78	0.24	0.29	0.23
Netherlands	0.50	0.49	0.48	0.39	0.39	0.29	0.92	0.84	0.92	0.86	0.83	0.85		0.75	0.82	0.27	0.30	0.23
Sweden	0.42	0.41	0.42	0.37	0.38	0.30	0.78	0.73	0.78	0.75	0.75	0.74	0.75		0.75	0.29	0.33	0.27
Switzerland	0.42	0.41	0.38	0.35	0.38	0.28	0.86	0.78	0.84	0.77	0.77	0.78	0.82	0.75		0.29	0.32	0.29
Nikkei	0.09	0.09	0.14	0.17	0.17	0.26	0.26	0.28	0.26	0.27	0.24	0.27	0.29	0.29		0.52	0.49	
Hang Seng	0.11	0.11	0.16	0.22	0.25	0.22	0.30	0.30	0.32	0.29	0.32	0.29	0.30	0.33	0.32	0.52		0.48
Australia	0.07	0.05	0.07	0.17	0.17	0.15	0.24	0.26	0.25	0.21	0.26	0.23	0.23	0.27	0.29	0.49	0.48	

Multicollinearity and the Variance Inflation Factor (VIF)

And when you have any number of covariates (features)...

$$\hat{\beta} \sim MVN\left(\beta, \sigma^2(\mathbf{x}^T \mathbf{x})^{-1}\right)$$

$$\widehat{\text{Var}}[\hat{\beta}_j] = \frac{\hat{\sigma}^2}{(n - 1)\widehat{\text{Var}}[X_j]} \cdot \frac{1}{1 - R_j^2} \quad [\text{VIF}]$$

where R_j^2 is the R^2 of X_j regressed on all the other X 's

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Centering X 's can decorrelate X and X^2 ...

Scaling X 's (to the same scale) numerically stabilizes the condition number

Half time

Assessing Model Fit (more Machine Learning-ish)

Residual Sum of Squares

$$RSS = \sum(Y_i - \hat{Y}_i)^2 = \sum \hat{\epsilon}_i^2$$

Total Sum of Squares

$$\begin{aligned} TSS &= \sum(Y_i - \bar{Y})^2 \\ &= \sum(\hat{Y}_i - \bar{Y})^2 + RSS \end{aligned}$$

Residual Standard Deviation

$$\begin{aligned} \hat{\sigma} &= \sqrt{\frac{1}{n-p-1} RSS} \\ &= \sqrt{\frac{\sum(Y_i - \hat{Y}_i)^2}{n-p-1}} \end{aligned}$$

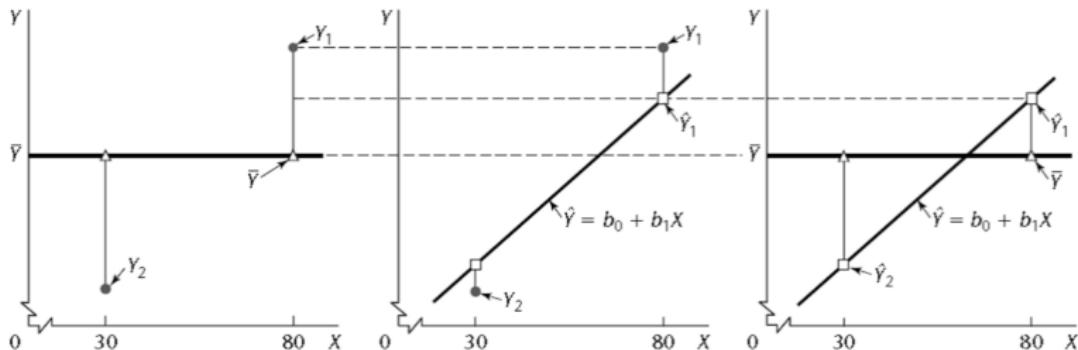
Proportion of Variance Explained

$$\begin{aligned} R^2 &= \frac{TSS - RSS}{TSS} \\ &= 1 - \frac{RSS}{TSS} \end{aligned}$$

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



$$\begin{aligned} TSS &= \sum(Y_i - \bar{Y})^2 = \sum(Y_i - \hat{Y}_i + \hat{Y}_i - \bar{Y})^2 \\ &= \sum(Y_i - \hat{Y}_i)^2 + 2\sum(Y_i - \hat{Y}_i)(\hat{Y}_i - \bar{Y}) + \sum(\hat{Y}_i - \bar{Y})^2 \\ &= \sum(Y_i - \hat{Y}_i)^2 + 2\sum\hat{\epsilon}_i(\hat{Y}_i - \bar{Y}) + \sum(\hat{Y}_i - \bar{Y})^2 \\ &\quad \sum\hat{\epsilon}_i = 0 \uparrow \uparrow \sum\hat{\epsilon}_i \hat{Y}_i = 0 \\ &= \sum(Y_i - \hat{Y}_i)^2 + \sum(\hat{Y}_i - \bar{Y})^2 = RSS + \sum(\hat{Y}_i - \bar{Y})^2 \end{aligned}$$

MODEL SELECTION!!!

- ▶ R^2 (model fit) is insufficient – more features means larger R^2

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

$$\text{Mallow's } C_p = \frac{1}{n}(RSS + 2p\hat{\sigma}^2)$$

$$AIC = -2 \log L + 2p$$

$$BIC = -2 \log L + p \log n$$

$$\text{Adjusted } R^2 = 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)}$$

$$D_M = -2 \log f(Y|\hat{\theta}^{M_p}) + 2 \log f(Y|Y)$$

$$D_M \stackrel{\text{approx.}}{\sim} \chi^2_{n-p-1}$$

Assessing Parameter Uncertainty (definitely Statistics)

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

$$f(\hat{\beta} | \beta, \sigma^2, \mathbf{x}) = MVN\left(\beta, \sigma^2(\mathbf{x}^T \mathbf{x})^{-1}\right)$$

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

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(where p is the number of coefficients) then we have that

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

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

Hypothesis Testing for Feature Selection

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

$F \sim F_{p,n-p-1}$ (tests if any coefficient is *non-zero*)

$\frac{\hat{\beta}_i - \beta_i}{\widehat{SD}(\hat{\beta}_i)} \sim t_{n-p-1}$ (tests if a *specific* coefficient is non-zero*)

*in the presence of all the others (this is a “last-in” test)

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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
x1	0.4687	0.026	17.751
x2	0.4836	0.104	4.659
x3	-0.0174	0.002	-7.507
const	5.2058	0.171	30.405

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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*in the presence of all the others (this is a “last-in” test)

- ▶ Forward Selection

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
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const	5.2058	0.171	30.405	0.000	4.861 5.550

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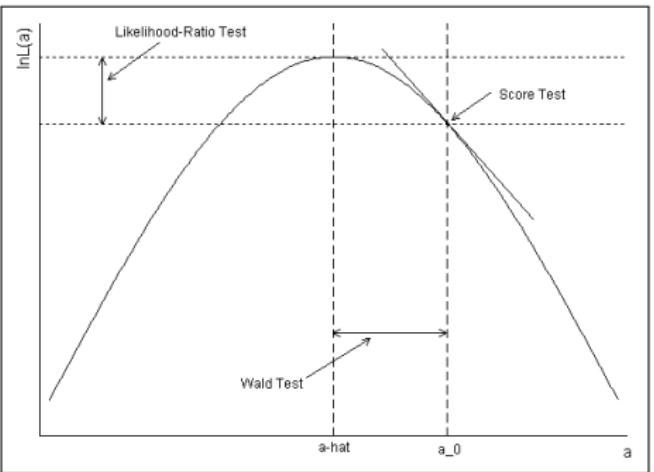
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- ▶ Backward Selection

- ▶ Both

Testing: other flavors



Wald test

$$\sqrt{\frac{(\hat{\theta} - \theta_0)^2}{\text{Var}(\hat{\theta})}} \underset{\text{approx.}}{\sim} N(0, 1) \text{ under } H_0$$

Likelihood-Ratio (LR) test

$$-2 \ln \left(\frac{L(\theta_0|x)}{L(\theta|x)} \right) \underset{\text{approx.}}{\sim} \chi_k^2 \text{ under } H_0$$

Score test

$$\frac{\left(\frac{\partial}{\partial \theta} \log L(\theta_0|x) \right)^2}{-\mathbb{E} \left[\frac{\partial^2}{\partial \theta^2} \log L(\theta_0|x) \right]} \underset{\text{approx.}}{\sim} \chi_1^2 \text{ under } H_0$$

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

Testing: demonstrated in simple linear regression

$$f(\mathbf{Y}|\mathbf{x}, \beta, \sigma^2) = MVN(\mathbf{x}\beta, \sigma^2 I)$$
$$\implies f(\hat{\beta}|\mathbf{x}, \beta, \sigma^2) = MVN\left(\beta, \sigma^2(\mathbf{x}^T \mathbf{x})^{-1}\right)$$

For simple linear regression then

$$\hat{\beta} \sim MVN\left(\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \frac{\sigma^2}{n \sum (x_i - \bar{x})^2} \begin{bmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{bmatrix}\right)$$

where

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x} \quad \hat{\beta}_1 = \frac{\sum_{i=1}^n (Y_i - \bar{Y})(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{R_{xY} S_Y}{S_x}$$

$$\text{Var}(\hat{\beta}_1) = \sigma^2 \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad \text{Var}(\hat{\beta}_0) = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right]$$

$$\text{SD}(\hat{\beta}_0) = \sqrt{\text{Var}(\hat{\beta}_0)} \quad \text{SD}(\hat{\beta}_1) = \sqrt{\text{Var}(\hat{\beta}_1)}$$

Testing: extra credit

- ▶ What is $\text{Var}(\hat{Y}_0)$? (Suppose we know σ^2)

Hint: $\hat{Y}_0 = \hat{\beta}_0 + x_0\hat{\beta}_1$

Hint: $\text{Var}[aX + bY] = ?$

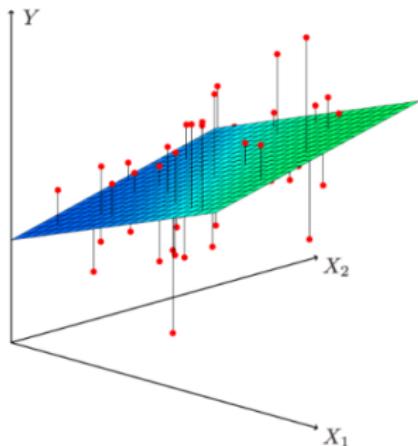
- ▶ $\text{Var}(Y_0)$? For a *new observation* Y_0 according to our model?
(Suppose we know σ^2)
- ▶ *Hint:* $Y_0 = \hat{\beta}_0 + \hat{\beta}_1x_0 + \epsilon$

Linear Models

- ▶ Linear model... that sounds too simple...

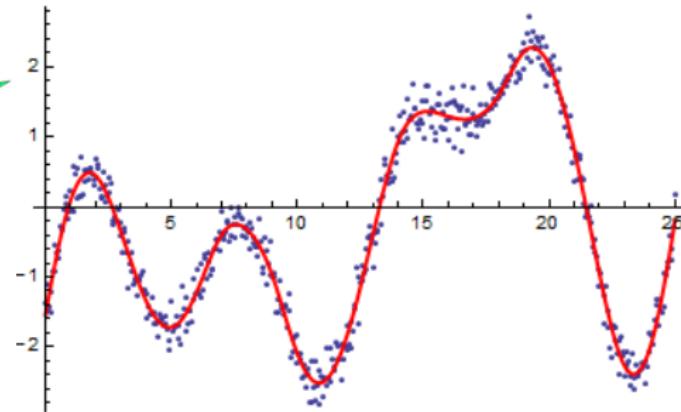
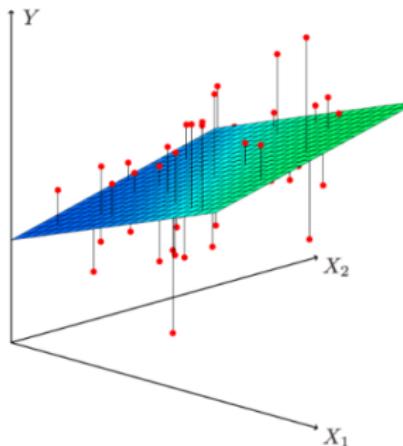
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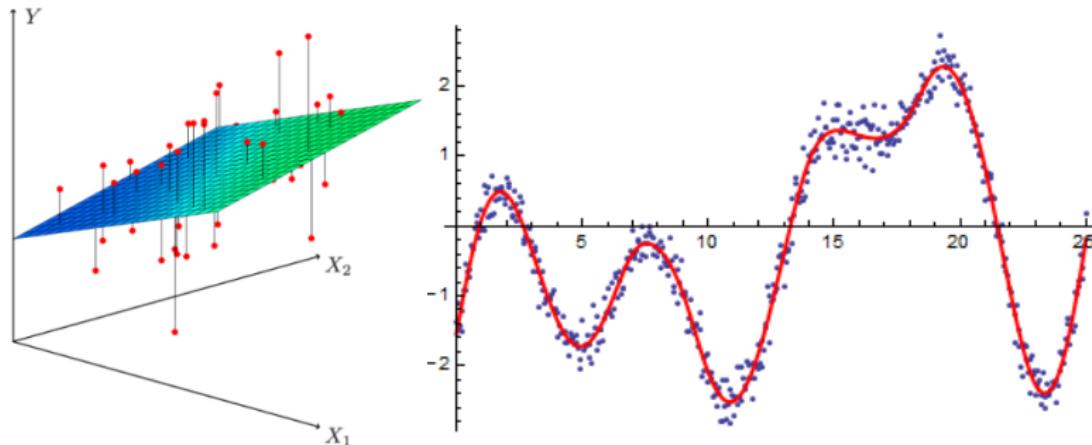
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Linear Models

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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...

Features that produce “non-linear” response surfaces?

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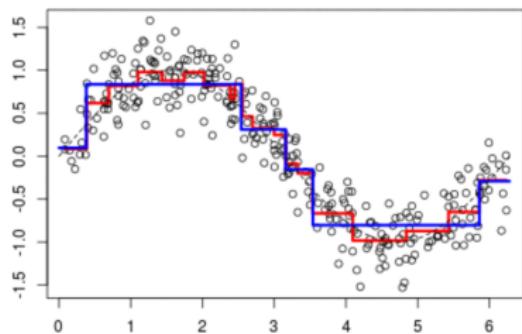
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- ▶ Step functions

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

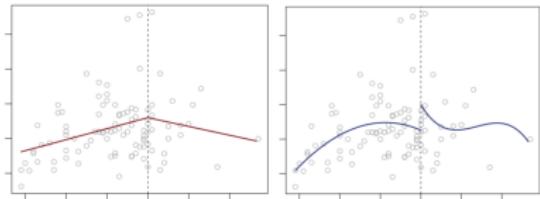


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- ▶ Step functions
- ▶ Regression Splines



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

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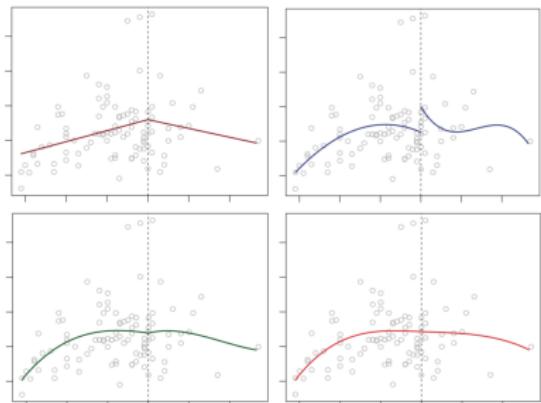
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$$h(X_i, \xi) = \begin{cases} (x - \xi)^3 & : \text{if } X_i > \xi \\ 0 & : \text{if } X_i \leq \xi \end{cases}$$

basis functions & knots

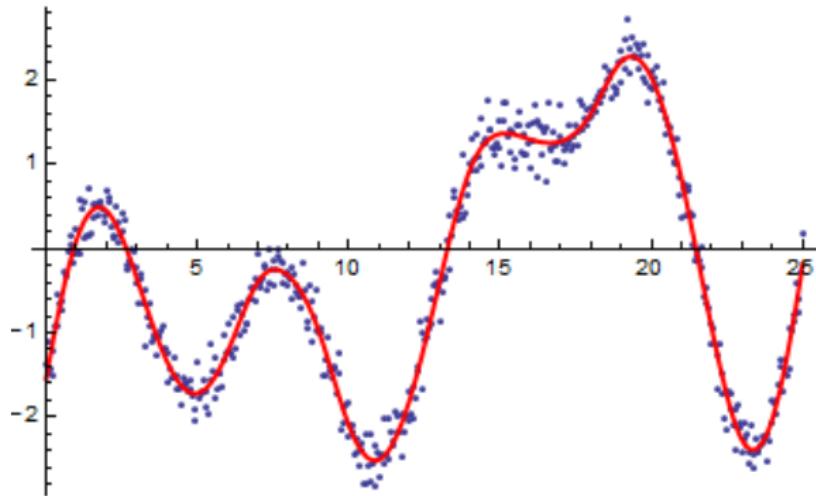
$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 + \beta_{s1} h(X_i, \xi_1) + \dots + \epsilon_i$$



Linear models aren't really so “linear”

Other ways to get “non linear regressions”

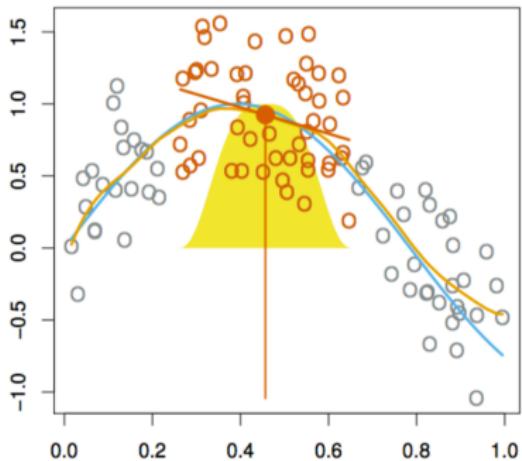
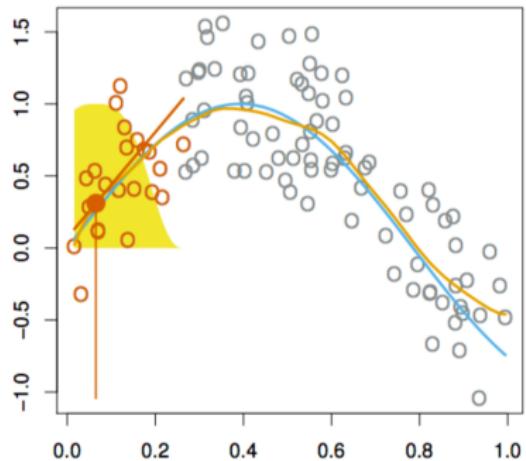
- ▶ Smoothing Splines



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

Other ways to get “non linear regressions”

- ▶ Local Regression (LOESS)



Other ways to get “non linear regressions”

- ▶ Generalized Additive Models

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

