# Regression

Schwartz

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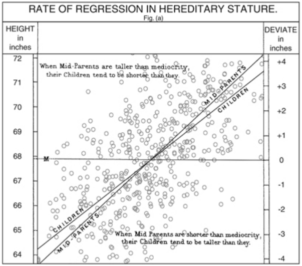
# The Sophomore Slump

...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. 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

- Terminology
- Least squares fit
- Normal distribution theory
- Coefficient testing
- Linear models and Multiple variables and Alternatives
- Model fit and Model selection
- Model diagnostics and Model evaluation

# Terminology

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

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Coefficient

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Intercept Error Noise

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

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Fitted value Residual

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Residual Standard Error (RSE)

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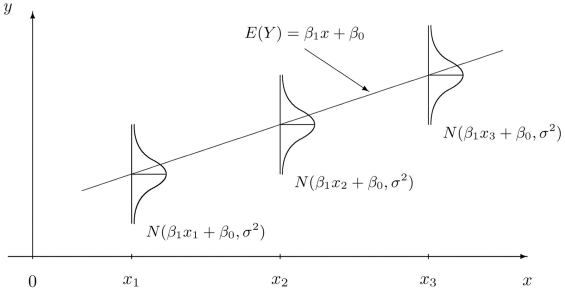


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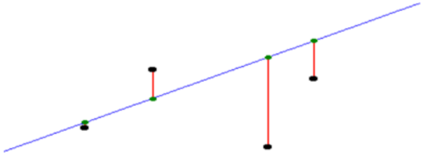

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where $\mathbf{x}_i^T = [1, x_i]$ and $\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$

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

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

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

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

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

# Least Squares Fit *bonus*

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

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

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

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2. Maximum likelihood estimation (MLE) is equivalent

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

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

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

$$= \underset{\beta}{argmin}(\mathbf{Y} - \mathbf{x}_i\beta)^T(\mathbf{Y} - \mathbf{x}\beta)$$

# The *Multivariate Normal Distribution* (MVN)

$$f(\mathbf{Y}|\mathbf{x}, \beta, \sigma^2) = \prod_{i=1}^{n} f(Y_i|\mathbf{x}_i, \beta, \sigma^2)$$

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

$$f(\mathbf{Y}|\mathbf{x}, \beta, \sigma^2) = MVN(\mathbf{x}\beta, \sigma^2 I)$$

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For simple linear regression then

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

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where

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

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

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

# Testing *Extra Credit I*

- What is $\mathrm{Var}(\hat{Y}_0)$? (Suppose we know $\sigma^2$)

- *Hint:* $\hat{Y}_0 = \hat{\beta}_0 + x_0\hat{\beta}_1$
- *Hint:* $Var[aX + bY] = ?$

# Testing *Extra Credit II*

- $\mathrm{Var}(Y_0)$? For a *new observation* $Y_0$ according to our model?
  (Suppose we know $\sigma^2$)

- *Hint:* $Y_0 = \hat{\beta}_0 + \hat{\beta}_1 x_0 + \epsilon$

# A SERIOUSLY MAJOR TRANSITION JUST HAPPENED

And you didn't even notice

# Coefficient Testing

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

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

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and if we estimate

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

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

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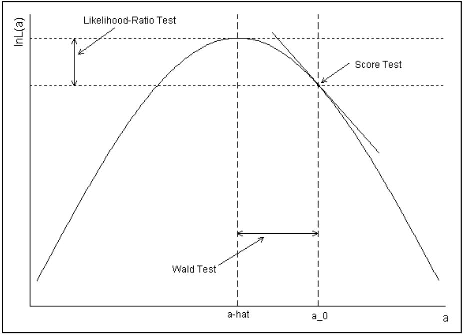
And this works for any number of covariates...

# More Coefficient Testing




Wald test

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

Likelihood-Ratio (LR) test

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

Score test

$$\frac{\left(\frac{\partial}{\partial\theta}\log L(\theta_0|x)\right)^2}{-\mathrm{E}\left[\frac{\partial^2}{\partial\theta^2}\log L(\theta_0|x)\right]} \overset{approx.}{\sim} \chi^2_1 \text{ under } H_0$$

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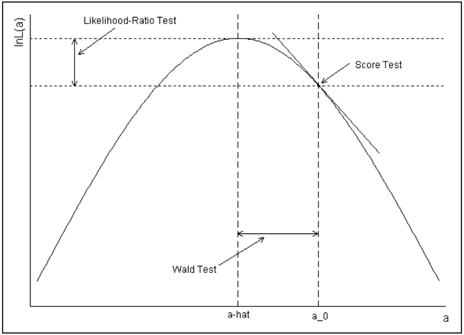


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# Multicollinearity and the Variance Inflation Factor (VIF)

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

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

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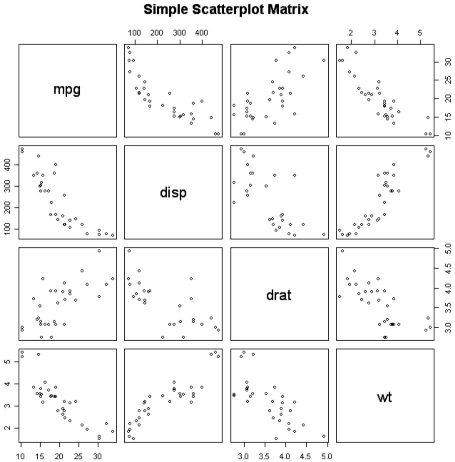

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| | DJIA | S&P 500 | Nasdaq | Canada | Mexico | Brazil | Stoxx 50 | FTSE 100 | CAC 40 | DAX | IBEX | Italy | Netherlands | Sweden | Switzerland | Nikkei | Hang Seng | Australia |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **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 | 0.17 | 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)...

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

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

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

# Multivariate Regression

That seriously major transition that just happened that you didn't even notice?

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

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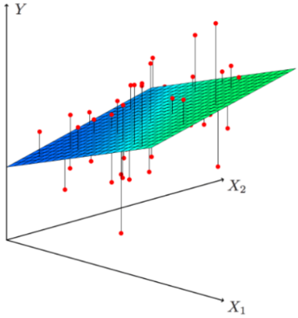

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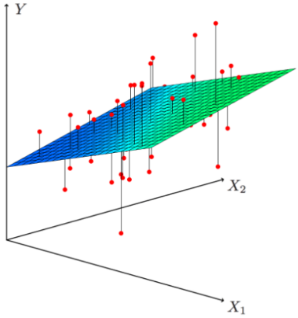


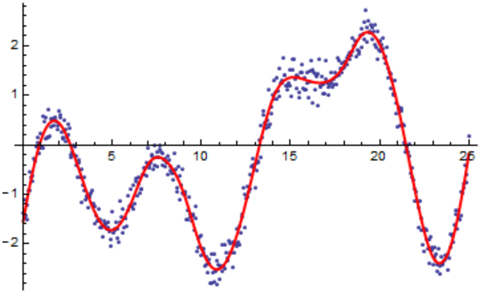

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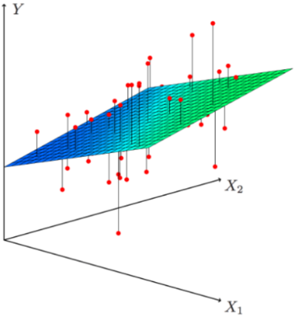


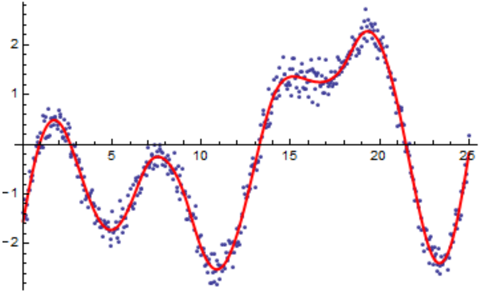


- "Linear" models are only linear in the coefficients

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

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

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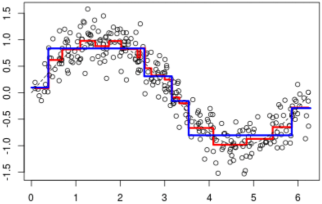
Step functions

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



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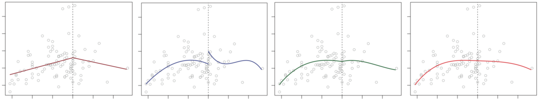

$$Y_i = \begin{cases} \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 + \epsilon_i & : if \;\; X_i \leq c \\ \beta_0^* + \beta_1 X_i + \beta_2^* X_i^2 + \beta_3^* X_i^3 + \epsilon_i & : if \;\; X_i > c \end{cases}$$

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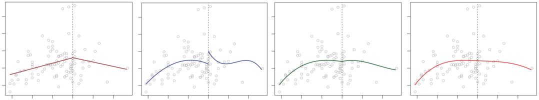

$$h(X_i, \xi) = \begin{cases} (x - \xi)^3 & : \mathit{if}\ X_i > \xi \\ 0 & : \mathit{if}\ X_i \leq \xi \end{cases} \qquad Y_i = \begin{array}{l} \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \beta_3 X_i^3 \\ + \beta_{s1} h(X_i, \xi_1) + \cdots + \epsilon_i \end{array}$$

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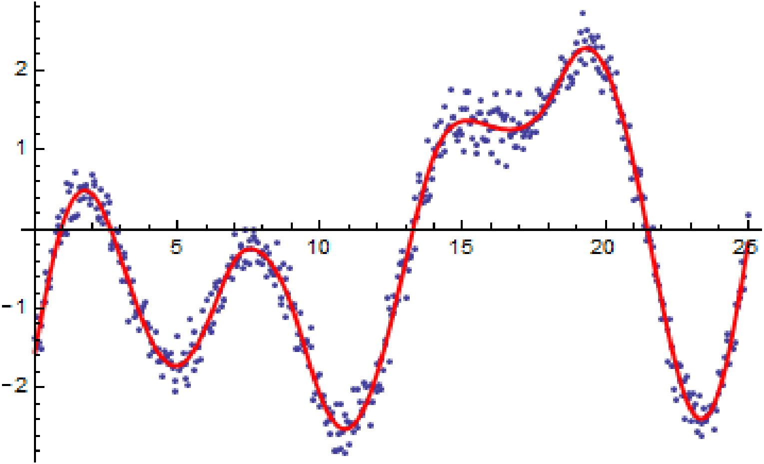
Step functions
Regression Splines
Smoothing Splines

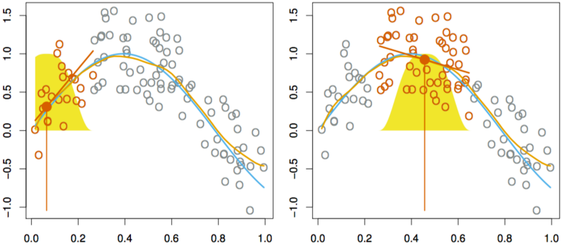
$$\min_g \sum_{i=1}^{n} (Y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

# Linear models aren't really so "linear"



# Other ways to get "non linear" response surfaces

- Local Regression (LOESS)



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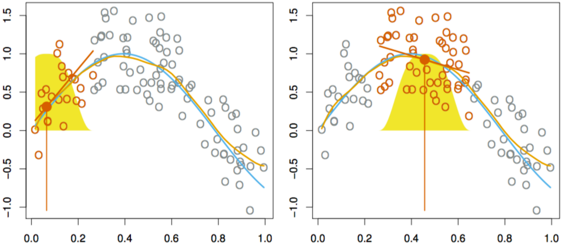
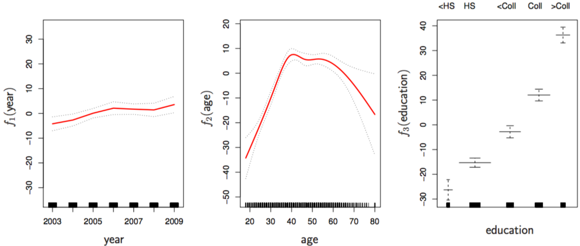



- Generalized Additive Models

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



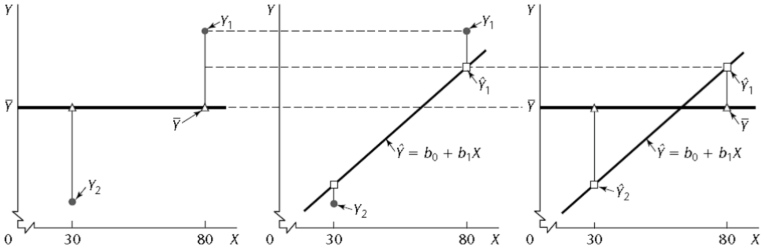
# Model Fit

| | |
|---|---|
| Residual Variation<br><br>$RSS = \sum(Y_i - \hat{Y}_i)^2 = \sum \hat{\epsilon}_i^2$ | Total Variation<br><br>$TSS = \sum(Y_i - \bar{Y})^2$<br>$= RSS + \sum(\hat{Y}_i - \bar{Y})^2$ |
| Residual Standard Error<br><br>$RSE = \sqrt{\frac{1}{n-p-1} RSS}$<br>$= \sqrt{\frac{\sum(Y_i - \hat{Y}_i)^2}{n-p-1}}$ | Proportion of Variance Explained<br><br>$R^2 = \frac{TSS-RSS}{TSS}$<br>$= 1 - \frac{RSS}{TSS}$ |

$F$-test

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

# 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\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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                            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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- Classical Model Selection Criterion

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

# Assumptions, violations, and remedial measures

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

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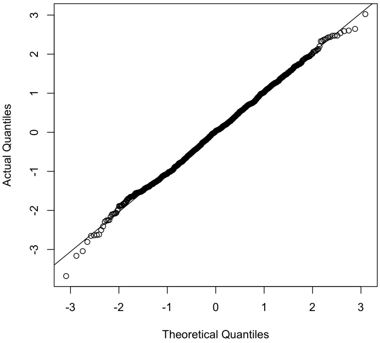


Q-Q Plot

Hypothesis testing depends on distributional assumptions

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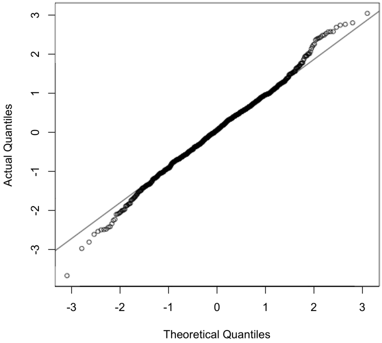


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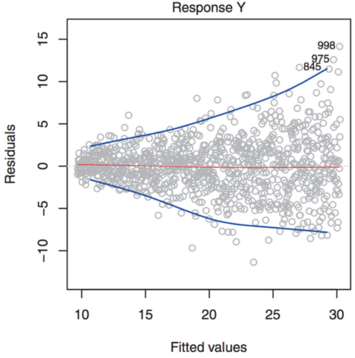


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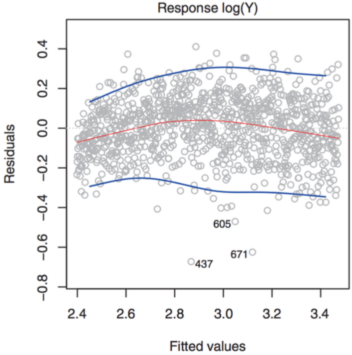


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$$\mathrm{Cov}[\boldsymbol{Y} - \boldsymbol{X}\beta] = (\boldsymbol{Y} - \boldsymbol{X}\beta])^T(\boldsymbol{Y} - \boldsymbol{X}\beta])$$

$$\approx \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix}$$

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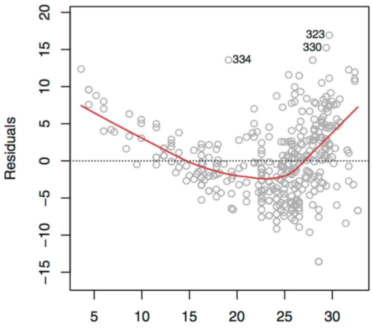


Residuals versus Feature Values

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

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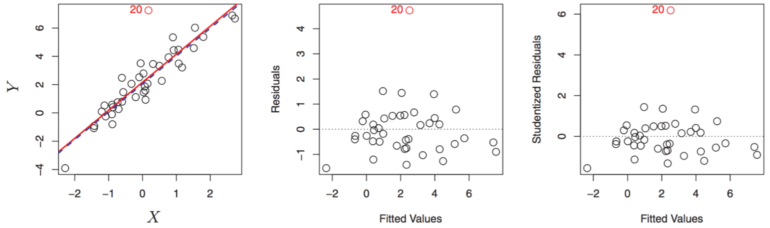
# Concerns: Outliers

Studentized Residuals (as in "Student's t-distributioned" residuals)

$$r_i = \frac{\hat{\epsilon}_i}{\hat{s}igma^2} = \frac{\text{residual}_i}{\text{RSE}}$$

have a t-distribution



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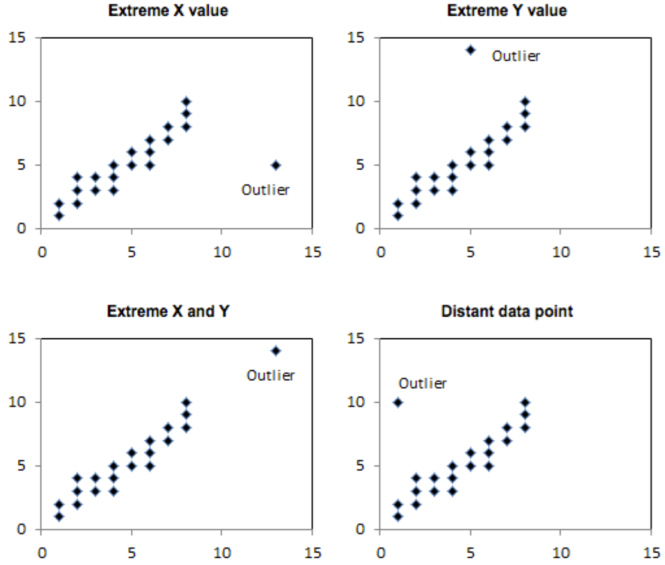

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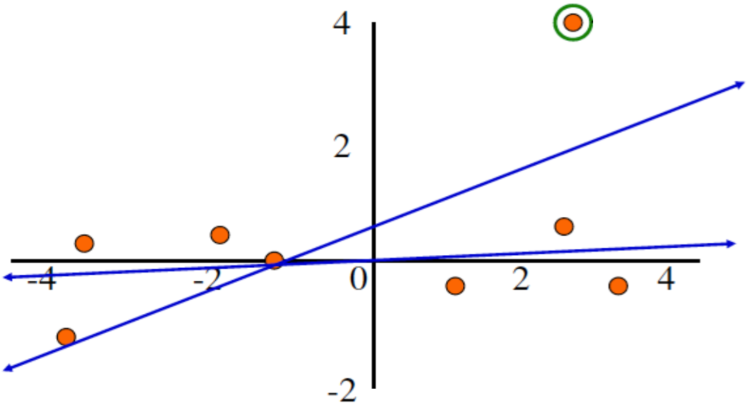

# Concerns: High Leverage Points

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

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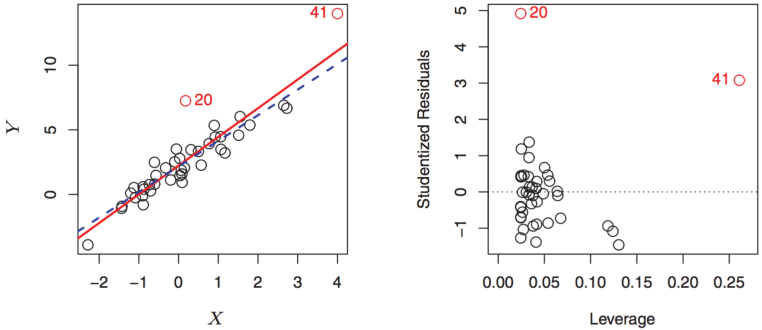

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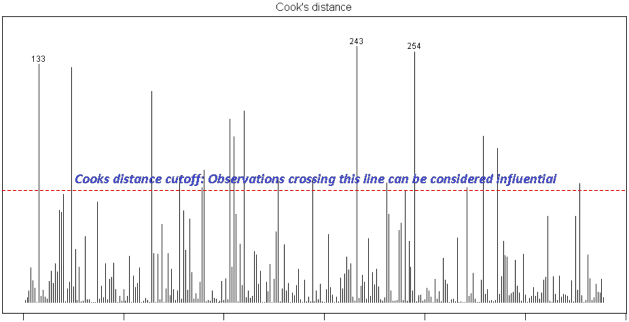

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