Regression

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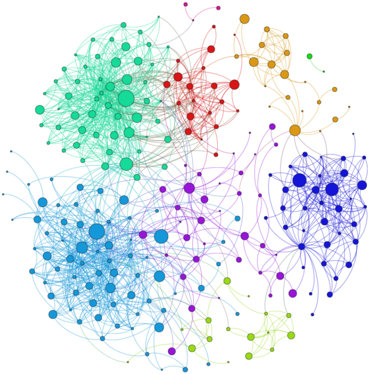

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Linear Regression

The linear regression model[1] is a discriminative model with $f(x) = E[y|x]$[2] as the target function and $\mathcal{H} = \{h(x)\}$ consisting of linear functions[3]:

$$h(x) = x'\beta$$

, where $x = (1, x_1, \ldots, x_p)'$ and $\beta = (\beta_0, \beta_1, \ldots, \beta_p)'$.

The goal is to find $g \in \mathcal{H}$ that best approximates f.

---

[1] Note on terminology: linear regression can refer broadly to the use of any linear models for regression purposes. However, historically it often refers more narrowly to least squares linear regression. Here we start by discussing the least squares linear regression model.

[2] The **conditional expectation function** (**CEF**), $E[y|x]$, is also known as the **regression function**.

[3] Since each $h(x)$ is associated with a unique β, $h(x)$ is said to be **parametrized** by β. In this case, choosing a hypothesis h is equivalent to choosing a parameter β.

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- Error measures:

$$E_{out}(h) = E\left[(y - h(x))^2\right] \tag{1}$$

$$E_{in}(h) = \frac{1}{N}\sum_{i=1}^{N}(y_i - h(x_i))^2 \tag{2}$$

- The VC dimension of a linear model is $p + 1$[4]. For $N \gg p$, the linear model generalizes well from E_{in} to E_{out}.

[4] p is the dimension of the input space.

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Linear Regression

Let

$$\begin{aligned}\beta^* &= \arg\min_{\beta} E\left[\left(y - x'\beta\right)^2\right] \\ &= \underbrace{E\left(xx'\right)^{-1}}_{(p+1)\times(p+1)} \underbrace{E\left(xy\right)}_{(p+1)\times 1}\end{aligned} \tag{3}$$

β^* is the *population* regression coefficient.

$x'\beta^*$ is the best[5] linear predictor of y given x in the underlying population.

[5]in the sense of minimizing the L2 loss function.

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Linear Regression

Recall that the CEF $f(x) = E[y|x]$ is the best[6] predictor of y given x in the class of all functions of x.

The function $x'\beta^*$ provides the best[6] linear approximation to the CEF:

$$\beta^* = \arg\min_{\beta} E\left[\left(E[y|x] - x'\beta\right)^2\right]$$

[6] minimum L2 loss

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Let $e^* \equiv y - x'\beta^*$. By construction,

$$\underbrace{E\left(xe^*\right)}_{(p+1)\times 1} = 0 \tag{4}$$

In particular, if x contains a constant term, then (4) $\Rightarrow E\left(e^*\right) = 0$. In this case e^* and x are uncorrelated.

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Linear Regression

We can separate the constant term and write the linear model as

$$y = \beta_0 + \widetilde{x}'\widetilde{\beta} + e$$

, where $\widetilde{x} = (x_1, \ldots, x_p)'$ and $\widetilde{\beta} = (\beta_1, \ldots, \beta_p)'$.

Then (3) $\Rightarrow$

$$\begin{aligned} \widetilde{\beta}^* &= Var\left(\widetilde{x}\right)^{-1} Cov\left(\widetilde{x}, y\right) \\ \beta_0^* &= E\left(y\right) - E\left(\widetilde{x}\right)' \widetilde{\beta}^* \end{aligned} \tag{5}$$

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Linear Regression

When $p = 1$,

$$y = \beta_0 + \beta_1 x_1 + e$$

(5) $\Rightarrow$

$$\beta_1^* = \frac{Cov\left(x_1, y\right)}{Var\left(x_1\right)} \tag{6}$$

When $p > 1$, (5) $\Rightarrow$ for any $j \in \{1, \ldots, p\}$,

$$\beta_j^* = \frac{Cov\left(u_j^*, y\right)}{Var\left(u_j^*\right)} \tag{7}$$

, where u_j^* is the residual from a regression of x_j on all the other inputs.

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Linear Regression

- $\beta^* = E\left(xx'\right)^{-1} E\left(xy\right)$ is the $(p+1) \times 1$ vector with the $j^{th} \, (j > 1)$ element being $\beta_j^* = \frac{Cov\left(u_j^*, y\right)}{Var\left(u_j^*\right)}$.

- Each β_j^* is the slope coefficient on a scatter plot with y on the $y-$axis and u_j^* on the $x-$axis.

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The OLS Estimator

Given observed data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_N, y_N)\} \sim^{i.i.d.} p(x, y)$, we have, for $i = 1, \ldots, N$,

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + e_i$$

, which can be written as

$$Y = X\beta + e$$

, where $Y = [y_1, \ldots, y_N]'$, $e = [e_1, \ldots, e_N]'$, and

$$X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & \cdots & x_{Np} \end{bmatrix} = \begin{bmatrix} x_1' \\ \vdots \\ x_N' \end{bmatrix}$$

, where $x_i = [1, x_{i1}, \ldots, x_{ip}]'$.

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The OLS Estimator

Minimizing the in-sample error (2) $\Rightarrow$

$$\widehat{\beta} = \left[\sum_{i=1}^{N} x_i x_i'\right]^{-1} \sum_{i=1}^{N} x_i y_i \tag{8}$$
$$= \left(X'X\right)^{-1} X'Y$$

$\widehat{\beta}$ is the *least squares* regression coefficient – the sample estimate of β^*.

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The OLS Estimator

When $p = 1$,

$$\widehat{\beta}_0 = \overline{y} - \widehat{\beta}_1 \overline{x}_{i1}$$
$$\widehat{\beta}_1 = \frac{\sum_{i=1}^{N} \left(x_{i1} - \overline{x}_{i1}\right) y_i}{\sum_{i=1}^{N} \left(x_{i1} - \overline{x}_{i1}\right)^2}$$

, where $\overline{x}_{i1} = \frac{1}{N}\sum_{i=1}^{N} x_{i1}$.

When $p > 1$, for any $j \in \{1, \ldots, p\}$,

$$\widehat{\beta}_j = \frac{\sum_{i=1}^{N} \widehat{u}_{ij} y_i}{\sum_{i=1}^{N} \widehat{u}_{ij}^2} = \frac{\widehat{u}_j' Y}{\widehat{u}_j' \widehat{u}_j} \tag{9}$$

, where $\widehat{u}_j = (\widehat{u}_{1j}, \ldots, \widehat{u}_{Nj})'$, and $\widehat{u}_{ij}$ is the estimated residual from a regression of x_{ij} on $\left(1, \{x_{ik}\}_{k \neq j}\right)$.

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The OLS Estimator

Generate some data:

$$
\begin{aligned}
x_1 &\sim U(0,1) \\
x_2 &= 0.5x_1 + 0.5r, \;\; r \sim U(0,1) \\
y &= 1 - 2.5x_1 + 5x_2 + e, \;\; e \sim \mathcal{N}(0,1)
\end{aligned}
$$

```r
n <- 500
e <- rnorm(n)
x1 <- runif(n)
x2 <- 0.5*x1 + 0.5*runif(n)
y <- 1 - 2.5*x1 + 5*x2 + e
```

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The OLS Estimator

```
require(AER)
reg <- lm(y ~ x1 + x2)
coeftest(reg)

##
## t test of coefficients:
##
##              Estimate Std. Error  t value  Pr(>|t|)
## (Intercept)  1.01013    0.11884   8.4997 2.233e-16 ***
## x1          -2.59166    0.22529 -11.5039 < 2.2e-16 ***
## x2           5.06250    0.31213  16.2193 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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The OLS Estimator

```
X <- cbind(rep(1,n),x1,x2)
beta <- solve(t(X)%*%X)%*%t(X)%*%y
t(beta)

##                      x1       x2
## [1,] 1.010133 -2.591657 5.062497

x1reg <- lm(x1~x2)
u1 <- residuals(x1reg)
b1 <- cov(u1,y)/var(u1)

x2reg <- lm(x2~x1)
u2 <- residuals(x2reg)
b2 <- cov(u2,y)/var(u2)

b0 = mean(y) - b1*mean(x1) - b2*mean(x2)
cbind(b0,b1,b2)

##            b0        b1       b2
## [1,] 1.010133 -2.591657 5.062497
```

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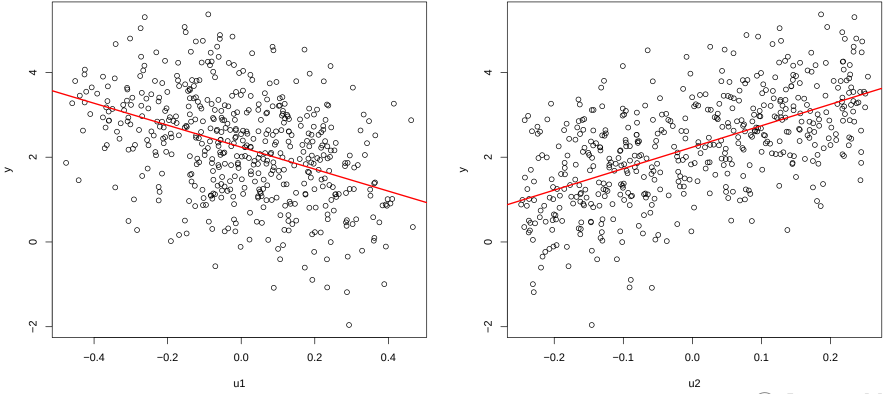
The OLS Estimator

```
plot(u1,y)
abline(lm(y~u1),col="red",lwd=2)
plot(u2,y)
abline(lm(y~u2),col="red",lwd=2)
```



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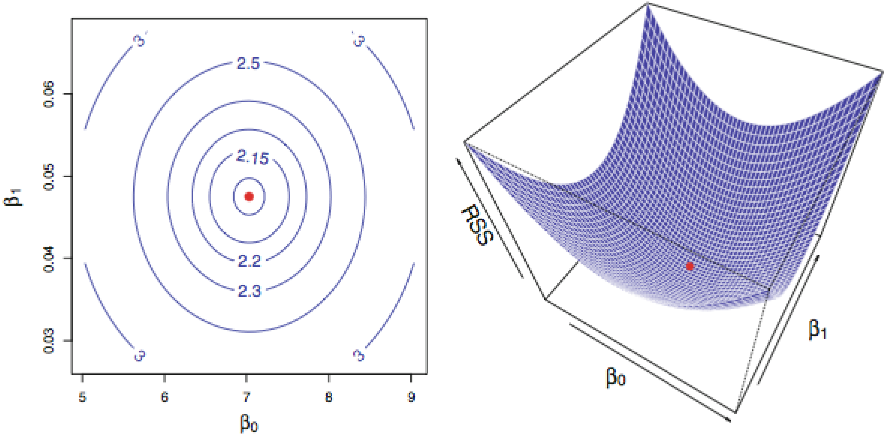
Searching for the best hypothesis



Contour and three-dimensional plots of RSS $= \sum_{i=1}^{N} (y_i - x_i' \beta)^2$

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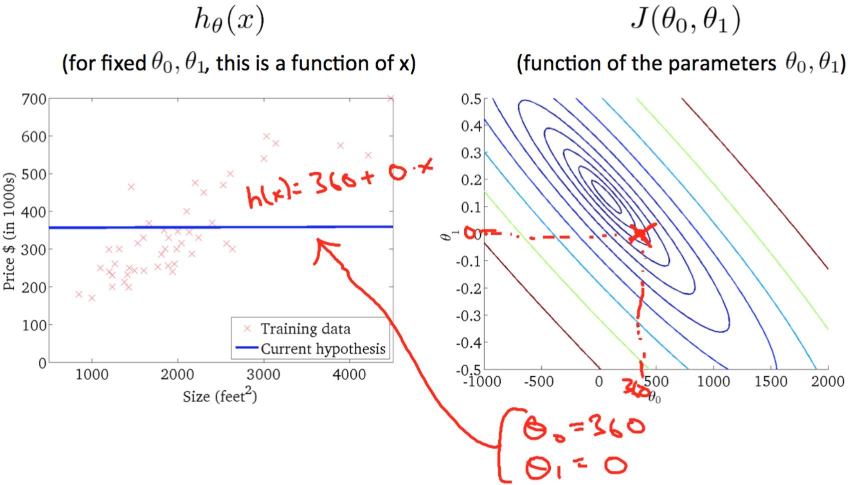
Searching for the best hypothesis



$$\mathcal{H} = \{h_\theta(x) = \theta_0 + \theta_1 x\}$$

Left: training data and $h_\theta(x)$ for a particular $\theta = (\theta_0, \theta_1)$

Right: RSS: $J(\theta_0, \theta_1) = \sum_i (y_i - \theta_0 - \theta_1 x_i)^2$

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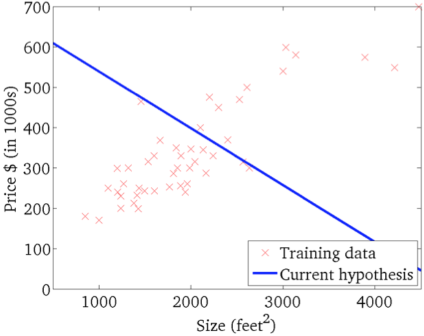
Searching for the best hypothesis

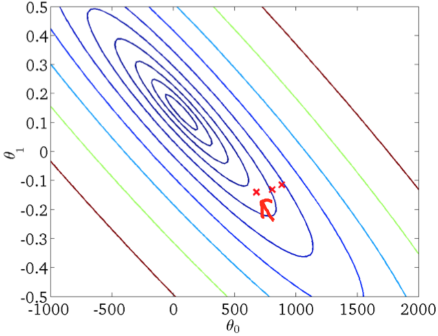
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



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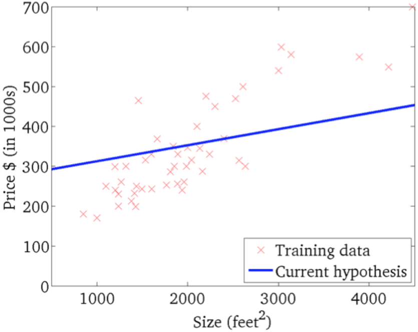
Searching for the best hypothesis

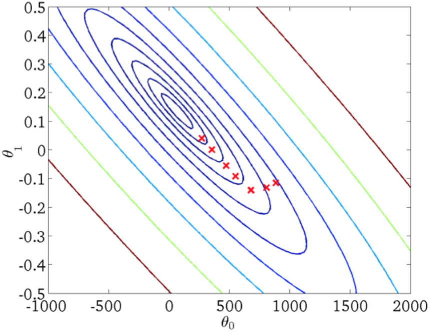
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



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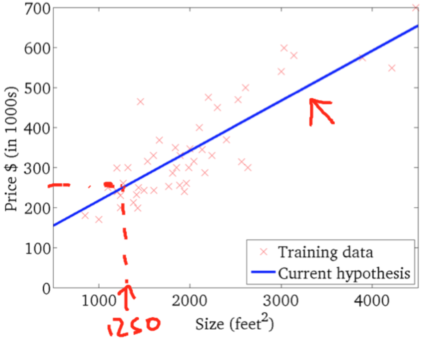
Searching for the best hypothesis

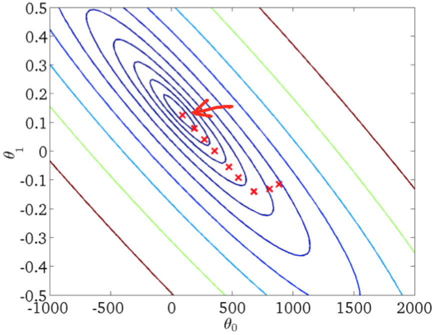
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



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Geometric Interpretation

Consider two $n-$dimensional vectors: $a = (a_1, \ldots, a_n)$ and $b = (b_1, \ldots, b_n)$. The **Euclidean distance** between a and b is:

$$\|a - b\| = \sqrt{\sum_{i=1}^{n} (a_i - b_i)^2} = \sqrt{(a-b) \cdot (a-b)}$$

The cosine of the angle between a and b is:

$$\cos\theta = \frac{a \cdot b}{\|a\| \, \|b\|}$$

, where $\|a\| = \|a - 0\|$ is the length of a.

When $a \cdot b = 0$, a and b are **orthogonal**, denoted by $a \perp b$.

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Geometric Interpretation

The linear space spanned by a, denoted by $\mathcal{R}(a)$, is the collection of points $\beta a = (\beta a_1, \ldots, \beta a_n)$ for any real number β.

The **projection** of b onto $\mathcal{R}(a)$ is the point b^* in $\mathcal{R}(a)$ that is closest to b in terms of Euclidean distance:

$$b^* = \left(\frac{a \cdot b}{\|a\|^2}\right) a$$

- $(b - b^*) \perp a$

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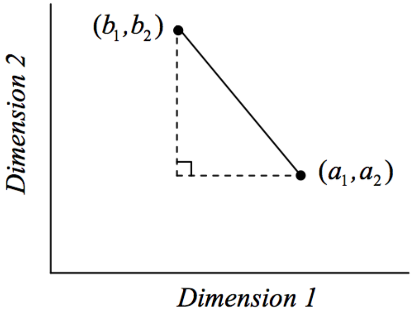
Geometric Interpretation



Euclidean Distance in two Dimensions

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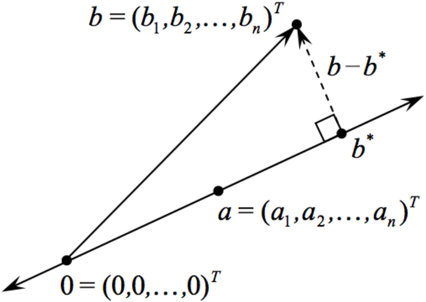
Geometric Interpretation



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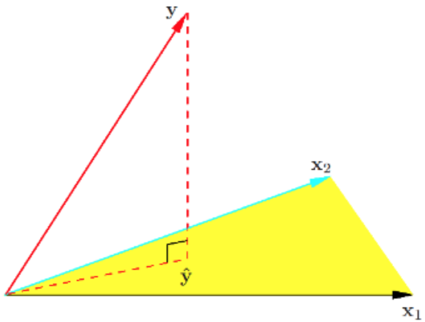
Geometric Interpretation

The linear regression fit $\widehat{Y}$ is the projection of Y onto the linear space spanned by $\{\mathbf{1}, X_1, \ldots, X_p\}$[7].



[7] $X_j = (x_{1j}, \ldots, x_{Nj})'$ for $j = 1, \ldots, p$.

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Geometric Interpretation

- **Projection matrix** $\mathbb{H} = X\left(X'X\right)^{-1}X'$

$$\mathbb{H}Y = \widehat{Y}$$

  - $\mathbb{H}$ is also called the **hat matrix**[8,9].

- $\widehat{e} \; = Y - X\widehat{\beta} = \left(\mathbb{I} - \mathbb{H}\right)Y \; \perp \; \mathcal{R}\left(\mathbf{1}, X_1, \ldots, X_p\right)$.

  - $\widehat{e} \perp X_j \; \forall j$.
  - $\widehat{e} \perp \mathbf{1} \Rightarrow \sum_i \widehat{e}_i = 0$.

[8] Since it "puts a hat" on Y.

[9] The hat matrix has many special properties such as: $\mathbb{H}^2 = \mathbb{H}$, $\left(\mathbb{I} - \mathbb{H}\right)^2 = \left(\mathbb{I} - \mathbb{H}\right)$, and $\text{trace}\left(\mathbb{H}\right) = 1 + p$.

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Asymptotic Properties

- $\widehat{\beta}$ is unbiased: $E\left(\widehat{\beta}\right) = \beta^*$.
- But how much does $\widehat{\beta}$ vary around β^*?

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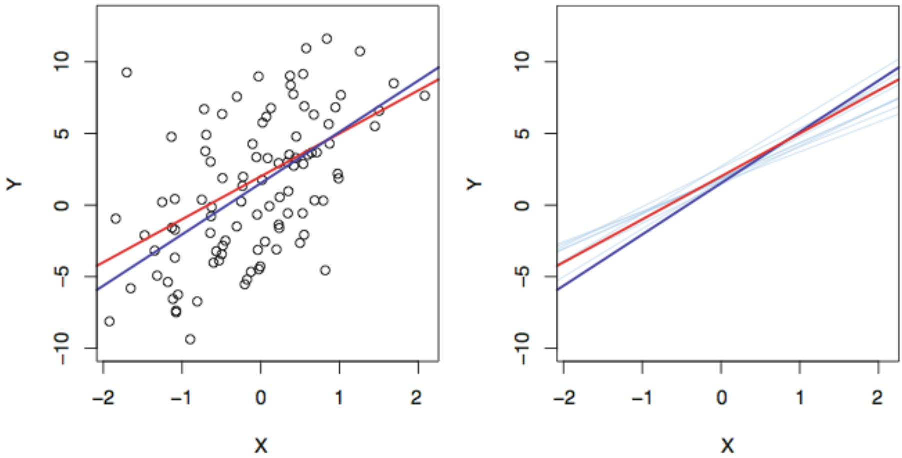
Asymptotic Properties



bed: $x'\beta^*$. blue: $x'\widehat{\beta}$
Right: $x'\widehat{\beta}$ based on 10 random set of observations.

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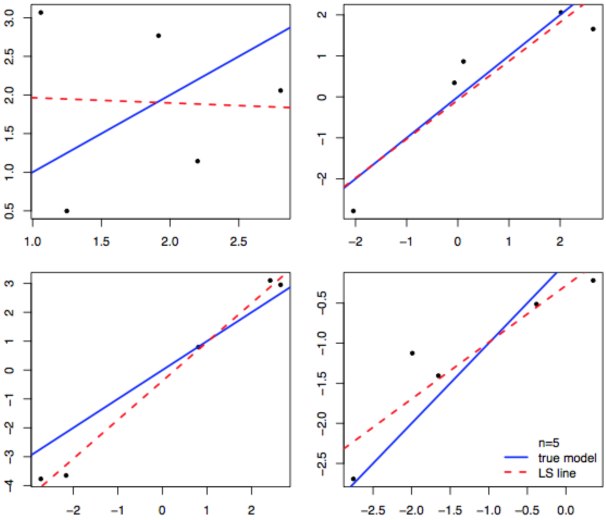
Asymptotic Properties



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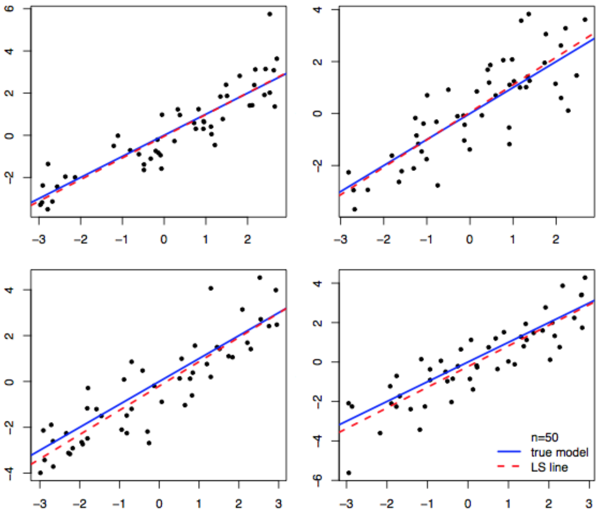
Asymptotic Properties



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Asymptotic Properties

By the central limit theorem,

$$\sqrt{N}\left(\widehat{\beta}-\beta^*\right)\longrightarrow^d \mathcal{N}\left(0, E\left(xx'\right)^{-1} E\left[xx'\left(e^*\right)^2\right] E\left(xx'\right)^{-1}\right)$$

- $V\left(\widehat{\beta}\right)=\underbrace{N^{-1}E\left(xx'\right)^{-1} E\left[xx'\left(e^*\right)^2\right] E\left(xx'\right)^{-1}}_{(p+1)\times(p+1)}$ is the **asymptotic variance** of $\widehat{\beta}$ conditional on x.
- $V\left(\widehat{\beta}\right)$ quantifies the uncertainty of $\widehat{\beta}$ due to random sampling.

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Asymptotic Properties

$$\begin{aligned}\widehat{V}\left(\widehat{\beta}\right) &= \left[\sum_{i=1}^{N} x_i x_i'\right]^{-1} \left(\sum_{i=1}^{N} x_i x_i' \widehat{e}_i^2\right) \left[\sum_{i=1}^{N} x_i x_i'\right]^{-1} \\ &= \left(X'X\right)^{-1} \left(X'\Omega X\right) \left(X'X\right)^{-1} \\ &\to^{p} V\left(\widehat{\beta}\right)\end{aligned} \tag{10}$$

, where $\Omega = \mathrm{diag}\left(\widehat{e}_1^2, \ldots, \widehat{e}_N^2\right) = \begin{bmatrix} \widehat{e}_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \widehat{e}_N^2 \end{bmatrix}$.

Asymptotic Properties

Homoskedasticity: $E\left[\left.(e^*)^2\right| x\right] = \sigma^2$

Heteroskedasticity: $E\left[\left.(e^*)^2\right| x\right] = \sigma^2(x)$

Under homoskedasticity,

$$\sqrt{N}\left(\widehat{\beta} - \beta^*\right) \longrightarrow^d \mathcal{N}\left(0, E\left(xx'\right)^{-1}\sigma^2\right)$$

$$\widehat{V}\left(\widehat{\beta}\right) = \left(X'X\right)^{-1}\widehat{\sigma}^2 \tag{11}$$

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Asymptotic Properties

From (9), we can also derive the homoskedastic asymptotic variance of $\widehat{\beta}_j$ – the $(j+1)^{th}$ diagonal element of $V\left(\widehat{\beta}\right)$ – as:

For $j = 1, \ldots, p$,

$$\sqrt{N}\left(\widehat{\beta}_j - \beta_j^*\right) \longrightarrow^d \mathcal{N}\left(0, \frac{\sigma^2}{Var\left(u_j\right)}\right)$$

$$\widehat{V}\left(\widehat{\beta}_j\right) = \frac{\widehat{\sigma}^2}{\widehat{u}_j'\widehat{u}_j} \tag{12}$$

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Asymptotic Properties

- **t-statistic**

$$t_j = \frac{\widehat{\beta}_j - \beta_j^*}{\widehat{se}\left(\widehat{\beta}_j\right)} \rightarrow^d \mathcal{N}(0,1)$$

, where $\widehat{se}\left(\widehat{\beta}_j\right) = \sqrt{\widehat{V}\left(\widehat{\beta}_j\right)}$.

- 95% **confidence interval** for β_j^*:

$$\left[\widehat{\beta}_j - 1.96 \times \widehat{se}\left(\widehat{\beta}_j\right), \widehat{\beta}_j + 1.96 \times \widehat{se}\left(\widehat{\beta}_j\right)\right]$$

  - The interval represents a set estimate of β_j^*.

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Hypothesis Testing

$\mathbb{H}_0 : \beta_j^* = 0$ vs. $\mathbb{H}_1 : \beta_j^* \neq 0$

Under H_0,

$$t_j = \frac{\widehat{\beta}_j}{\widehat{se}\left(\widehat{\beta}_j\right)} \to^d \mathcal{N}(0,1) \tag{13}$$

P-value: probability of observing any value more extreme than $|t_j|$ under $\mathbb{H}_0$. (13) $\Rightarrow$ in large sample,

$$p-\text{value} \approx 2\left(1-\Phi\left(|t_j|\right)\right) \tag{14}$$

, where Φ is the CDF of $\mathcal{N}(0,1)$.

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Hypothesis Testing

For significance level α, reject $\mathbb{H}_0$ if $|t_j| > c_\alpha = \Phi^{-1}(1 - \alpha/2)$, or equivalently, if $p-$value $< \alpha$[10].

- c_α is called the **asymptotic critical value**.
- Common practice: $\alpha = 5\%$ ($c_{.05} \approx 1.96$), $\alpha = 10\%$ ($c_{.10} \approx 1.64$), $\alpha = 1\%$ ($c_{.01} \approx 2.58$).

[10]It is worth emphasizing that (14) is only valid *in large samples*, since it is based on the asymptotic distribution of t_j. Any $p-$values calculated using (14) on small samples should *not* be trusted. In general, hypothesis tests based on the asymptotic properties of test statistics are only valid for large samples.

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Hypothesis Testing

Hypothesis Testing Decisions

	Accept $\mathbb{H}_0$	Reject $\mathbb{H}_0$
$\mathbb{H}_0$ true	Correct Decision	Type I Error
$\mathbb{H}_1$ true	Type II Error	Correct Decision

- α is the **size** of the test – the probability of making a Type I error: $\Pr(\text{reject } \mathbb{H}_0 | \mathbb{H}_0 \text{ is true})$.
- The **power** or **sensitivity** of a test, is the probability of rejecting $\mathbb{H}_0$ when $\mathbb{H}_1$ is true. Thus $(1 - \text{power})$, denoted by β, is the probability of making a Type II error: $\Pr(\text{fail to reject } \mathbb{H}_0 | \mathbb{H}_1 \text{ is true})$.
    - Power $\uparrow$ as $\alpha \uparrow$, or sample size $N \uparrow$, or the true (population) parameter value is further away from its hypothesized value under $\mathbb{H}_0$.

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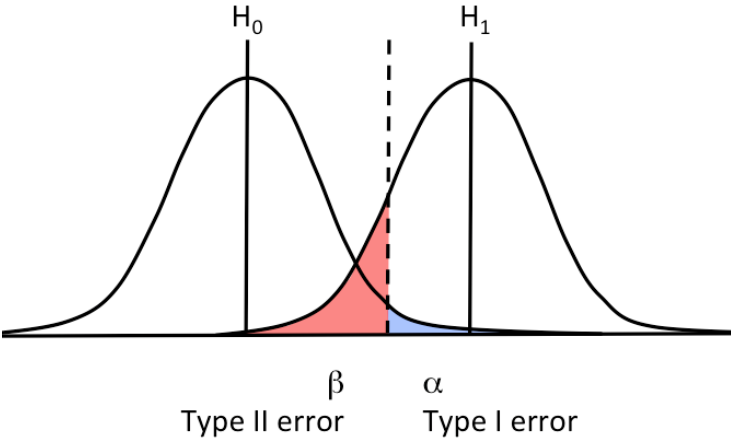
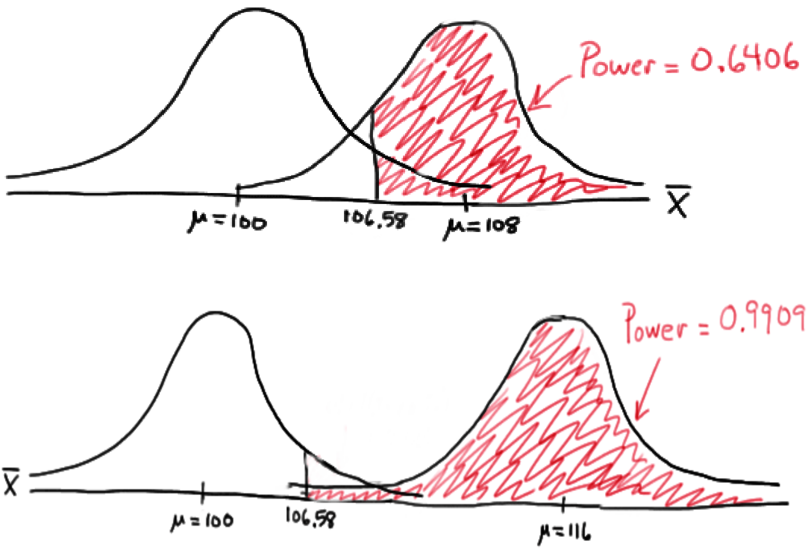
Hypothesis Testing



Hypothesis Testing



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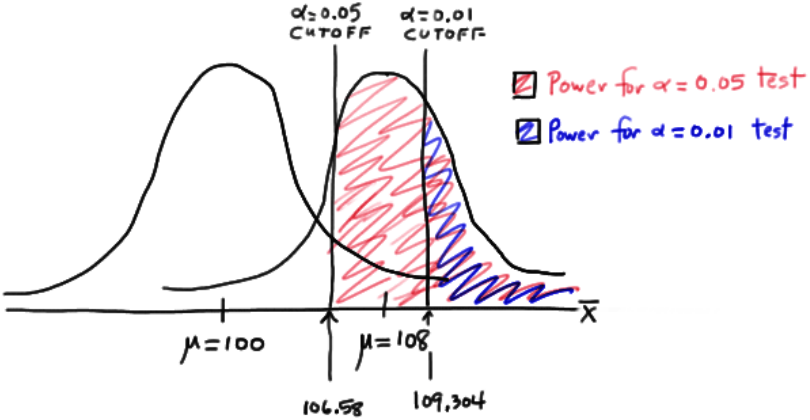
Hypothesis Testing



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R^2

$$R^2 = \frac{\sum_{i=1}^{N}(\widehat{y}_i - \overline{y})^2}{\sum_{i=1}^{N}(y_i - \overline{y})^2} = 1 - \frac{\sum_{i=1}^{N}\widehat{e}_i^2}{\sum_{i=1}^{N}(y_i - \overline{y})^2}$$

- measures the amount of variation in y_i accounted for by the model: $1 =$ perfect, $0 =$ perfect misfit.
- cannot go down when you add regressors.
  - Intuition: adding more regressors always allow us to fit the training data more accurately (i.e., reduce E_{in}, but not necessary E_{out})[11].

[11]Technically, $\widehat{\beta}$ is chosen to minimize $\sum_i \widehat{e}^2$. if you add a regressor, you can always set the coefficient of that regressor equal to zero to get the same $\sum_i \widehat{e}^2$. Therefore R^2 cannot go down.

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Robust Standard Errors

(10) is known as **heteroskedasticity-consistent (HC) standard error**, **robust standard error**, or **White standard error**.

Let's generate some data:

$$
\begin{aligned}
x &= U(0, 100) \\
y &= 5x + e, \;\; e \sim \mathcal{N}(0, \exp(x))
\end{aligned}
$$

```r
n <- 1e3
x <- 100*runif(n)
y <- rnorm(n,mean=5*x,sd=exp(x))
```

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Robust Standard Errors

```
require(AER)
coeftest(lm(y~x)) # homoskedastic standard error

##
## t test of coefficients:
##
##                 Estimate  Std. Error t value Pr(>|t|)
## (Intercept)  1.0116e+41  9.0736e+40  1.1148  0.26519
## x           -3.0822e+39  1.5634e+39 -1.9715  0.04895 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

coeftest(lm(y~x),vcov=vcovHC) # robust standard error

##
## t test of coefficients:
##
##                 Estimate  Std. Error t value Pr(>|t|)
## (Intercept)  1.0116e+41  8.6253e+40  1.1728   0.2412
## x           -3.0822e+39  2.6314e+39 -1.1713   0.2417
```

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The Bootstrap

- The bootstrap is a statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical method.
  - For example, it can provide an estimate of the standard error of a coefficient.
- The term is believed to derive from "The Surprising Adventures of Baron Munchausen" by Rudolph Erich Raspe[12]:

  The Baron had fallen to the bottom of a deep lake. Just when it looked like all was lost, he thought to pick himself up by his own bootstraps.

[12] We also have the Munchausen number – a number that is equal to the sum of each digit raised to the power of itself. E.g., $3435 = 3^3 + 4^4 + 3^3 + 5^5$.

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The Bootstrap

Baron Munchausen pulls himself out of a mire by his own hair (illustration by Oskar Herrfurth)

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The Bootstrap

Suppose we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y. Suppose our goal is to minimize the total risk, or variance, of our investment. Then the problem is to choose α such that

$$\alpha = \arg\min_{\gamma} Var\left[\gamma X + (1-\gamma)\, Y\right] \tag{15}$$

(15) $\Rightarrow$

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}} \tag{16}$$

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The Bootstrap

Suppose we do not know $\sigma_X^2, \sigma_Y^2, \sigma_{XY}$ but have access to a random sample $\mathcal{D}$ that is drawn from $p(X, Y)$. Then we can compute $\widehat{\sigma}_X^2, \widehat{\sigma}_Y^2, \widehat{\sigma}_{XY}$ from $\mathcal{D}$ and calculate $\widehat{\alpha}$.

Simulation:

- $\sigma_X^2 = 1, \sigma_Y^2 = 1.25, \sigma_{XY} = 0.5$ ($\Rightarrow \alpha = 0.6$)
- Draw random samples $\mathcal{D} = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ from $p(X, Y)$.

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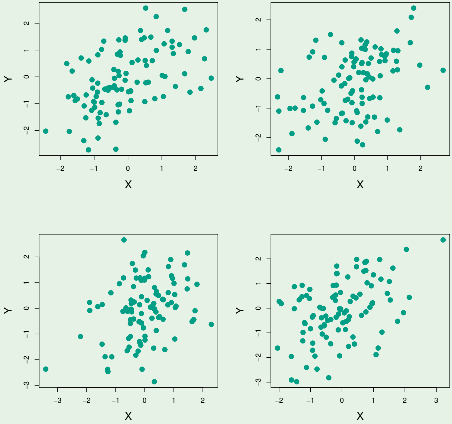
The Bootstrap



Each panel displays 100 simulated returns for investments X and Y .
The resulting estimates for α are 0.576, 0.532, 0.657, and 0.651 clockwise.

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The Bootstrap

To estimate the standard deviation of α, we simulate R random samples $\mathcal{D}$ from $p(X, Y)$ and estimate α R times $\Rightarrow$

$$\widehat{\alpha} = \frac{1}{R}\sum_{r=1}^{R}\widehat{\alpha}_r$$

$$\widehat{se}(\widehat{\alpha}) = \sqrt{\frac{1}{R-1}\sum_{r=1}^{R}(\widehat{\alpha}_r - \widehat{\alpha})^2}$$

- Let $n = 100$ and $R = 1000$. One run of this simulation $\Rightarrow \widehat{\alpha} = 0.5996$ and $\widehat{se}(\widehat{\alpha}) = 0.083$.

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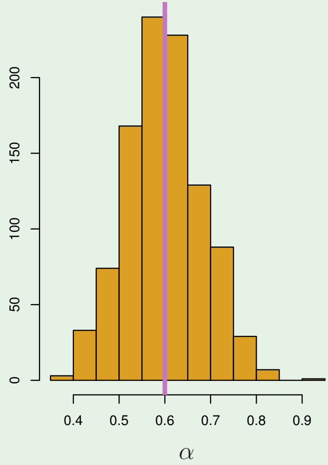
The Bootstrap



A histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population.

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The Bootstrap

- In practice, we cannot generate new samples from the true population.
- Instead, The bootstrap approach generates new samples from the observed sample itself, by repeatedly drawing observations from the observed sample with replacement.
- Each generated bootstrap sample contains the same number of observations as the original observed sample. As a result, some observations may appear more than once in a given bootstrap sample and some not at all.

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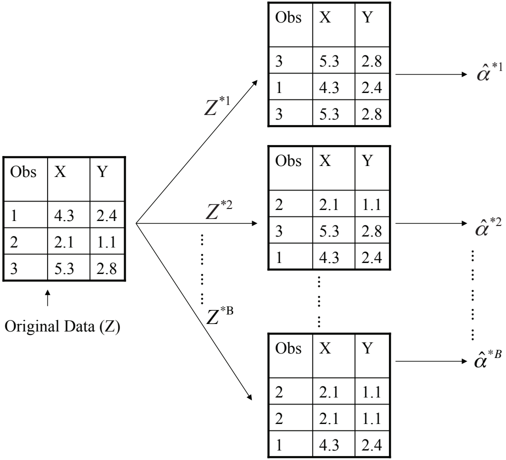
The Bootstrap



The bootstrap approach on a sample containing 3 observations.

© Jiaming Mao

The Bootstrap

```r
# Function to calculate alpha
alpha <- function(data,index){
  X <- data$X[index]
  Y <- data$Y[index]
  return((var(Y)-cov(X,Y))/(var(X)+var(Y)-2*cov(X,Y)))
}
#
# 'Portfolio' is a simulated data set containing the returns of X and Y
require(ISLR) # contains 'Portfolio'
n <- nrow(Portfolio)
bootsample <- sample(n,n,replace=T) # generate one bootstrap sample
alpha(Portfolio,bootsample) # calculate alpha based on the bootstrap sample

## [1] 0.4896806
```

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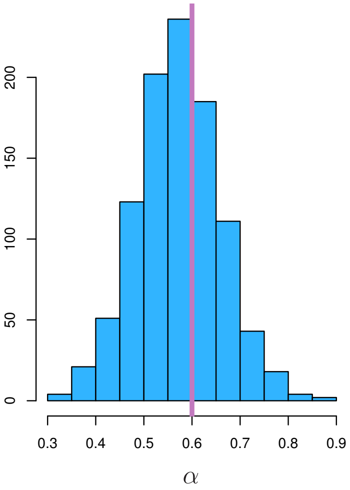
The Bootstrap

```r
# Calculate alpha based on 1000 bootstrap samples
require(boot)
boot(Portfolio,alpha,R=1000)

##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = Portfolio, statistic = alpha, R = 1000)
##
##
## Bootstrap Statistics :
##      original      bias    std. error
## t1* 0.5758321 0.002353412  0.08752433
```

© Jiaming Mao

The Bootstrap



A histogram of the estimates of α obtained from 1,000 bootstrap samples from a single data set

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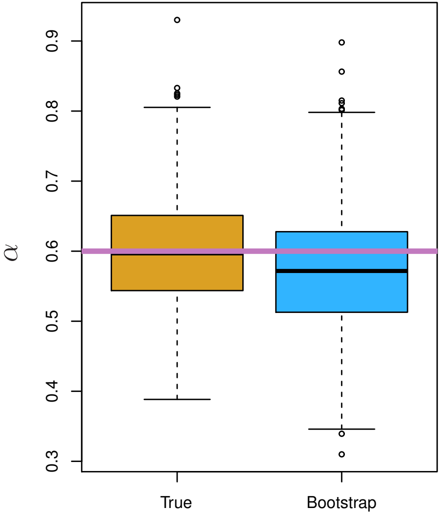
The Bootstrap



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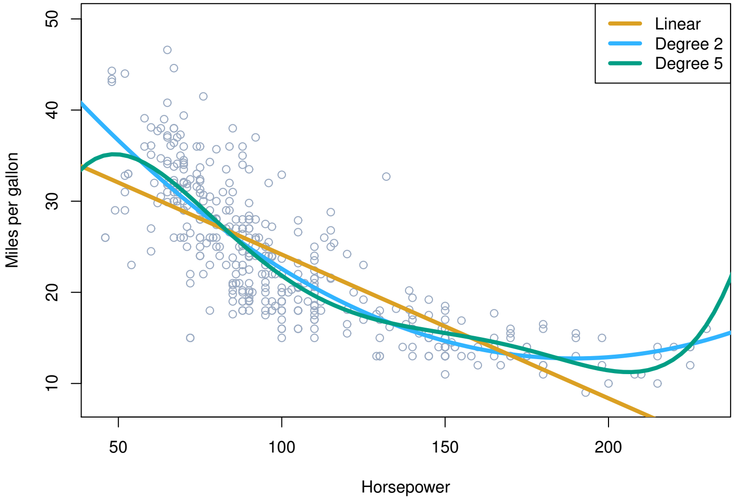
MPG and Horsepower



© Jiaming Mao

MPG and Horsepower

```r
require(ISLR) # contains the data set 'Auto'
require(boot)
beta <- function(data,index){
  coef(lm(mpg~horsepower,data=data,subset=index))
}
boot(Auto,beta,R=1000)

##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = Auto, statistic = beta, R = 1000)
##
##
## Bootstrap Statistics :
##       original        bias    std. error
## t1* 39.9358610  0.0269563085 0.859851825
## t2* -0.1578447 -0.0002906457 0.007402954
```

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MPG and Horsepower

```
require(AER)
coeftest(lm(mpg ~ horsepower,data=Auto)) # homoskedastic std err

##
## t test of coefficients:
##
##               Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 39.9358610  0.7174987  55.660 < 2.2e-16 ***
## horsepower  -0.1578447  0.0064455 -24.489 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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MPG and Horsepower

```r
coeftest(lm(mpg ~ horsepower,data=Auto),vcov=vcovHC) # robust std err

##
## t test of coefficients:
##
##               Estimate Std. Error t value  Pr(>|t|)
## (Intercept) 39.9358610  0.8644903  46.196 < 2.2e-16 ***
## horsepower  -0.1578447  0.0074943 -21.062 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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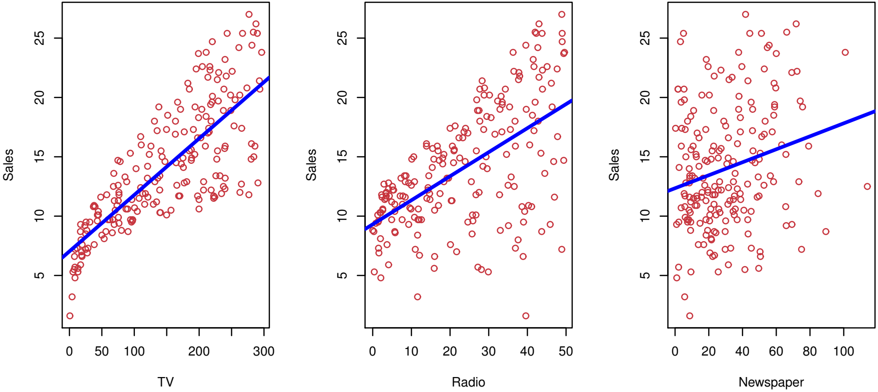
Advertising and Sales



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Advertising and Sales

	Coefficient	Std. error	t-statistic	p-value
Intercept	7.0325	0.4578	15.36	< 0.0001
TV	0.0475	0.0027	17.67	< 0.0001

	Coefficient	Std. error	t-statistic	p-value
Intercept	9.312	0.563	16.54	< 0.0001
radio	0.203	0.020	9.92	< 0.0001

	Coefficient	Std. error	t-statistic	p-value
Intercept	12.351	0.621	19.88	< 0.0001
newspaper	0.055	0.017	3.30	< 0.0001

Simple regression of sales on TV, radio and newspaper respectively.

© Jiaming Mao

Advertising and Sales

	Coefficient	Std. error	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	−0.001	0.0059	−0.18	0.8599

$$sales = \beta_0 + \beta_1 TV + \beta_2 radio + \beta_3 newspaper + e$$

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Advertising and Sales

	TV	radio	newspaper	sales
TV	1.0000	0.0548	0.0567	0.7822
radio		1.0000	0.3541	0.5762
newspaper			1.0000	0.2283
sales				1.0000

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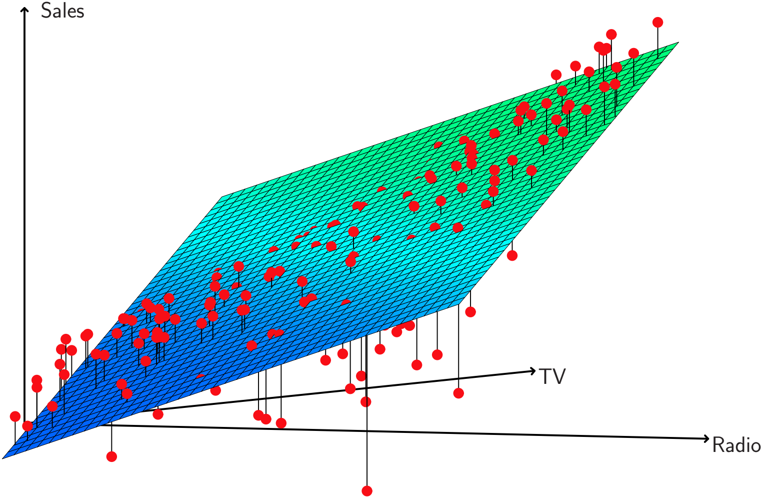
Advertising and Sales



$$sales = \beta_0 + \beta_1 TV + \beta_2 radio + e$$

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Advertising and Sales

	Coefficient	Std. error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

$$sales = \beta_0 + \beta_1 TV + \beta_2 radio + \beta_3 (TV \times radio) + e$$

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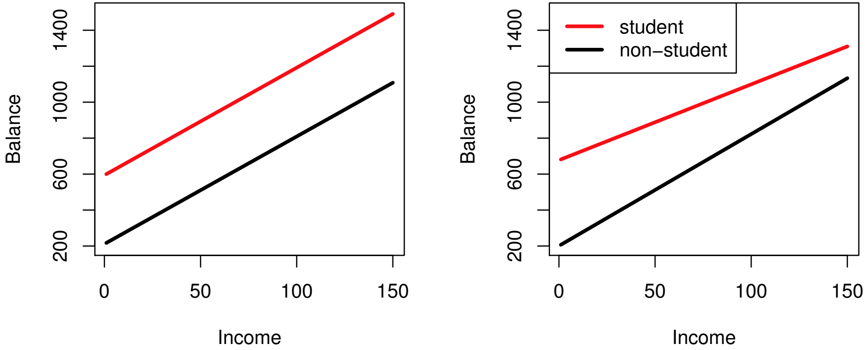
Credit Card Balance



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Credit Card Balance

Let *student* $\in \{0, 1\}$ indicate student status. Two models:

$$\begin{aligned} balance &= \beta_0 + \beta_1 income + \beta_2 student + e \\ &= \begin{cases} \beta_0 + \beta_1 income + e & \text{if not student} \\ (\beta_0 + \beta_2) + \beta_1 income + e & \text{if student} \end{cases} \end{aligned}$$

$$\begin{aligned} balance &= \beta_0 + \beta_1 income + \beta_2 student + \beta_3 income \times student + e \\ &= \begin{cases} \beta_0 + \beta_1 income + e & \text{if not student} \\ (\beta_0 + \beta_2) + (\beta_1 + \beta_3)\, income + e & \text{if student} \end{cases} \end{aligned}$$

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Interaction Terms and the Hierarchy Principle

- Sometimes an interaction term has a very small p-value, but the associated main effects do not.
- **The hierarchy principle**: If we include an interaction in a model, we should also include the main effects, even if the p-values associated with their coefficients are not significant.

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Log-Linear Regression

When y changes on a multiplicative or percentage scale, it is often appropriate to use $\log(y)$ as the dependent variable[13]:

$$y = Ae^{\beta x + e} \Rightarrow \log(y) = \log(A) + \beta x + e$$

e.g.,

$$\log(\text{GDP}) = \alpha + g \times t + e$$

, where $t =$ years, $\alpha = \log(\text{base year GDP})$, and $g =$ annual growth rate.

[13] Suppose y grows at a rate i. If i is continuously compounded, then $y_t = y_0 \lim_{n\to\infty} \left(1 + \frac{i}{n}\right)^{nt} = y_0 e^{it} \Rightarrow \log(y_t) = \log(y_0) + i \times t$. If i is not continuously compounded, then $y_t = y_0 (1+i)^t \Rightarrow \log(y_t) = \log(y_0) + t \log(1+i) \approx \log(y_0) + i \times t$.

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Elasticity and Log-Log Regression

In a log-log model:

$$\log(y) = \beta_0 + \beta_1 \log(x) + e$$

β_1 can often be interpreted as an elasticity measure:

$$\beta_1 = \frac{\partial \log(y)}{\partial \log(x)} = \frac{\partial y / y}{\partial x / x} \approx \frac{\% \Delta y}{\% \Delta x}$$

e.g.,

$$\log(\text{sales}) = \beta_0 + \beta_1 \log(\text{price}) + e$$

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Target Transform

[14]

[14] Note: in general, $E[f(y)] \neq f(E[y])$. In particular, by the Jensen's inequality, $E[\log(y)] < \log(E[y])$. Therefore, if $E[\log(y)|\, x] = \alpha + \beta x$, then $E[y|x] > \exp(\alpha + \beta x)$.

If we are willing to assume

$$\log(y) = \alpha + \beta x + e, \;\; e \sim \mathcal{N}\left(0, \sigma^2\right)$$

, then we have: $E[y|x] = \exp\left(\alpha + \beta x + \frac{1}{2}\sigma^2\right) = \exp\left(E[\log(y)|\, x] + \frac{1}{2}\sigma^2\right)$.

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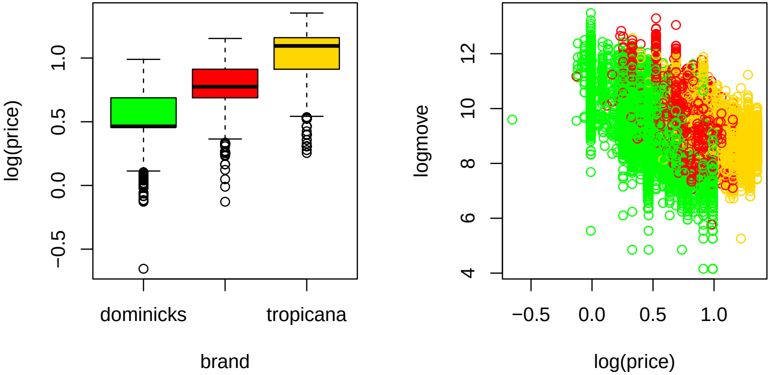
Orange Juice

Three brands: Tropicana, Minute Maid, Dominick's

Data from 83 stores on price, sales (units moved), and whether featured in the store



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Orange Juice

$$\log(\text{sales}) = \alpha + \beta \log(\text{price}) + e$$

```
require(AER)
oj <- read.csv('oj.csv')
reg1 = lm(logmove ~ log(price), data=oj)
coeftest(reg1)

##
## t test of coefficients:
##
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  10.4234     0.0154   679.0   <2e-16 ***
## log(price)   -1.6013     0.0184   -87.2   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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Orange Juice

$\log(\text{sales}) = \alpha_b + \beta_b \log(\text{price}) + e$, where b denotes brand

```
reg2 = lm(logmove ~ log(price)*brand, data=oj)
coeftest(reg2)
```

```
##
## t test of coefficients:
##
##                              Estimate Std. Error t value Pr(>|t|)
## (Intercept)                   10.9547     0.0207  529.14   <2e-16 ***
## log(price)                    -3.3775     0.0362  -93.32   <2e-16 ***
## brandminute.maid               0.8883     0.0416   21.38   <2e-16 ***
## brandtropicana                 0.9624     0.0464   20.72   <2e-16 ***
## log(price):brandminute.maid    0.0568     0.0573    0.99     0.32
## log(price):brandtropicana      0.6658     0.0535   12.44   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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Orange Juice

$$\log(\text{sales}) = (\alpha_{0b} + \text{feature} \times a_{1b}) + (\beta_{0b} + \text{feature} \times \beta_{1b}) \times \log(\text{price}) + e$$

```
reg3 = lm(logmove ~ log(price)*brand*feat, data=oj)
coeftest(reg3)
```

```
##
## t test of coefficients:
##
##                                  Estimate Std. Error t value  Pr(>|t|)    
## (Intercept)                       10.4066     0.0234  445.67  < 2e-16 ***
## log(price)                        -2.7742     0.0388  -71.45  < 2e-16 ***
## brandminute.maid                   0.0472     0.0466    1.01     0.31    
## brandtropicana                     0.7079     0.0508   13.94  < 2e-16 ***
## feat                               1.0944     0.0381   28.72  < 2e-16 ***
## log(price):brandminute.maid        0.7829     0.0614   12.75  < 2e-16 ***
## log(price):brandtropicana          0.7358     0.0568   12.95  < 2e-16 ***
## log(price):feat                   -0.4706     0.0741   -6.35  2.2e-10 ***
## brandminute.maid:feat              1.1729     0.0820   14.31  < 2e-16 ***
## brandtropicana:feat                0.7853     0.0987    7.95  1.9e-15 ***
## log(price):brandminute.maid:feat  -1.1092     0.1222   -9.07  < 2e-16 ***
## log(price):brandtropicana:feat    -0.9861     0.1241   -7.95  2.0e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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Orange Juice

- Elasticity[15]: -1.6
- Brand-specific elasticities:

  Dominick's: -3.4, Minute Maid: -3.4, Tropicana: -2.7
- How does featuring a product affect its elasticity?

	Dominick's	Minute Maid	Tropicana
not featured	-2.8	-2.0	-2.0
featured	-3.2	-3.6	-3.5

[15] What economic assumptions need to be satisfied in order for the coefficients to be interpreted as price elasticities of demand?

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CAPM

The Capital Asset Pricing Model (CAPM) for asset A relates return $R_{A,t}$ to the market return, $R_{M,t}$:

$$R_{A,t} = \alpha + \beta R_{M,t} + e$$

When asset A is a mutual fund, this CAPM regression can be used as a performance benchmark for fund managers.

```
# 'mfunds.csv' contains data on the historical returns of
#              6 mutual funds as well as the market return
mfund <- read.csv('mfunds.csv')
mu <- apply(mfund,2,mean)
stdev <- apply(mfund,2,sd)
```

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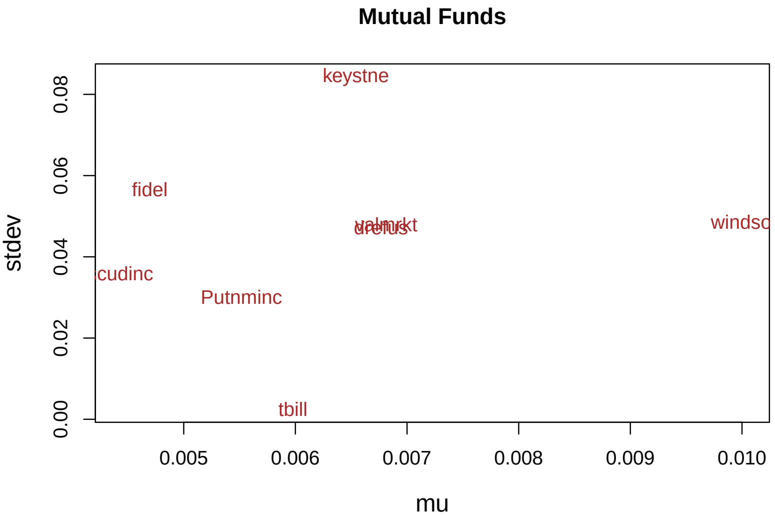
Mutual Funds
keystne
fidel
valmrkt
drefus
windsor
cudinc
Putnminc
tbill
stdev
0.00
0.02
0.04
0.06
0.08
0.005
0.006
0.007
0.008
0.009
0.010
mu

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CAPM

```r
CAPM <- lm(as.matrix(mfund[,1:6]) ~ mfund$valmrkt)
CAPM
```

```
##
## Call:
## lm(formula = as.matrix(mfund[, 1:6]) ~ mfund$valmrkt)
##
## Coefficients:
##                 drefus      fidel       keystne     Putnminc    scudinc
## (Intercept)      0.0003462  -0.0029655  -0.0037704   0.0028271   0.000281
## mfund$valmrkt    0.9424286   1.1246549   1.5137186   0.3948280   0.609202
##                 windsor
## (Intercept)      0.0036469
## mfund$valmrkt    0.9357170
```

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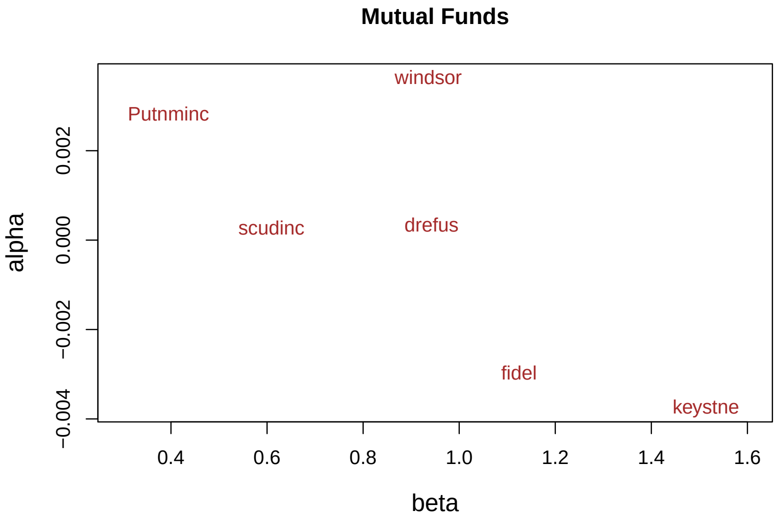
CAPM



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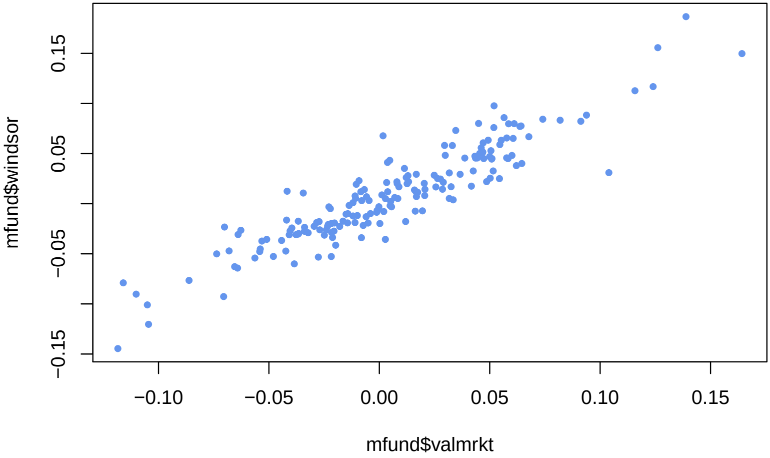
Look at windsor (which dominates the market):



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CAPM

Does Windsor have an "alpha" over the market?

$\mathbb{H}_0 : \alpha = 0$ vs. $\mathbb{H}_1 : \alpha \neq 0$

```
require(AER)
reg <- lm(mfund$windsor ~ mfund$valmrkt)
coeftest(reg)

##
## t test of coefficients:
##
##                 Estimate Std. Error t value Pr(>|t|)
## (Intercept)    0.0036469  0.0014094  2.5876  0.01046 *
## mfund$valmrkt 0.9357170  0.0291499 32.1002  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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CAPM

Now look at beta:

$\mathbb{H}_0 : \beta = 1$, Windsor is just the market (+ alpha).
$\mathbb{H}_1 : \beta \neq 1$, Windsor softens or exaggerates market moves.

```
linearHypothesis(reg, "mfund$valmrkt = 1")

## Linear hypothesis test
##
## Hypothesis:
## mfund$valmrkt = 1
##
## Model 1: restricted model
## Model 2: mfund$windsor ~ mfund$valmrkt
##
##   Res.Df      RSS Df Sum of Sq      F  Pr(>F)
## 1    179 0.064082
## 2    178 0.062378  1 0.0017042 4.8632 0.02872 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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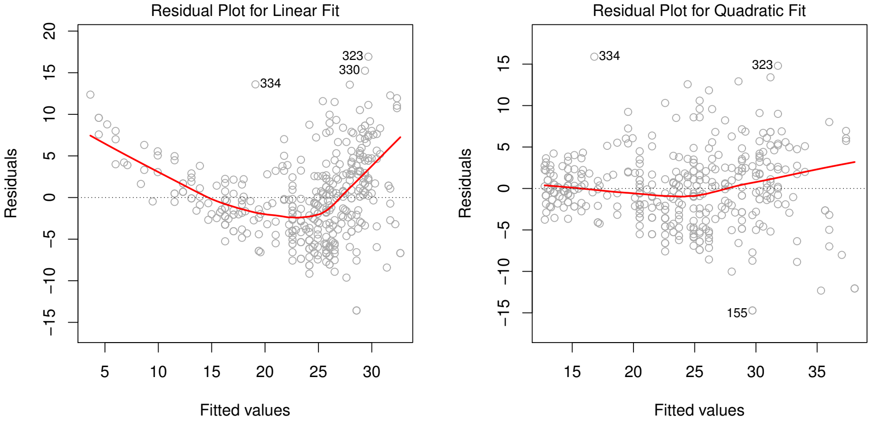
Rregression Diagnostics: Is the CEF linear?



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Rregression Diagnostics: Is the CEF linear?

Anscombe's quartet comprises four datasets that have similar statistical properties …

```
attach(anscombe <- read.csv("anscombe.csv"))
c(x.m1=mean(x1), x.m2=mean(x2), x.m3=mean(x3), x.m4=mean(x4))

## x.m1 x.m2 x.m3 x.m4
##    9    9    9    9

c(y.m1=mean(y1), y.m2=mean(y2), y.m3=mean(y3), y.m4=mean(y4))

##     y.m1     y.m2     y.m3     y.m4
## 7.500909 7.500909 7.500000 7.500909
```

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Rregression Diagnostics: Is the CEF linear?

```r
c(x.sd1=sd(x1), x.sd2=sd(x2), x.sd3=sd(x3), x.sd3=sd(x4))

##    x.sd1    x.sd2    x.sd3    x.sd3
## 3.316625 3.316625 3.316625 3.316625

c(y.sd1=sd(y1), y.sd2=sd(y2), y.sd4=sd(y3), y.sd4=sd(y4))

##    y.sd1    y.sd2    y.sd4    y.sd4
## 2.031568 2.031657 2.030424 2.030579

c(cor1=cor(x1,y1), cor2=cor(x2,y2), cor3=cor(x3,y3), cor4=cor(x4,y4))

##      cor1      cor2      cor3      cor4
## 0.8164205 0.8162365 0.8162867 0.8165214
```

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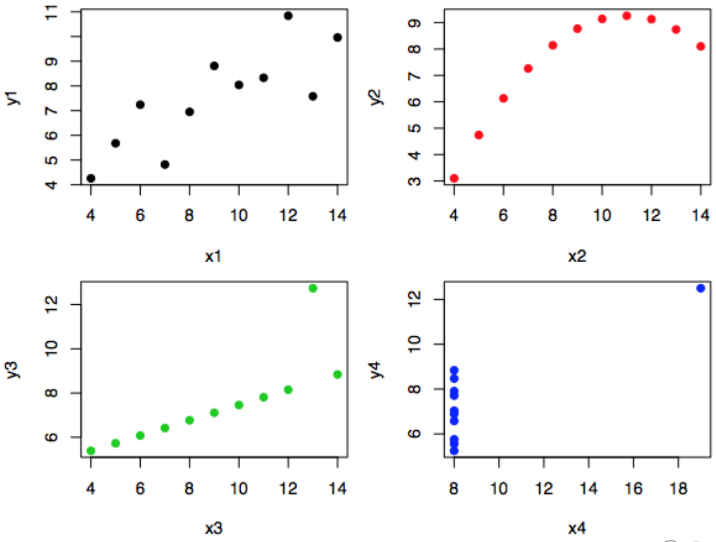
Rregression Diagnostics: Is the CEF linear?

...but vary considerably when graphed:



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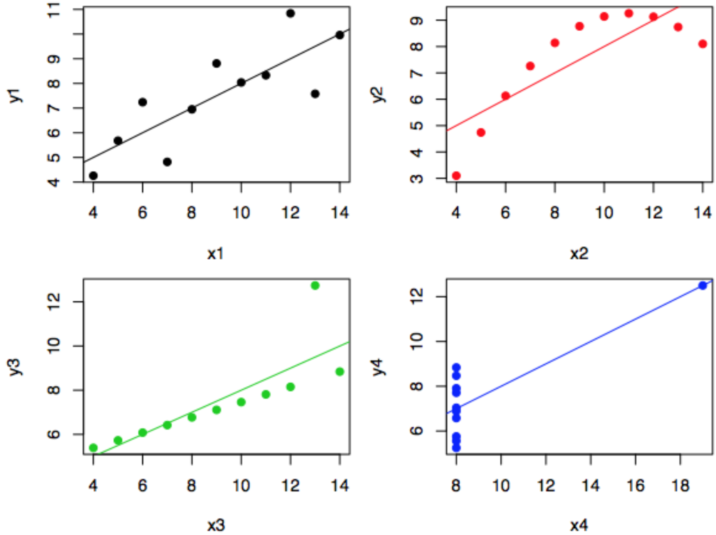
Rregression Diagnostics: Is the CEF linear?

Linear regression on each dataset:



Rregression Diagnostics: Is the CEF linear?

The regression lines and R^2 values are the same...

```
areg <- list(areg1=lm(y1~x1), areg2=lm(y2~x2), areg3=lm(y3~x3),
             areg4=lm(y4~x4))
attach(areg)
cbind(areg1$coef, areg2$coef, areg3$coef, areg4$coef)

##                  [,1]     [,2]      [,3]      [,4]
## (Intercept) 3.0000909 3.000909 3.0024545 3.0017273
## x1          0.5000909 0.500000 0.4997273 0.4999091

s <- lapply(areg, summary)
c(s$areg1$r.sq, s$areg2$r.sq,s$areg3$r.sq, s$areg4$r.sq)

## [1] 0.6665425 0.6662420 0.6663240 0.6667073
```

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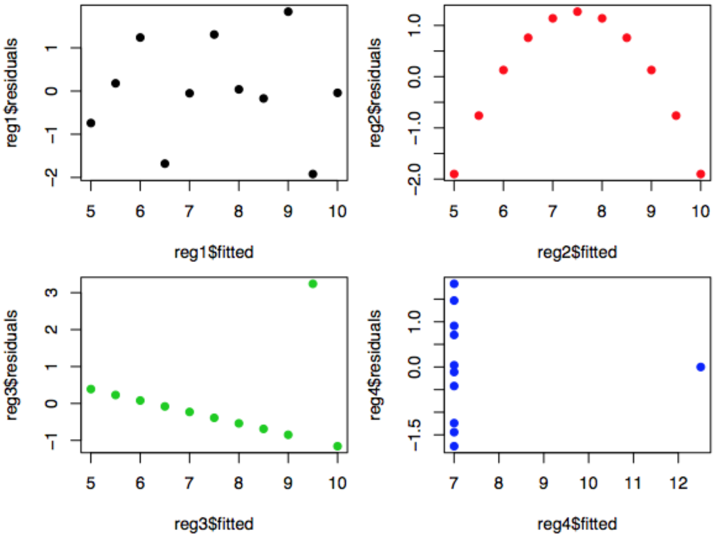
Rregression Diagnostics: Is the CEF linear?

...but residual plots show the differences:



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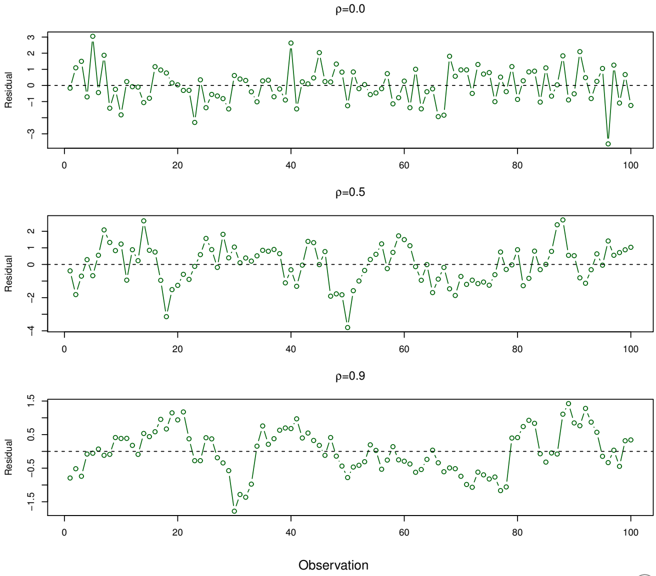
Rregression Diagnostics: Nonrandom Sampling



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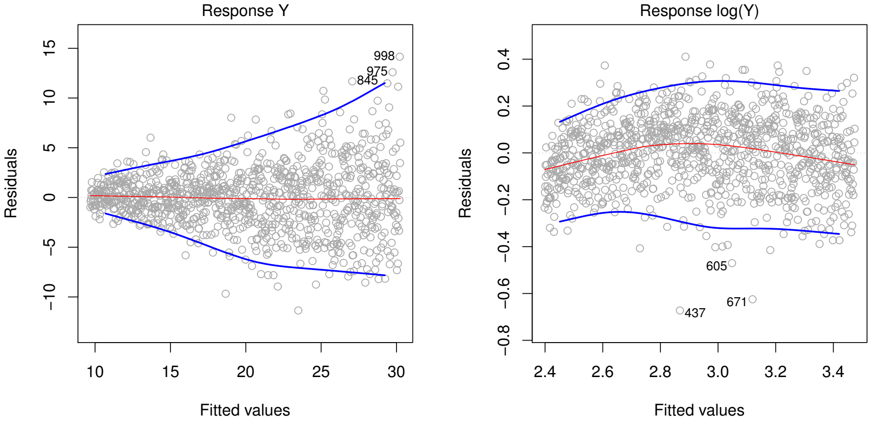
Rregression Diagnostics: Heteroskedasticity



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Rregression Diagnostics: Collinearity

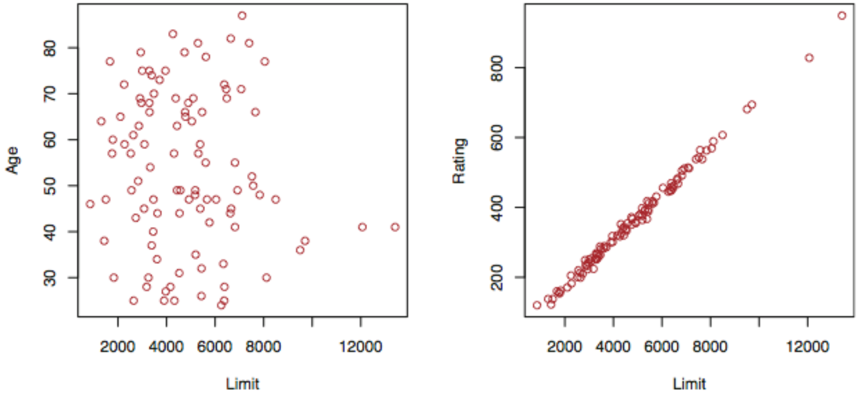

FIGURE 3.14. *Scatterplots of the observations from the* `Credit` *data set.* Left: *A plot of* `age` *versus* `limit`. *These two variables are not collinear.* Right: *A plot of* `rating` *versus* `limit`. *There is high collinearity.*

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Rregression Diagnostics: Collinearity

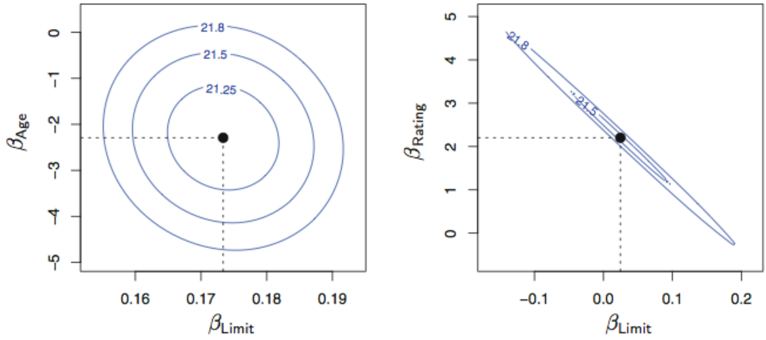

FIGURE 3.15. *Contour plots for the RSS values as a function of the parameters β for various regressions involving the* `Credit` *data set. In each plot, the black dots represent the coefficient values corresponding to the minimum RSS.* Left: *A contour plot of RSS for the regression of* `balance` *onto* `age` *and* `limit`*. The minimum value is well defined.* Right: *A contour plot of RSS for the regression of* `balance` *onto* `rating` *and* `limit`*. Because of the collinearity, there are many pairs $(\beta_{\text{Limit}}, \beta_{\text{Rating}})$ with a similar value for RSS.*

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Rregression Diagnostics: Collinearity

From (9), we can see that:

- If $X_1, \ldots, X_p$ are orthogonal, $\widehat{\beta}_j$ is equal to the simple regression coefficient of y on $(\mathbf{1}, X_j)$.
  - $\widehat{u}_j = X_j - \overline{X}_j$
- If $X_1, \ldots, X_p$ are correlated – in particular – if X_j is highly correlated with the other predictors, then $\widehat{u}_j$ will be close to 0. This makes $\widehat{\beta}_j$ unstable, as both the denominator and the numerator are small.

From (12), we can see that:

- If X_j is highly correlated with the other predictors, the variance of $\widehat{\beta}_j$ is inflated, making it less likely to be significant.

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Rregression Diagnostics: Collinearity

		Coefficient	Std. error	t-statistic	p-value
Model 1	`Intercept`	−173.411	43.828	−3.957	< 0.0001
	`age`	−2.292	0.672	−3.407	0.0007
	`limit`	0.173	0.005	34.496	< 0.0001
Model 2	`Intercept`	−377.537	45.254	−8.343	< 0.0001
	`rating`	2.202	0.952	2.312	0.0213
	`limit`	0.025	0.064	0.384	0.7012

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Rregression Diagnostics: Collinearity

- A simple way to detect collinearity is to look at the correlation matrix of the predictors.
- However, it is possible for collinearity to exist between three or more variables even if no pair of variables has a particularly high correlation. This is called **multicollinearity**.
- **Variance inflation factor (VIF)**:

$$VIF\left(\widehat{\beta}_j\right) = \frac{1}{1 - R^2_{X_j|X_{-j}}}$$

, where $R^2_{X_j|X_{-j}}$ is the R^2 from a regression of X_j onto all of the other predictors.

  - $VIF \geq 1$. Large VIF indicates a problematic amount of collinearity.

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Rregression Diagnostics: Collinearity

- When faced with the problem of collinearity, a simple solution is to drop one of the problematic variables.
- Suppose two variables both contribute in explaining y, but are highly correlated with each other.
  - Both will be insignificant if both are included in the regression model.
  - Dropping one will likely make the other significant.
- This is why we can't remove two (or more) supposedly insignificant predictors *at a time*: significance depends on what other predictors are in the model!

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Maximum Likeliood Estimation

- While least squares regression learns a deterministic function $f(x)$ that directly maps each x into a prediction of y, an alternative approach is to learn the conditional distribution $p(y|x)$ and use the estimated $p(y|x)$ to form a prediction of y.

- To do so, let $\mathcal{H} = \{q_\theta(y|x) : \theta \in \Theta\}$, where the hypotheses $q_\theta(y|x)$ are conditional distributions parametrized by $\theta \in \Theta$.

- We select a $q_\theta(y|x) \in \mathcal{H}$, or equivalently, a $\theta \in \Theta$, by minimizing the empirical KL divergence, or equivalently, by maximizing the (log) likelihood function.

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The log likelihood function[16]:

$$\log \mathcal{L}(\theta) = \sum_{i=1}^{N} \log q_\theta(y_i | x_i)$$

The maximum likelihood estimator chooses

$$\widehat{\theta} = \arg\max_{\theta \in \Theta} \log \mathcal{L}(\theta)$$

[16] Also written as $\log \mathcal{L}(\theta | \mathcal{D})$ to emphasize its dependence on sample $\mathcal{D}$.

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Normal Linear Model

The normal linear regression model is $\mathcal{H} = \{q_\theta(y|x)\}$, where

$$q_\theta(y|x) = \mathcal{N}\left(x'\beta, \sigma^2\right) \tag{17}$$

, where $\theta = (\beta, \sigma)$.

This is equivalent to assuming[17]:

$$y = x'\beta + e,\ e \sim \mathcal{N}\left(0, \sigma^2\right) \tag{18}$$

[17] Notice the strong assumptions imposed by (17) and (18). In addition to assuming a linear regression function, we are now assuming that (1) at each x, the scatter of y around the regression function is Gaussian (**Gaussianity**); (2) the variance of this scatter is constant (**homoskedasticity**); and (3) there is no dependence between this scatter and anything else (**error independence**).

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Normal Linear Model

Given sample $\mathcal{D}$ and model (17),

$$\log \mathcal{L} = \sum_{i=1}^{N} \log \left\{ \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} \left(y_i - x_i' \beta \right)^2 \right) \right\}$$
$$= -\frac{N}{2} \log(2\pi) - N \log \sigma - \frac{1}{2\sigma^2} \underbrace{\sum_{i=1}^{N} \left(y_i - x_i' \beta \right)^2}_{\text{RSS}} \tag{19}$$

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Normal Linear Model

Maximizing (19) with respect to β and $\sigma \Rightarrow$

$$\frac{\partial \log \mathcal{L}}{\partial \beta} = 0 \Rightarrow \widehat{\beta} = \left[\sum_{i=1}^{N} x_i x_i'\right]^{-1} \sum_{i=1}^{N} x_i y_i = \left(X'X\right)^{-1} X'Y$$

$$\frac{\partial \log \mathcal{L}}{\partial \sigma} = 0 \Rightarrow \widehat{\sigma} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - x_i'\widehat{\beta}\right)^2}$$

Thus, maximum likelihood estimation of the normal linear model produces the same estimate of β as least squares regression.

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Normal Linear Model

Let's fit the normal linear model (17) on the data we generated on page 14:

```
# Define the negative log likelihood function
nll <-function(theta){
  beta0 <- theta[1]
  beta1 <- theta[2]
  beta2 <- theta[3]
  sigma <- theta[4]
  N <- length(y)
  z <- (y - beta0 - beta1*x1 - beta2*x2)/sigma
  logL <- -1*N*log(sigma) - 0.5*sum(z^2)
  return(-logL)}
#
# Minimize the negative likelihood function
mlefit <- optim(c(0,0,0,1),nll) # initial value for theta: (0,0,0,1)
mlefit$par # parameter estimate

## [1]  1.010153 -2.591790  5.062709  1.004935
```

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Normal Linear Model

```
# Alternatively, use the mle2 function from the bbmle package
require(bbmle)
parnames(nll) <- c("beta0","beta1","beta2","sigma")
result <- mle2(nll,start=c(beta0=0,beta1=0,beta2=0,sigma=1))
summary(result)

## Maximum likelihood estimation
##
## Call:
## mle2(minuslogl = nll, start = c(beta0 = 0, beta1 = 0, beta2 = 0,
##     sigma = 1))
##
## Coefficients:
##        Estimate Std. Error  z value     Pr(z)
## beta0  1.010134   0.118487   8.5253 < 2.2e-16 ***
## beta1 -2.591654   0.224609 -11.5385 < 2.2e-16 ***
## beta2  5.062493   0.311189  16.2682 < 2.2e-16 ***
## sigma  1.004913   0.031778  31.6227 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

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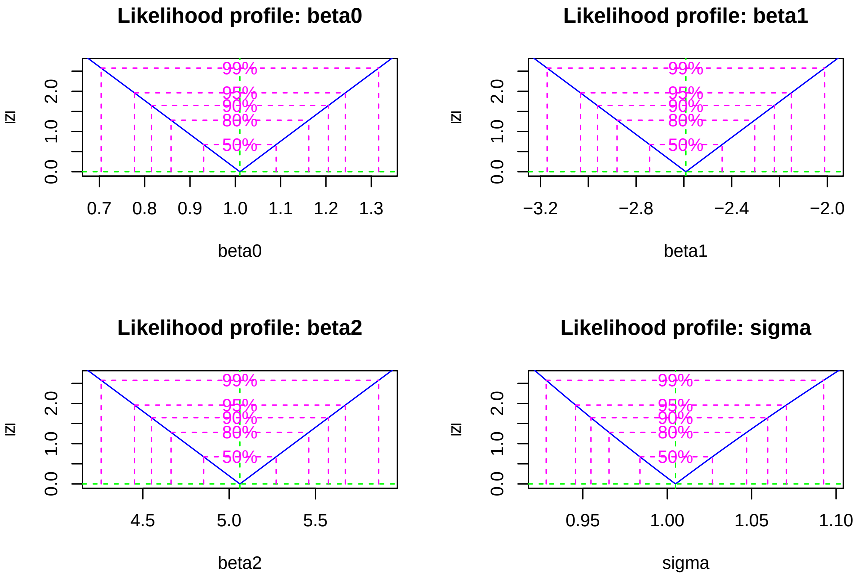
Normal Linear Model



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Moving Beyond Linearity

- The CEF $f(x) = E(y|x)$ is seldom linear. The least squares linear regression model, however, doesn't have to be linear in x either. We can move beyond linearity in inputs x as long as we retain linearity in parameters β[18].

- Polynomial regression is a standard way to extend linear regression to settings in which the relationship between x and y is nonlinear.

[18] We have already seen examples of including nonlinear terms in x such as $\log(x)$ and interaction effects $(x_1 x_2)$ in the regression model.

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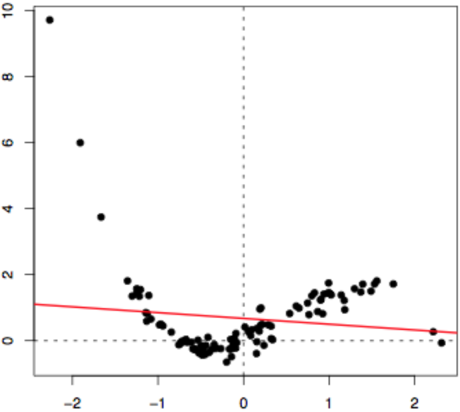
Polynomial Regression



$$h(x) = \beta_0 + \beta_1 x$$

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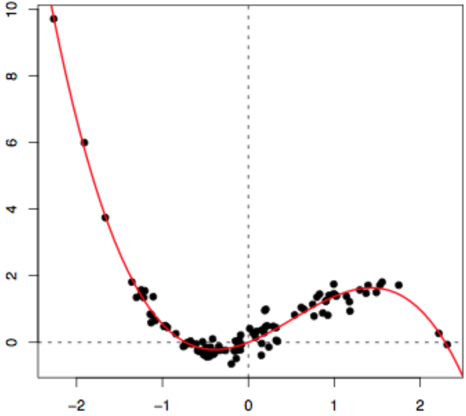
Polynomial Regression



$$h(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$

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Wage Profile

Data: income survey for men in central Atlantic region of USA

```
require(AER)
require(ISLR) # contains the data set 'Wage'
fit = lm(wage ~ poly(age,4,raw=T),data=Wage) # degree-4 polynomial
coeftest(fit)

##
## t test of coefficients:
##
##                         Estimate  Std. Error t value  Pr(>|t|)
## (Intercept)          -1.8415e+02  6.0040e+01 -3.0672 0.0021803 **
## poly(age, 4, raw = T)1  2.1246e+01  5.8867e+00  3.6090 0.0003124 ***
## poly(age, 4, raw = T)2 -5.6386e-01  2.0611e-01 -2.7357 0.0062606 **
## poly(age, 4, raw = T)3  6.8107e-03  3.0659e-03  2.2214 0.0263978 *
## poly(age, 4, raw = T)4 -3.2038e-05  1.6414e-05 -1.9519 0.0510386 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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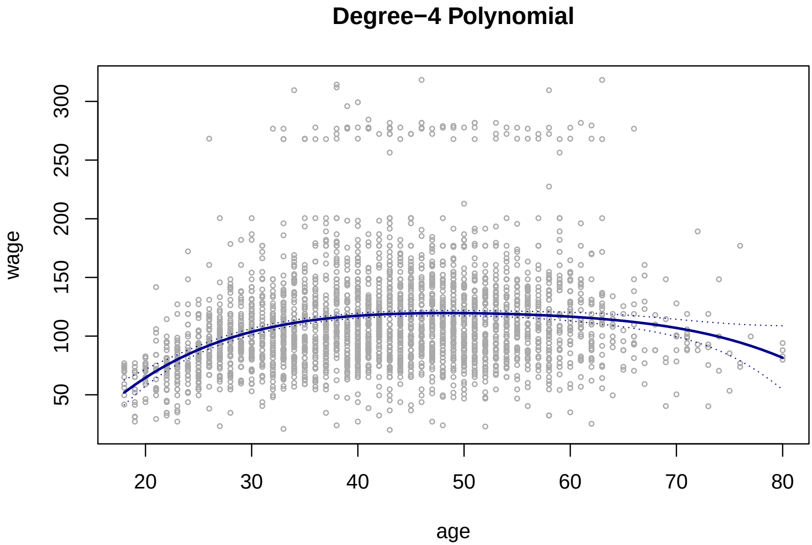
Wage Profile



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Piecewise Constant Regression

- For the following analysis, consider modeling the relationship between y and a single input variable x.
- So far we have imposed a ☼`global`☽ structure on the relationship between x and y.
- Piecewise regression breaks the input space into distinct regions and fit a different relationship in each region.

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Piecewise Constant Regression

How it works:

1. Divide the range of x into M regions by creating $M-1$ cutpoints, or **knots**, $\xi_1, \ldots, \xi_{M-1}$. Then construct the following dummy variables:

Region	$\phi(x)$
R_1	$\phi_1(x) = \mathcal{I}(x < \xi_1)$
R_2	$\phi_2(x) = \mathcal{I}(\xi_1 \leq x < \xi_2)$
$\vdots$	$\vdots$
R_M	$\phi_M(x) = \mathcal{I}(\xi_{M-1} \leq x)$

This amounts to converting a continuous variable into an *ordered categorical variable*.

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Piecewise Constant Regression

How it works:

2. Fit the following model:

$$y = \beta_1 \phi_1 (x) + \beta_2 \phi_2 (x) + \cdots + \beta_M \phi_M (x) + e \tag{20}$$

$\sum_{m=1}^{M} \beta_m \phi_m (x)$ is a **step function** or **piecewise constant function**, and (20) is called a **piecewise constant regression** model.

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Piecewise Constant Regression

Solving (20) by least squares $\Rightarrow$

$$\widehat{\beta}_m = \overline{y}_m$$

, where $\overline{y}_m \equiv \frac{1}{n_m} \sum_{x_i \in R_m} y_i$[19].

i.e., for every $x \in R_m$, we make the same prediction, which is simply the mean of the response values for the training observations in R_m.

[19] n_m is the number of observations in R_m.

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Wage Profile

```r
# cut(x,M) divides x into M pieces of equal length
#          and generates the corresponding dummy variables
fit = lm(wage ~ 0 + cut(age,4),data=Wage) # no intercept
coeftest(fit)

##
## t test of coefficients:
##
##                         Estimate Std. Error t value  Pr(>|t|)
## cut(age, 4)(17.9,33.5]  94.1584     1.4761  63.790 < 2.2e-16 ***
## cut(age, 4)(33.5,49]   118.2119     1.0808 109.379 < 2.2e-16 ***
## cut(age, 4)(49,64.5]   117.8230     1.4483  81.351 < 2.2e-16 ***
## cut(age, 4)(64.5,80.1] 101.7990     4.7640  21.368 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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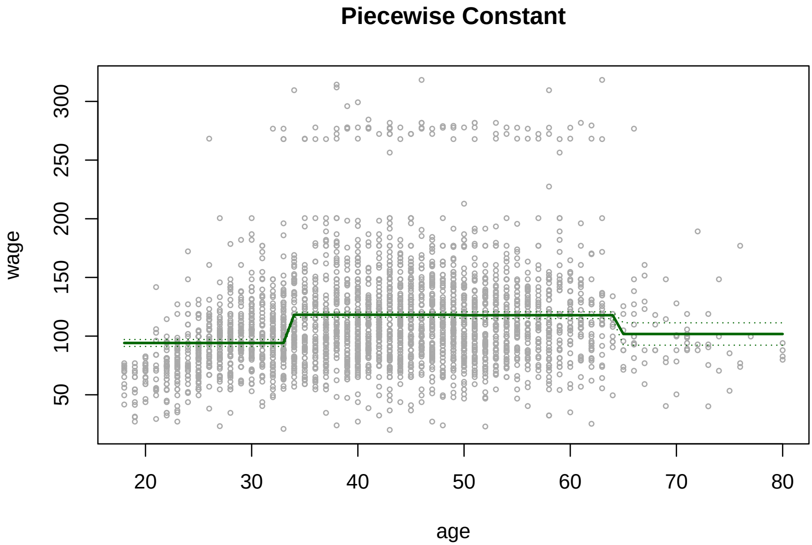
Wage Profile



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Basis Functions

In general, $\phi(x)$ are called **basis functions** and do not have to be dummy variables. They can be any functions of x.

A **linear basis function model** is defined as[20]:

$$y = \beta_1 \phi_1(x) + \beta_2 \phi_2(x) + \cdots + \beta_M \phi_M(x) + e = \beta' \Phi(x) + e \tag{21}$$

, where $\beta = (\beta_1, \ldots, \beta_M)'$ and $\Phi = (\phi_1, \ldots, \phi_M)'$.

Solving (21) by least squares $\Rightarrow$

$$\widehat{\beta} = \left(\Phi'\Phi\right)^{-1} \Phi' Y$$

, where $\Phi = \Phi(X)$.

[20] Notice that (21) is the same as (20), except now $\phi(x)$ can be any function of x.

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Regression Splines

- Polynomial and piecewise constant regression models are special cases of linear basis function models[21].

- We can also do **piecewise polynomial regression**, which involves fitting different polynomials over different regions of x.

[21] For example, for $K-$degree polynomial regressions, $\phi_1(x) = 1, \phi_2(x) = x, \phi_3(x) = x^2, \ldots, \phi_K(x) = x^K$.

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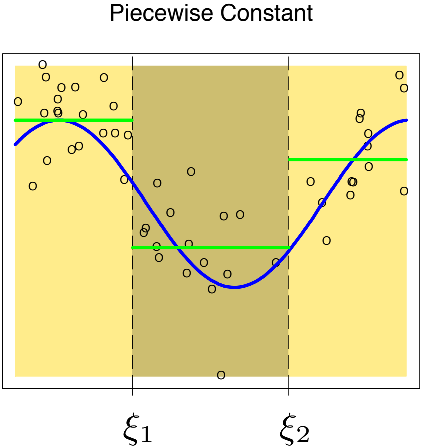
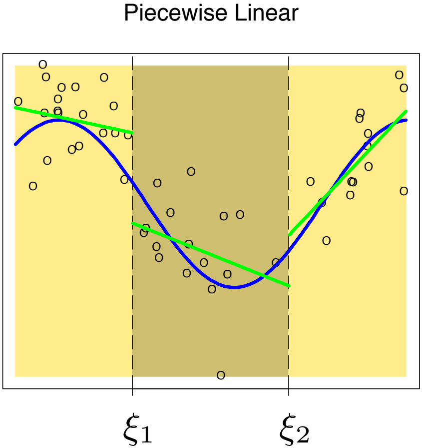
Regression Splines





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Regression Splines

Oftentimes it is desired that the fitted curve is continuous over the range of x, i.e. there should be no jump at the knots.

For piecewise linear regression with one knot (ξ), this means:

$$y = \begin{cases} \alpha_{10} + \alpha_{11} x + e & x < \xi \\ \alpha_{20} + \alpha_{21}(x - \xi) + e & x \geq \xi \end{cases} \tag{22}$$

under the constraint that

$$\alpha_{10} + \alpha_{11}\xi = \alpha_{20} \tag{23}$$

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Regression Splines

(22) and (23) $\Rightarrow$ the continuous piecewise linear model can be parametrized as

$$y = \beta_0 + \beta_1 x + \beta_2 (x - \xi)_+ + e \tag{24}$$

, where $\beta_0 = \alpha_{10}$, $\beta_1 = \alpha_{11}$, $\beta_2 = \alpha_{21} - \alpha_{11}$, and $(x - \xi)_+ \equiv (x - \xi) \mathcal{I} (x \geq \xi)$.

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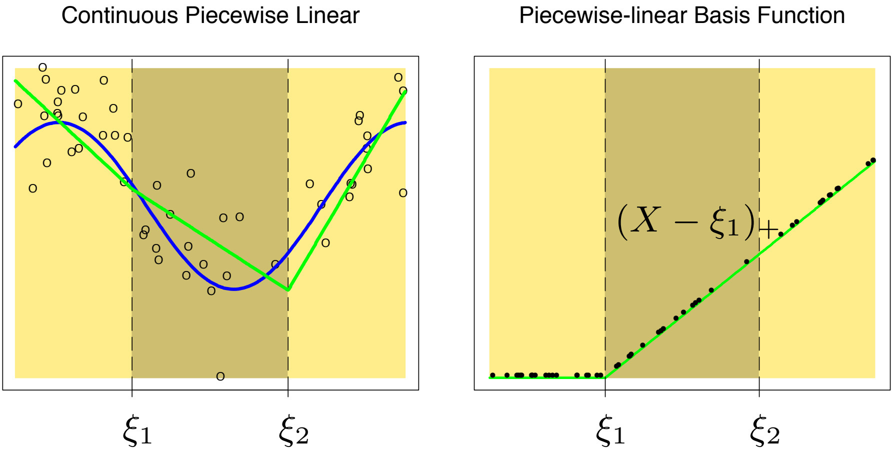
Regression Splines



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Regression Splines

For higher-order piecewise polynomial regression, in addition to the fitted curve being continuous, we may also want it to be smooth by requiring the derivatives of the piecewise polynomials to be also continuous at the knots.

For piecewise cubic polynomial regression with one knot (ξ), this means:

$$y = \begin{cases} \alpha_{10} + \alpha_{11}x + \alpha_{12}x^2 + \alpha_{13}x^3 + e & x < \xi \\ \alpha_{20} + \alpha_{21}(x-\xi) + \alpha_{22}(x-\xi)^2 + \alpha_{23}(x-\xi)^3 + e & x \geq \xi \end{cases} \tag{25}$$

subject to the constraints that the piecewise polynomials as well as their 1^{st} and 2^{nd} derivatives are continuous at ξ:

$$\begin{aligned} \alpha_{10} + \alpha_{11}\xi + \alpha_{12}\xi^2 + \alpha_{13}\xi^3 &= \alpha_{20} \\ \alpha_{11} + 2\alpha_{12}\xi + 3\alpha_{13}\xi^2 &= \alpha_{21} \\ \alpha_{12} + 3\alpha_{13}\xi &= \alpha_{22} \end{aligned} \tag{26}$$

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Regression Splines

(25) and (26) $\Rightarrow$

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - \xi)_+^3 + e \tag{27}$$

, where $\beta_0 = \alpha_{10}$, $\beta_1 = \alpha_{11}$, $\beta_2 = \alpha_{12}$, $\beta_3 = \alpha_{13}$, and $\beta_4 = \alpha_{23} - \alpha_{13}$.

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Regression Splines

(24) and (27) are examples of **regression splines**. (24) is called a *linear spline* and (27) is called a *cubic spline*.

Regression Spline

A degree$-d$ spline is a piecewise degree$-d$ polynomial, with continuity in derivatives up to degree $d-1$ at each knot.

- In general, a degree$-d$ spline with $M-1$ knots has $d+M$ degrees of freedom[22].

[22] For example, a linear spline has $1+M$ degrees of freedom (see (24)). A cubic spline has $3+M$ degress of freedom (see (27)). In comparison, a degree$-d$ polynomial has $d+1$ degrees of freedom.

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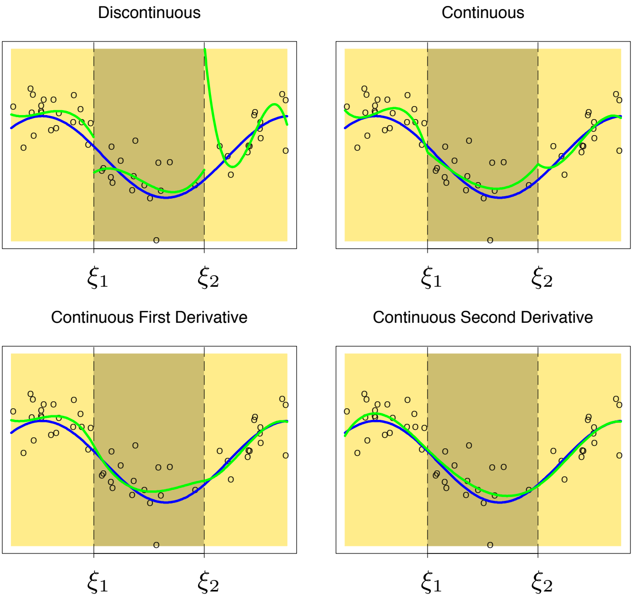
Piecewise Cubic Polynomials



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Natural Splines

- Splines tend to have high variance at the boundary ($x < \xi_1$ or $x \geq \xi_{M-1}$, where $M-1$ is the total number of knots).

- A **natural spline** is a regression spline with additional boundary constraints: the function is required to be *linear* beyond the boundary knots, in order to produce more stable estimates.

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Wage Profile

```r
require(splines)

# Cubic Spline
# ------------
# bs() generates B-spline basis functions with specified degrees
#      of polynomials and knots
fit = lm(wage ~ bs(age,knots=c(25,40,60),degree=3),data=Wage)
#     knots at age 25,40,60

# Natural Cubic Spline
# --------------------
# ns() fits a natural cubic spline
fit2 = lm(wage ~ ns(age,knots=c(25,40,60)))
```

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Wage Profile

```
coeftest(fit)

##
## t test of coefficients:
##
##                                          Estimate Std. Error t value
## (Intercept)                               60.4937     9.4604  6.3944
## bs(age, knots = c(25, 40, 60), degree = 3)1   3.9805    12.5376  0.3175
## bs(age, knots = c(25, 40, 60), degree = 3)2  44.6310     9.6263  4.6364
## bs(age, knots = c(25, 40, 60), degree = 3)3  62.8388    10.7552  5.8426
## bs(age, knots = c(25, 40, 60), degree = 3)4  55.9908    10.7063  5.2297
## bs(age, knots = c(25, 40, 60), degree = 3)5  50.6881    14.4018  3.5196
## bs(age, knots = c(25, 40, 60), degree = 3)6  16.6061    19.1264  0.8682
##                                            Pr(>|t|)
## (Intercept)                               1.863e-10 ***
## bs(age, knots = c(25, 40, 60), degree = 3)1 0.7508987
## bs(age, knots = c(25, 40, 60), degree = 3)2 3.698e-06 ***
## bs(age, knots = c(25, 40, 60), degree = 3)3 5.691e-09 ***
## bs(age, knots = c(25, 40, 60), degree = 3)4 1.815e-07 ***
## bs(age, knots = c(25, 40, 60), degree = 3)5 0.0004387 ***
## bs(age, knots = c(25, 40, 60), degree = 3)6 0.3853380
```

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Wage Profile

```
coeftest(fit2)

##
## t test of coefficients:
##
##                                Estimate Std. Error t value  Pr(>|t|)
## (Intercept)                     54.7595     5.1378 10.6581 < 2.2e-16 **
## ns(age, knots = c(25, 40, 60))1  67.4019     5.0134 13.4442 < 2.2e-16 **
## ns(age, knots = c(25, 40, 60))2  51.3828     5.7115  8.9964 < 2.2e-16 **
## ns(age, knots = c(25, 40, 60))3  88.5661    12.0156  7.3709 2.181e-13 **
## ns(age, knots = c(25, 40, 60))4  10.6369     9.8332  1.0817    0.2795
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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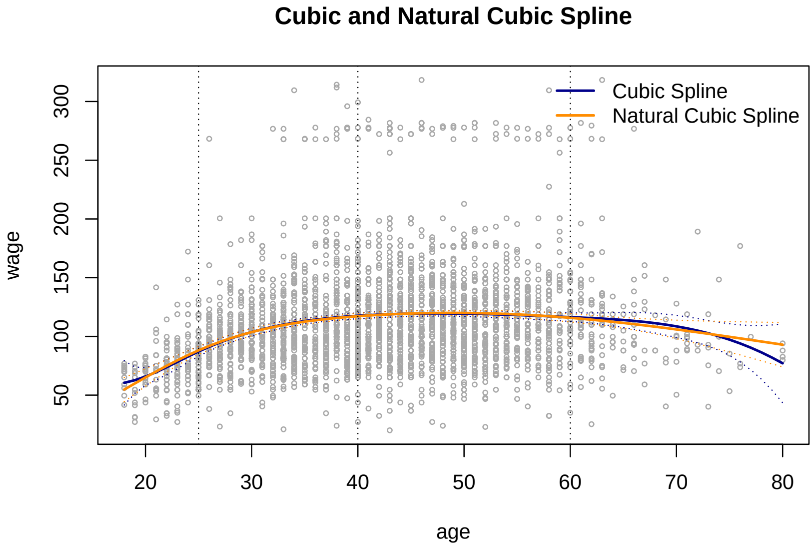
Wage Profile



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Generalized Additive Models

So far we have been dealing with a single input x in our discussion of polynomial regression and regression splines. A natural way to extend this discussion to multiple inputs is to assume the following model:

$$y = \omega_0 + \omega_1(x_1) + \omega_2(x_2) + \cdots \omega_p(x_p) + e \tag{28}$$

, where

$$\omega_j(x_j) = \sum_{m=1}^{M_j} \beta_{jm}\phi_{jm}(x_j)$$

(28) is called a **generalized additive model (GAM)**.

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Generalized Additive Models

The GAM allows for flexible nonlinear relationships in each dimension of the input space while maintaining the additive structure of linear models.

- For example, we can fit a linear relationship in x_1, a polynomial in x_2, a cubic spline in x_3, etc.
- The GAM remains a linear basis function model and therefore can be fit by least squares[23].

[23] (28) is equivalent to

$$y = \beta' \Phi(x) + e$$

, where $\Phi = \left(\mathbf{1}, \phi_{11}, \ldots, \phi_{1M_1}, \ldots, \phi_{p1}, \ldots, \phi_{pM_p}\right)'$.

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Wage Profile

```
fit = lm(wage ~ poly(year,2) + ns(age,knots=c(25,40,60)) + education)
coeftest(fit)

##
## t test of coefficients:
##
##                                Estimate Std. Error t value  Pr(>|t|)
## (Intercept)                     47.5751     4.8992  9.7108 < 2.2e-16 **
## poly(year, 2)1                 130.4942    35.2930  3.6974 0.0002217 **
## poly(year, 2)2                 -36.3005    35.2579 -1.0296 0.3032959
## ns(age, knots = c(25, 40, 60))1  51.1072     4.4572 11.4662 < 2.2e-16 **
## ns(age, knots = c(25, 40, 60))2  33.1989     5.0767  6.5394 7.237e-11 **
## ns(age, knots = c(25, 40, 60))3  53.5004    10.6621  5.0178 5.532e-07 **
## ns(age, knots = c(25, 40, 60))4  12.3733     8.6866  1.4244 0.1544320
## education2. HS Grad             10.8174     2.4305  4.4507 8.871e-06 **
## education3. Some College        23.3191     2.5626  9.0997 < 2.2e-16 **
## education4. College Grad        37.9867     2.5464 14.9176 < 2.2e-16 **
## education5. Advanced Degree     62.5184     2.7629 22.6275 < 2.2e-16 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

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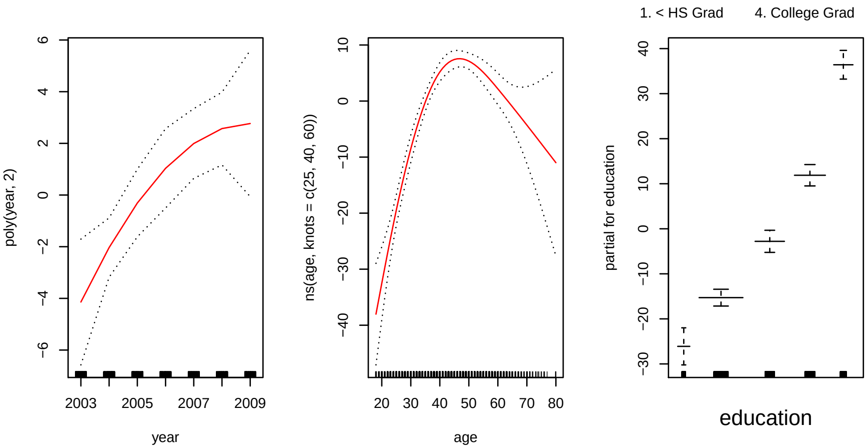
Wage Profile



A GAM model of wage with a quadratic polynomial in `year`, a natural cubic spline in `age`, and a step function in `education`

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Generalization Issues

Fitting a linear basis function model (21) can be thought of as a two-step process:

1. Transform x into $\Phi(x)$[24].
   - Let $z = \Phi(x) \in \mathcal{Z}$. $\Phi : \mathcal{X} \to \mathcal{Z}$ is called a **feature transform**.
2. Fit the linear model: $\mathcal{H}_\Phi = \{h : h(z) = \beta' z\}$, where $\mathcal{H}_\Phi$ denotes the hypothesis set corresponding to the feature transform Φ.

[24] x can be multi-dimensional: $x = (x_1, \ldots, x_p)$

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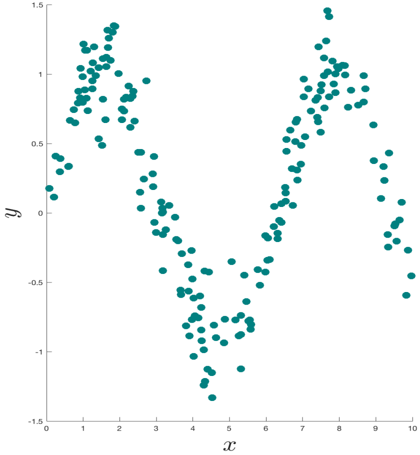
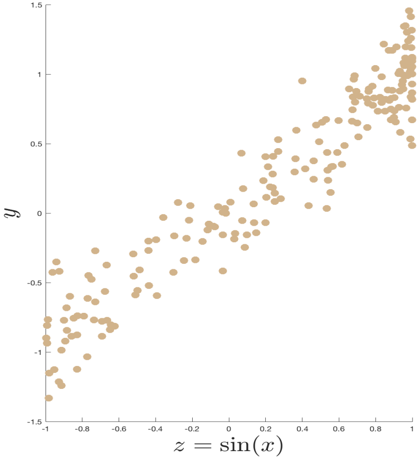
Feature Transform





Left: data in $\mathcal{X}-$space; Right: data in $\mathcal{Z}-$space

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Generalization Issues

If we decide on the feature transform Φ *before* seeing the data, then the VC generalization bound holds with $d_{VC}(\mathcal{H}_\Phi)$ as the VC dimension.

I.e., for any $g \in \mathcal{H}_\Phi$, with probability at least $1-\delta$,

$$\begin{aligned} E_{out}(g) &\leq E_{in}(g) + \sqrt{\frac{8}{N} \ln \frac{4\left((2N)^{d_{VC}}+1\right)}{\delta}} \\ &= E_{in}(g) + \mathcal{O}\left(\sqrt{\frac{d_{VC}}{N} \ln N}\right) \end{aligned} \tag{29}$$

, where $d_{VC} = d_{VC}(\mathcal{H}_\Phi)$.

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Generalization Issues

Therefore, when choosing a high-order polynomial, or a spline with many degrees of freedom, or a GAM with complex nonlinearities in many dimensions, we cannot avoid the approximation-generalization tradeoff:

- More complex $\mathcal{H}_\Phi$ $(d_{VC}(\mathcal{H}_\Phi)\uparrow) \Rightarrow E_{in}\downarrow$
- Less complex $\mathcal{H}_\Phi$ $(d_{VC}(\mathcal{H}_\Phi)\downarrow) \Rightarrow |E_{out} - E_{in}|\downarrow$

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Generalization Issues

What if we try a transformation Φ_1 first, and then, finding the results unsatisfactory, decide to use Φ_2? Then we are effectively using a model that contains both $\{\beta'\Phi_1(x)\}$ and $\{\beta'\Phi_2(x)\}$.

- For example, if we try a linear model first, then a quadratic polynomial, then a piecewise constant model, before settling on a cubic spline, then d_{VC} in (29) should be the VC dimension of a hypothesis set that contains not only the cubic spline model, but all of the aforementioned models.
- The process of trying a series of models until we get a satisfactory result is called **specification search** or **data snooping**. In general, the more models you try, the poorer your final result will generalize out of sample.

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Acknowledgement I

Part of this lecture is adapted from the following sources:

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- Shalizi, C. R. 2019. *Advanced Data Analysis from an Elementary Point of View*. Manuscript.

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Acknowledgement II

- Taddy, M. *Big Data*. Lecture at the University of Chicago Booth School of Business, retrieved on 2017.01.01. [link]

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