Data Mining
W4240 Section 001

Giovanni Motta

Columbia University, Department of Statistics

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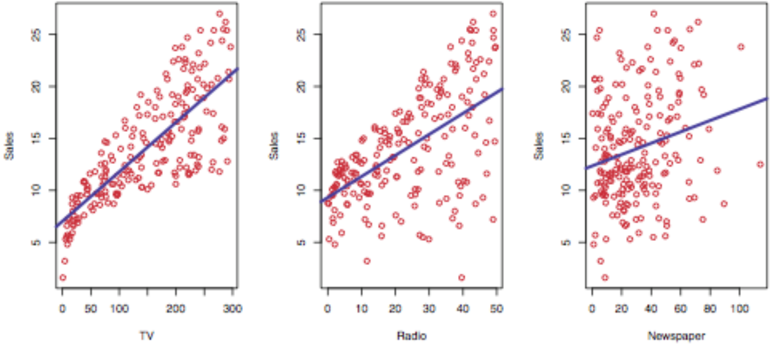
Outline

Advertising Data

Recall from before:

$$\texttt{sales} = f(\texttt{TV}, \texttt{radio}, \texttt{newspaper}) + \epsilon$$



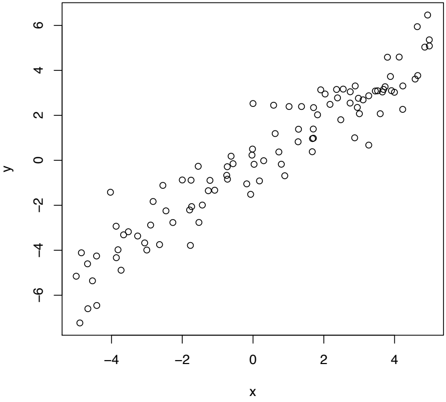
Advertising Data

Questions:

1. Is there a relationship between the advertising budget and sales?
2. How strong is the relationship between advertising budget and sales?
3. Which media contribute to sales?
4. How accurately can we estimate the effects of each medium on sales?
5. How accurately can we predict future sales?
6. Is the relationship linear?
7. Is there synergy between media? (Synergy means $f(a \text{ and } b) > f(a) + f(b)$)

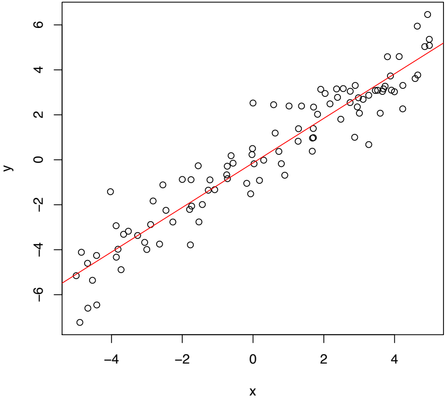
Can we use kNN to answer these questions? What type of model can answer these questions?

Linear Regression



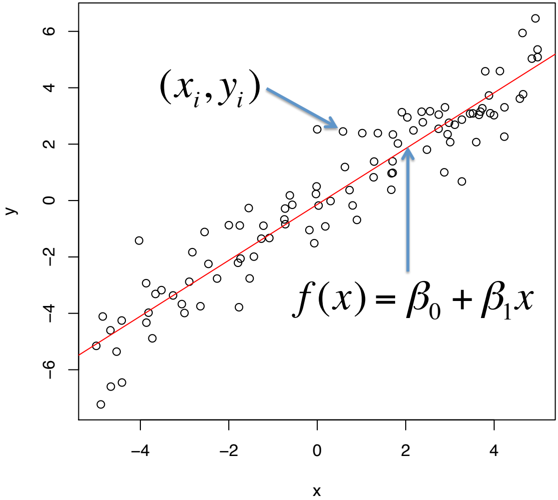
Training data are the set of inputs and outputs, $\mathcal{T} = \{(x_i, y_i)\}_{i=1}^{n}$

Linear Regression



In *linear regression*, the goal is to predict Y from X using a linear function

Linear Regression



Why am I now showing β and not $\mathbf{w}$ (a notational apology)?

Linear Regression

Model:

$$f(X) \approx \beta_0 + \beta_1 X$$

...but we don't know β_0 and β_1. How can we estimate them from the data?

Let's begin by looking at the *residual sum of squares* (RSS):

$$\begin{aligned} RSS(\beta_0, \beta_1) &= \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 \end{aligned}$$

The i^{th} *residual* is the difference between the observed value and the predicted value, $y_i - \beta_0 - \beta_1 x_i$. (Compare to MSE...)

Linear Regression

Notice that RSS is a *function* of (β_0, β_1). Let's pick the pair that **minimizes RSS**:

$$(\hat{\beta}_0, \hat{\beta}_1) = \arg\min \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

- Hold on! Last lecture you told us that picking a model that minimizes training MSE can lead to overfitting!
- Does this *model* minimize training MSE?

Linear Regression

Let's take the derivative of $RSS(\beta_0, \beta_1)$ with respect to β_0 and set it equal to 0:

$$\frac{\partial}{\partial \beta_0} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) \ \ (= 0)$$

$$n\beta_0 = -\beta_1 \sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i$$

$$\beta_0 = \bar{y} - \beta_1 \bar{x}$$

<u>What does this last line mean?</u>

Linear Regression

Now let's take the derivative of $RSS(\beta_0, \beta_1)$ with respect to β_1 and set it equal to 0:

$$\frac{\partial}{\partial \beta_1} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 = -2 \sum_{i=1}^{n} x_i \left(y_i - \beta_0 - \beta_1 x_i\right) \ (= 0)$$

$$\beta_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i - \beta_0 \sum_{i=1}^{n} x_i$$

$$\beta_1 = \frac{\sum_{i=1}^{n} y_i x_i - n\beta_0 \bar{x}}{\sum_{i=1}^{n} x_i^2}$$

Linear Regression

Now we have two equations and two unknowns, so let's solve for β_0 and β_1:

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

$$\hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i - \hat{\beta}_0 \sum_{i=1}^{n} x_i$$

$$\hat{\beta}_1 \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i - \left(\bar{y} - \hat{\beta}_1 \bar{x}\right) \sum_{i=1}^{n} x_i$$

$$\hat{\beta}_1 \left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 \right) = \sum_{i=1}^{n} x_i y_i - n\bar{x}\bar{y}$$

$$\underline{\hat{\beta}_1} = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$

Outline

How Accurate are the Coefficients?

We can approximate

$$Y = f(X) + \epsilon_1$$

by a linear model

$$Y = \beta_0 + \beta_1 X + \epsilon_2.$$

This is called the **population regression line.**

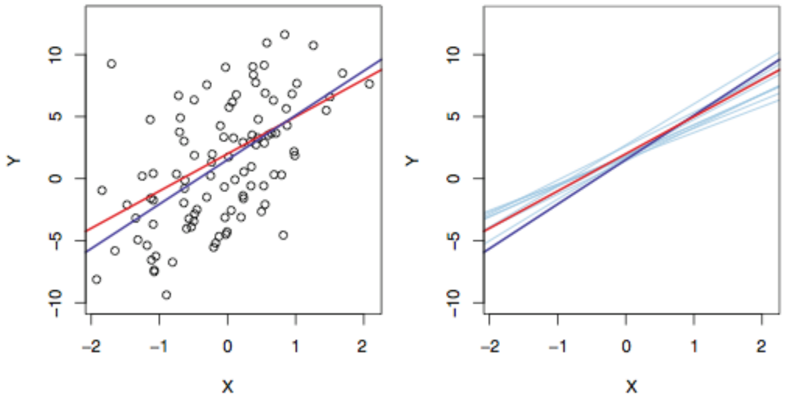
However, $\hat{\beta}_0$ and $\hat{\beta}_1$ produce a **least squares line**,

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

How different are these?

How Accurate are the Coefficients?

The red line: $f(X) = 2 + 3X$. The dots: $y_i = 2 + 3x_i + \epsilon_i$



Ten blue lines: different data produce different $(\hat{\beta}_0, \hat{\beta}_1)$.[1]

[1]Some images are taken from *An Introduction to Statistical Learning* by James, Witten, Hastie and Tibshirani.

How Accurate are the Coefficients?

Population regression line:

$$Y = \beta_0 + \beta_1 X + \epsilon_2$$

Least squares line:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

What can we say about $\hat{\beta}_0$ vs β_0 and $\hat{\beta}_1$ vs β_1:

- $\hat{\beta}_0$ and $\hat{\beta}_1$ are ***unbiased*** estimators of β_0 and β_1

$$\mathbb{E}\left[\hat{\beta}_0\right] = \beta_0, \quad \mathbb{E}\left[\hat{\beta}_1\right] = \beta_1$$

- (prove that for at least one of these)
- What about $\mathrm{Var}(\hat{\beta}_0)$? (Read James 3.1 or take W4315)
- This allows us to do hypothesis testing... why?

Assessing Model Accuracy

Let ϵ_i be iid with mean 0 and variance σ_ϵ^2. Then

$$\boxed{\begin{aligned} \mathbb{V}\text{ar}(\hat\beta_0) = [\mathrm{SE}(\hat\beta_0)]^2 &= \sigma_\epsilon^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right] \\ \mathbb{V}\text{ar}(\hat\beta_1) = [\mathrm{SE}(\hat\beta_1)]^2 &= \frac{\sigma_\epsilon^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \end{aligned}}$$

95% confidence intervals

$$\hat\beta_0 \pm 1.96 \times \mathrm{SE}(\hat\beta_0) \qquad \hat\beta_1 \pm 1.96 \times \mathrm{SE}(\hat\beta_1)$$

Example: the null hypothesis states that there is no relationship between X and Y

$$H_0 : \beta = 0 \text{ (t-statistics under the null)}$$

$$t = \frac{\hat\beta_1 - 0}{\mathrm{SE}(\hat\beta_1)} \sim t_{(n-2)}$$

Assessing Model Accuracy

So how well does this model represent the data?

- let's try to see how much of the data spread this model captures
- $RSS(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$ is the total amount of error left in the model
- ...but there is some noise to begin with, measured by the *total sum of squares* $TSS = \sum_{i=1}^{n} (y_i - \bar{y})^2$
- the R^2 statistic is the proportion of error reduced by the model,

$$R^2 = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

Assessing Model Accuracy

Sum of squares

$$\begin{aligned}\underline{\mathrm{TSS}} &= \sum_{i=1}^{n}(y_i - \bar{y})^2\\ \underline{\mathrm{ESS}} &= \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2\\ \underline{\mathrm{RSS}} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2\end{aligned}$$

Error decomposition & R^2

$$\mathrm{TSS} = \mathrm{ESS} + \mathrm{RSS}, \qquad R^2 = \frac{\mathrm{ESS}}{\mathrm{TSS}} = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

Outline

Multiple Linear Regression

So what happens if we have more than one predictor? Well, we can just include those in the model as well,

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & X_{11} & \dots & X_{1p} \\ \vdots & & & \\ 1 & X_{n1} & \dots & X_{np} \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_0 \\ \vdots \\ w_p \end{bmatrix}$$

$$\begin{aligned} \mathbf{Y} &= \mathbf{X}\mathbf{w} + \epsilon \\ Y_i &= w_0 + w_1 X_{i1} + \dots + w_p X_{ip} \end{aligned}$$

Multiple Linear Regression

How do we find the least squares coefficients? Same as always...

- Find $RSS(\mathbf{w})$
- Take the gradient with respect to $\mathbf{w}$, set equal to 0
- Do some algebra ($p + 1$ equations, $p + 1$ unknowns)

Multiple Linear Regression

To find the best weights $\mathbf{w}$:

$$\begin{aligned}
\hat{\mathbf{w}} &= \arg\min \sum_{i=1}^{n} \left(y_i - \mathbf{w}^\top \mathbf{x}_i\right)^2 \\
&= \arg\min \sum_{i=1}^{n} y_i^2 - 2y_i \mathbf{w}^\top \mathbf{x}_i + \left(\mathbf{w}^\top \mathbf{x}_i\right)^2 \\
&= \arg\min \sum_{i=1}^{n} y_i^2 - 2\mathbf{w}^\top \left(\sum_{i=1}^{n} y_i \mathbf{x}_i\right) + \mathbf{w}^\top \left(\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top\right) \mathbf{w} \\
&= \arg\min \sum_{i=1}^{n} y_i^2 - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{Y} + \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w}
\end{aligned}$$

Now take the gradient in $\mathbf{w}$, set to 0, and...

$$\hat{\mathbf{w}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}$$

Multiple Linear Regression

$$\boxed{\begin{aligned}\mathbb{E}(\hat{\mathbf{w}}) &= \boldsymbol{\beta} \\ \mathbb{V}\mathsf{ar}(\hat{\mathbf{w}}) &= \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\boldsymbol{\Sigma}_\epsilon\mathbf{X}\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\end{aligned}}$$

Multivariate Linear Regression

What happens when $\mathbf{X} \in \mathbb{R}^{n\times(p+1)}$? (Remember the ones!)
Some caveats:

- we only have a solution if $\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}$ exists
- this happens when $\mathbf{X}^\top\mathbf{X}$ has full rank (here, $p+1$):
  - $\mathbf{X}$ has rank $p+1$ ($p+1$ linearly independent covariate observations)
  - happens with random sampling from a noisy continuous distribution
- if $\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}$ does not exist, there are infinitely many solutions that are optimal
- Example: $\mathbf{X} = [1\ 1],\ \mathbf{Y} = [1]$ vs
  $\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},\ \mathbf{y} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

Multivariate Linear Regression

So what about hypothesis tests with multiple β's?

$$\begin{aligned} H_0 &: \beta_1 = \beta_2 = \cdots = \beta_p = 0 \\ H_1 &: \text{at least one } \beta_j \neq 0 \end{aligned}$$

We can perform this hypothesis test by computing the $F-$statistic:

$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)}$$

- if linear assumption is true, $\mathbb{E}[RSS/(n-p-1)] = \sigma^2$
- if H_0 is true, $\mathbb{E}[(TSS - RSS)/p] = \sigma^2$
- so if H_0 is true, $F-$statistic should be close to 1, otherwise it should be greater
- rejection threshold depends on n and p (again, W4315)

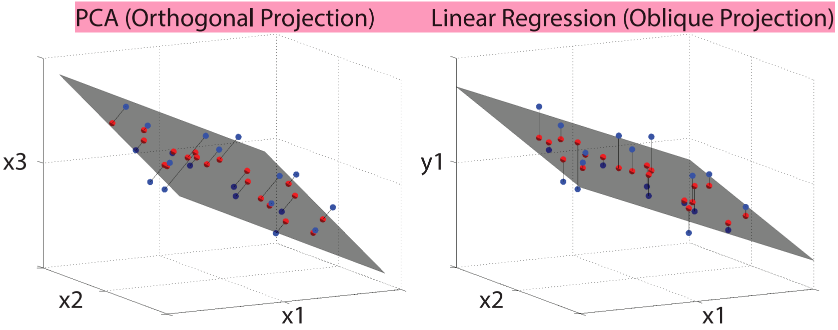
Linear Regression: (Almost) All You Need To Know

$$\boxed{\hat{\mathbf{w}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}}$$

Outline

Big Picture: Supervised vs Unsupervised

- Unsupervised learning seeks explanatory factors
- Supervised learning asserts explanatory factors



Multiple Linear Regression

To find the best weights $\mathbf{w}$:

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&= \arg\min \sum_{i=1}^{n} y_i^2 - 2\mathbf{w}^\top \left(\sum_{i=1}^{n} y_i \mathbf{x}_i\right) + \mathbf{w}^\top \left(\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^\top\right) \mathbf{w} \\
&= \arg\min \sum_{i=1}^{n} y_i^2 - 2\mathbf{w}^\top \mathbf{X}^\top \mathbf{Y} + \mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w}
\end{aligned}$$

Now take the gradient in $\mathbf{w}$, set to 0, and...

$$\hat{\mathbf{w}} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{Y}$$

Principal Component Analysis

To find the best weights $\mathbf{w}$:

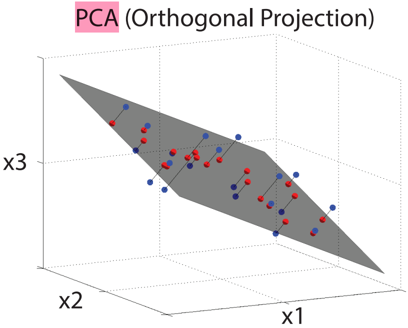
$$
\begin{aligned}
\hat{\mathbf{w}} &= \arg\min \sum_{i=1}^{n} ||\mathbf{x}_i - \mathbf{w}\mathbf{w}^\top \mathbf{x}_i||^2 \\
&= \arg\min \sum_{i=1}^{n} \left(\mathbf{x}_i - \mathbf{w}\mathbf{w}^\top \mathbf{x}_i\right)^\top \left(\mathbf{x}_i - \mathbf{w}\mathbf{w}^\top \mathbf{x}_i\right) \\
&= \arg\min \sum_{i=1}^{n} \mathbf{x}_i^\top \mathbf{x}_i - 2(\mathbf{w}^\top \mathbf{x}_i)^2 + (\mathbf{w}^\top \mathbf{x}_i)^2 \\
&= \arg\min \sum_{i=1}^{n} \mathbf{x}_i^\top \mathbf{x}_i - \mathbf{w}^\top \mathbf{X}^\top \mathbf{X}\mathbf{w}
\end{aligned}
$$

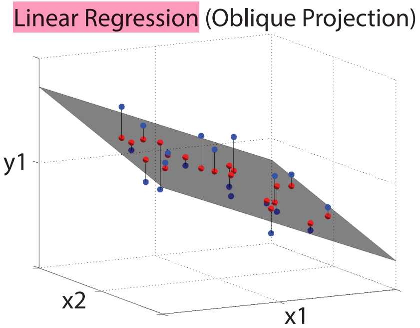
Now take the gradient in $\mathbf{w}$ (with the constraint $||\mathbf{w}|| = 1$), set to 0, and...

$$\hat{\mathbf{w}} = \mathrm{svd}\left(\mathbf{X}^\top \mathbf{X}\right)$$

Big Picture: Supervised vs Unsupervised

- Unsupervised learning seeks explanatory factors
- Supervised learning asserts explanatory factors





Outline

Advertising Data

Questions:

1. Is there a relationship between the advertising budget and sales?
2. How strong is the relationship between advertising budget and sales?
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6. Is the relationship linear?
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Advertising Data

Is there a relationship between the advertising budget and sales?

Use *hypothesis testing*!

Regress `sales` on `TV + newspaper + radio = advertising`;
$\texttt{sales} = \beta_0 + \beta_1 \texttt{advertising}$

$$\begin{aligned} H_0 &: \beta_1 = 0 \\ H_1 &: \beta_1 \neq 0 \end{aligned} \tag{1}$$

Advertising Data

How strong is the relationship between advertising budget and sales?

Use *a confidence interval*!

Regress `sales` on `TV + newspaper + radio = advertising`; $\texttt{sales} = \beta_0 + \beta_1 \texttt{advertising}$

- β_1 tells us the relationship between advertising budget and sales
- a confidence interval gives us more certainty about where the true parameter lies

Advertising Data

Which media contribute to sales?

Use coefficient $p-$*values*!

- from hypothesis testing against coefficient being equal to 0
- it is highly likely that coefficients with high p-values have a linear relationship with the output

Advertising Data

How accurately can we estimate the effects of each medium on sales?

Use a coefficient *confidence interval*!

How accurately can we predict future sales?

Use R^2!

Advertising Data

More questions:

1. Is the relationship linear?
2. Is there synergy between media?

Well, we can't answer these yet...

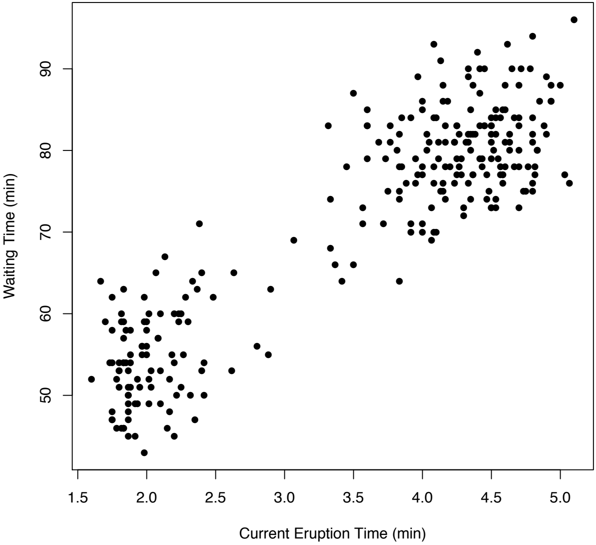
Example: Old Faithful

Example: Old Faithful

We will predict the time that we will have to wait to see the next eruption given the duration of the current eruption

```
>  library(datasets)
>  names(faithful)
[1] "eruptions" "waiting"
>  attach(faithful)
>  plot(eruptions,waiting,xlab="Current Eruption Time (min)",
+ ylab="Waiting Time (min)",pch=16)
```

Example: Old Faithful



Example: Old Faithful

To fit a linear model in R, use the `lm( )` function, which stands for "linear model"

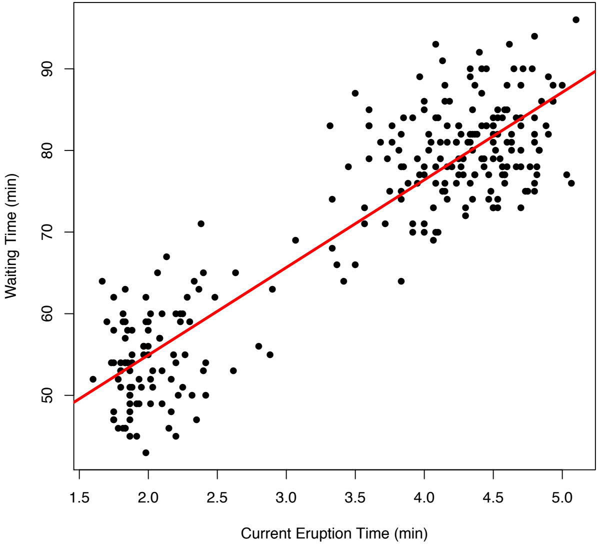
```
> fit.lm <- lm(waiting ~ eruptions)
> fit.lm

Call:
lm(formula = waiting ~ eruptions)

Coefficients:
(Intercept)    eruptions
      33.47        10.73

> names(fit.lm)
 [1] "coefficients"  "residuals"     "effects"
 [4] "rank"          "fitted.values" "assign"
 [7] "qr"            "df.residual"   "xlevels"
[10] "call"          "terms"         "model"
```

Example: Old Faithful

We can plot our data and make a function for new predictions

```
>  # Plot a line on the data
>  abline(fit.lm,col="red",lwd=3)
>
>  # Make a function for prediction
>  fit.lm$coefficients[1]
(Intercept)
    33.4744
>  fit.lm$coefficients[2]
eruptions
  10.72964
>  faithful.fit <- function(x) fit.lm$coefficients[1] +
fit.lm$coefficients[2]*x
>  x.pred <- c(2.0, 2.7, 3.8, 4.9)
>  faithful.fit(x.pred)
[1] 54.93368 62.44443 74.24703 86.04964
```

Example: Old Faithful



Example: Prostate Data

Data in Prostate.txt (also available on ESL website)

Predictors (columns 1–8): lcavol (log cancer volume), lweight (log weight), age, lbph (log amount of benign prostatic hyperplasia), svi (seminal vesicle inversion), lcp (log capsular penetration), gleason, pgg45 (percentage of Gleason scores 4 or 5)

outcome (column 9): lpsa (level of prostate-specific antigen)

train/test indicator (column 10)

```
> prostate <- read.table("Prostate.txt",header=TRUE, sep="\t")
> names(prostate)
 [1] "X"        "lcavol"  "lweight" "age"
 [5] "lbph"     "svi"     "lcp"     "gleason"
 [9] "pgg45"    "lpsa"    "train"
> prostate.train <- prostate[prostate$train==T,2:10]
> prostate.test <- prostate[prostate$train==F,2:10]
```

Example: Prostate Data

```
> prostate.lm <- lm(lpsa ~ lcavol + lweight + age + lbph
   + svi + lcp + gleason + pgg45, data=prostate.train)
> # Other way:
> # prostate.lm <- lm(lpsa ~., data=prostate.train)
> # Exclude intercept by:
> # prostate.lm <- lm(lpsa ~ lcavol + lweight + age + lbph
   + svi + lcp + gleason + pgg45 - 1, data=prostate.train)
> y.pred.lm <- predict(prostate.lm,prostate.test)
> mean((y.pred.lm-prostate.test$lpsa)^2)
[1] 0.521274
```

Note: the data in ESL was scaled before use, so $\hat{\beta}$ differs