# STAT 234 Lecture 24-25 Simple Linear Regression Model (Section 12.1-12.4) 

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## Outline

- Simple Linear Regression Models (Section 12.1)
- Least Square Estimate (Section 12.2)
- Hypothesis Tests \& Confidence Intervals for $\beta_{1}$ and $\beta_{0}$ (Section 12.3)
- Two Kinds of Conditional Predictions Problems (Section 12.4)


## Simple Linear Regression Models (Section 12.1)

## Simple Linear Regression Model (Review)

1. The condition mean of $Y$ given $X=x$ is a linear function of $x$, i.e.,

$$
\mathrm{E}(Y \mid X=x)=\beta_{0}+\beta_{1} x
$$

2. The conditional variance of $Y$ does not change with $x$, i.e.,

$$
\operatorname{Var}(Y \mid X=x)=\sigma^{2} \quad \text { for every } x
$$

3. (Optional) The conditional distribution of $Y$ given $X=x$ is normal,

$$
(Y \mid X=x) \sim N\left(\beta_{0}+\beta_{1} x, \sigma^{2}\right)
$$



## Simple Linear Regression Model

Equivalently, the SLR model asserts the values of $X$ and $Y$ for individuals in a population are related as follows

$$
Y=\beta_{0}+\beta_{1} X+\varepsilon,
$$

- the value of $\varepsilon$, called the error or the noise, varies from observation to observation, follows a normal distribution

$$
\varepsilon \sim N\left(0, \sigma^{2}\right)
$$

- In the model, the line $y=\beta_{0}+\beta_{1} x$ is called the population regression line.


## Data for a Simple Linear Regression Model

Suppose the data comprised of $n$ individuals/cases randomly sampled from a population.

From case $i$ we observe the response $y_{i}$ and the predictor $x_{i}$ :

$$
\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right),\left(x_{3}, y_{3}\right), \ldots,\left(x_{n}, y_{n}\right)
$$

The SLR model states that

$$
y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}
$$

How do we estimate intercept $\beta_{0}$ and the slope $\beta_{1}$ ?

Least-Square Estimates of the
Intercept and the Slope (Section
12.2)

## Residuals (Prediction Errors)

If one use the line $y=a+b x$ to predict $y$ from $x$, the predicted $y$ when $x=x_{i}$ is

$$
\hat{y}_{i}=a+b x_{i} .
$$

The residual $\left(e_{i}\right)$ of the $i$ th observation $\left(x_{i}, y_{i}\right)$ is

| $e_{i}$ | $=$ | $y_{i}$ | - | $\hat{y}_{i}$ |
| :---: | :---: | :---: | :---: | :---: |
| (Residual) |  | $($ Observed $y)$ |  | (Predicted $y$ ) |
|  | $=$ | $y_{i}$ | - | $\left(a+b x_{i}\right)$ |



Residuals are the (signed) vertical distances from data points to model line, not the shortest distances

## Least-Square Estimates of the Intercept and the Slope

We want a line $y=\widehat{\beta}_{0}+\widehat{\beta}_{1} x$ having small residuals:

- Using the line $y=\widehat{\beta}_{0}+\widehat{\beta}_{1} x$, the predicted $y$ when $x=x_{i}$ is

$$
\widehat{y}_{i}=\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}
$$

- The residual for $\left(x_{i}, y_{i}\right)$ is $e_{i}=y_{i}-\widehat{y}_{i}=y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}$.

For $\operatorname{SLR}$, the least squares estimate $\left(\widehat{\beta}_{0}, \widehat{\beta}_{1}\right)$ for $\left(\beta_{0}, \beta_{1}\right)$ is the intercept and slope of the straight line with the minimum sum of squared residuals.

$$
\sum_{i=1}^{n} e_{i}^{2}=\sum_{i=1}^{n}\left(y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}\right)^{2}
$$



## Solving the Least Squares Problem (1)

To find the $\left(\widehat{\beta}_{0}, \widehat{\beta}_{1}\right)$ that minimize

$$
L\left(\widehat{\beta}_{0}, \widehat{\beta}_{1}\right)=\sum_{i=1}^{n}\left(y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}\right)^{2}
$$

one can set the derivatives of $L$ with respect to $\widehat{\beta}_{0}$ and $\widehat{\beta}_{1}$ to 0

$$
\begin{aligned}
& \frac{\partial L}{\partial \widehat{\beta}_{0}}=-2 \sum_{i=1}^{n}\left(y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}\right)=0 \\
& \frac{\partial L}{\partial \widehat{\beta}_{1}}=-2 \sum_{i=1}^{n} x_{i}\left(y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}\right)=0
\end{aligned}
$$

This results in the 2 equations below in 2 unknowns $\widehat{\beta}_{0}$ and $\widehat{\beta}_{1}$.

$$
\begin{aligned}
n \widehat{\beta}_{0}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i} & =\sum_{i=1}^{n} y_{i} \\
\widehat{\beta}_{0} \sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} & =\sum_{i=1}^{n} x_{i} y_{i}
\end{aligned}
$$

## Solving the Least Squares Problem (2)

$$
\begin{aligned}
\widehat{\beta}_{0}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i} & =\sum_{i=1}^{n} y_{i} \\
\widehat{\beta}_{0} \sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} & =\sum_{i=1}^{n} x_{i} y_{i}
\end{aligned}
$$

## Solving the Least Squares Problem (2)

$$
\begin{array}{r}
\widehat{\beta}_{0}+\widehat{\beta}_{1} \overbrace{\sum_{i=1}^{n} x_{i}}^{=n \bar{x}}=\overbrace{\sum_{i=1}^{n} y_{i}}^{=n \bar{y}} \\
\widehat{\beta}_{0} \underbrace{\sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}}_{=n \bar{x}}=\sum_{i=1}^{n} x_{i} y_{i}
\end{array}
$$

## Solving the Least Squares Problem (2)

$$
\begin{aligned}
& n \widehat{\beta}_{0}+\widehat{\beta}_{1} \overbrace{\sum_{i=1}^{n} x_{i}}^{=n \bar{x}}=\overbrace{\sum_{i=1}^{n} y_{i}}^{=n \bar{y}} \stackrel{\text { divide by } n}{\Longrightarrow} \widehat{\beta}_{0}+\widehat{\beta}_{1} \bar{x}=\bar{y} \Rightarrow \widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \bar{x} \\
& \widehat{\beta}_{0} \underbrace{\sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i}}_{=n \bar{x}}
\end{aligned}
$$

## Solving the Least Squares Problem (2)

$$
\begin{gathered}
n \widehat{\beta}_{0}+\widehat{\beta}_{1} \overbrace{\sum_{i=1}^{n} x_{i}}^{=n \bar{x}}=\overbrace{\sum_{i=1}^{n} y_{i}}^{=n \bar{y}} \stackrel{\text { divide by } n}{\Longrightarrow} \widehat{\beta}_{0}+\widehat{\beta}_{1} \bar{x}=\bar{y} \Rightarrow \widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \bar{x} \\
\widehat{\beta}_{0} \underbrace{\sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i} \Longrightarrow \widehat{\beta}_{0} n \bar{x}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i}}_{=n \bar{x}}
\end{gathered}
$$

## Solving the Least Squares Problem (2)

$$
\begin{gathered}
n \widehat{\beta}_{0}+\widehat{\beta}_{1} \overbrace{\sum_{i=1}^{n} x_{i}}^{=n \bar{x}}=\overbrace{\sum_{i=1}^{n} y_{i}}^{=n \bar{y}} \stackrel{\text { divide by } n}{\Longrightarrow} \widehat{\beta}_{0}+\widehat{\beta}_{1} \bar{x}=\bar{y} \Rightarrow \widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \bar{x} \\
\widehat{\beta}_{0} \underbrace{\sum_{i=1}^{n} x_{i}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i} \Longrightarrow \widehat{\beta}_{0} n \bar{x}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i}}_{=n \bar{x}}
\end{gathered}
$$

Replacing $\widehat{\beta}_{0}$ with $\bar{y}-\widehat{\beta}_{1} \bar{x}$ in the second equation, we get

$$
\begin{aligned}
& \quad\left(\bar{y}-\widehat{\beta}_{1} \bar{x}\right) n \bar{x}+\widehat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2}=\sum_{i=1}^{n} x_{i} y_{i} \\
\Longleftrightarrow & \widehat{\beta}_{1}\left(\sum_{i=1}^{n} x_{i}^{2}-n \bar{x}^{2}\right)=\sum_{i=1}^{n} x_{i} y_{i}-n \bar{x} \bar{y} \\
\Longleftrightarrow & \widehat{\beta}_{1}=\frac{\sum_{i=1}^{n} x_{i} y_{i}-n \bar{x} \bar{y}}{\sum_{i=1}^{n} x_{i}^{2}-n \bar{x}^{2}}
\end{aligned}
$$

## Formulas for the Least Square Estimate for the Slope

Recall the shortcut formulas for sample covariance and variance:

$$
\begin{aligned}
s_{x y} & =\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{n-1}=\frac{\left(\sum_{i=1}^{n} x_{i} y_{i}\right)-n \bar{x} \bar{y}}{n-1}, \\
s_{x}^{2}=s_{x x} & =\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{n-1}=\frac{\left(\sum_{i=1}^{n} x_{i}^{2}\right)-n \bar{x}^{2}}{n-1} .
\end{aligned}
$$

The LS estimate of the slope is hence

$$
\widehat{\beta}_{1}=\frac{\sum_{i=1}^{n} x_{i} y_{i}-n \bar{x} \bar{y}}{\sum_{i=1}^{n} x_{i}^{2}-n \bar{x}^{2}}=\frac{s_{x y}}{s_{x}^{2}}=\frac{\text { sample covariance of } X \& Y}{\text { sample variance of } X} .
$$

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s_{x}^{2}=s_{x x} & =\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{n-1}=\frac{\left(\sum_{i=1}^{n} x_{i}^{2}\right)-n \bar{x}^{2}}{n-1} .
\end{aligned}
$$

The LS estimate of the slope is hence

$$
\widehat{\beta}_{1}=\frac{\sum_{i=1}^{n} x_{i} y_{i}-n \bar{x} \bar{y}}{\sum_{i=1}^{n} x_{i}^{2}-n \bar{x}^{2}}=\frac{s_{x y}}{s_{x}^{2}}=\frac{\text { sample covariance of } X \& Y}{\text { sample variance of } X} .
$$

Another formula:

$$
\widehat{\beta}_{1}=\frac{s_{x y}}{s_{x}^{2}}=\underbrace{\left(\frac{s_{x y}}{s_{x} s_{y}}\right)}_{=r} \frac{s_{y}}{s_{x}}=r \frac{s_{y}}{s_{x}}, \quad \text { where } r=\frac{s_{x y}}{s_{x} s_{y}}=\binom{\text { sample }}{\text { correlation }}
$$

## Properties of the LS Regression Line

$$
\begin{aligned}
\widehat{y} & =\overbrace{\widehat{\beta}_{0}}^{=\bar{y}-\widehat{\beta}_{1} \bar{x}}+\widehat{\beta}_{1} \cdot x \\
\Leftrightarrow \widehat{y}-\bar{y} & =\widehat{\beta}_{1} \cdot(x-\bar{x})=r \frac{s_{y}}{s_{x}}(x-\bar{x}) \\
\Leftrightarrow \underbrace{\frac{s^{\text {score of }} \bar{y}}{s_{y}}}_{z} & =r \cdot \underbrace{\frac{x-\bar{x}}{s_{x}}}_{z \text {-score of } x}
\end{aligned}
$$

- The LS regression line always passes through $(\bar{x}, \bar{y})$
- As $x$ goes up by 1 SD of $x$, the predicted value $\widehat{y}$ only goes up by $r \times$ (SD of y )
- When $r=0$, the LS regression line is horizontal $y=\bar{y}$, and the predicted value $\hat{y}$ is always the mean $\bar{y}$


## Example: Armor Strength — Least Square



$$
\begin{aligned}
n & =20 \\
\bar{x} & =733.4 \\
\bar{y} & =79.34 \\
\sum x_{i}^{2} & =10792614 \\
\sum y_{i}^{2} & =130028 \\
\sum x_{i} y_{i} & =1172708
\end{aligned}
$$

The LS estimates are

$$
\begin{aligned}
\widehat{\beta}_{1} & =\frac{\sum_{i=1}^{n} x_{i} y_{i}-n \bar{x} \bar{y}}{\sum_{i=1}^{n} x_{i}^{2}-n \bar{x}^{2}} \\
& =\frac{1172708-20(733.4)(79.34)}{10792614-20(733.4)^{2}}=\frac{8949}{35103} \approx 0.2549 \\
\widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \bar{x} & =79.34-0.2549(733.4) \approx-107.63
\end{aligned}
$$

## Example: Armor Strength — Least Square Line (2)



|  | Velocity <br> $(x)$ | Penetration <br> Area $(y)$ |
| :--- | :---: | :---: |
| mean | $\bar{x}=733.4$, | $\bar{y}=79.34$ |
| SD | $s_{x} \approx 42.983$ | $s_{y}=14.745$ |
|  | correlation | $r=0.7431$ |

The slope and the intercept of the least square regression line is

$$
\begin{aligned}
\text { slope } & =\widehat{\beta}_{1}=r \frac{s_{y}}{s_{x}}=0.7431 \times \frac{14.745}{42.983}=0.2549 \\
\text { intercept } & =\widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \cdot \bar{x}=79.34-0.2549(733.4) \approx-107.6
\end{aligned}
$$

The equation of the least square regression line is thus

$$
\widehat{y}=-107.6-0.2549 x
$$

## Least Square Regression in $\mathbf{R}$

Regression in $R$ is as simple as $\operatorname{lm}(y \sim x)$, in which $\operatorname{lm}$ stands for "linear models".

```
armor = read.table(
    "http://www.stat.uchicago.edu/~yibi/s234/ArmorStrength.txt",
    header=TRUE)
lm(penetration.area ~ velocity, data=armor)
```

Call:
$\operatorname{lm}(f o r m u l a=$ penetration.area $\sim$ velocity, data $=$ armor)

Coefficients:

```
(Intercept) velocity
    -107.632 0.255
```

The R output says the least square regression line is penetration area $\left(\mathrm{mm}^{2}\right)=-107.632+0.255$ (firing velocity in $\mathrm{m} / \mathrm{s}$ ).

Our calculation is slightly off due to rounding errors.

## Interpretation of Slope

The slope indicates how much the response changes associated with a unit change in $x$ on average (may NOT be causal, unless the data are from an experiment).
penetration area $\left(\mathrm{mm}^{2}\right)=-107.632+0.255$ (firing velocity in $\mathrm{m} / \mathrm{s}$ ).

- When the firing velocity increases by $1 \mathrm{~m} / \mathrm{s}$ the penetration area is estimated to increase by $0.255 \mathrm{~mm}^{2}$ on average.
- When the firing velocity increases by $10 \mathrm{~m} / \mathrm{s}$ the penetration area is estimated to increase by $2.55 \mathrm{~mm}^{2}$ on average.


## Interpretation of the Intercept

The intercept is the predicted value of response when $x=0$, which might have no practical meaning if $x=0$ is not a possible value. penetration area $\left(\mathrm{mm}^{2}\right)=-107.632+0.255$ (firing velocity in $\mathrm{m} / \mathrm{s}$ ).
e.g., when the firing velocity is $0 \mathrm{~m} / \mathrm{s}$, the predicted penetration area is $-107.632 \mathrm{~mm}^{2}$ ?

- extrapolation, not reliable


## R: Adding the LS Regression Line on the Scatterplot

```
p = ggplot(armor, aes(x=velocity, y=penetration.area)) +
    geom_point(col=rgb(0,0,1,0.5), size=2) +
    xlab("Velocity (m/s)") +
    ylab("Penetration Area (mm^2)")
```

p + geom_smooth(method='lm', col="red")
p + geom_smooth(method='lm', col="red", se=FALSE)



## Prediction

One can plug in an $x$-value to the equation of the least-square regression line to predict the response $y$.
e.g., when the firing velocity is $750 \mathrm{~m} / \mathrm{s}$, the predicted penetration area in $\mathrm{mm}^{2}$ is

$$
\widehat{y}=-107.632+0.255 \times 750=83.57 \mathrm{~mm}^{2}
$$



## Extrapolation

Applying a model estimate to values outside of the realm of the original data is called extrapolation.


The variable $X=$ velocity range from 660 to $800 \mathrm{~m} / \mathrm{s}$. Prediction made using $X$-values outside of this range is extrapolation.

## Hypothesis Tests \& Confidence Intervals for $\beta_{1}$ and $\beta_{0}$ (Section 12.3)

## Sample Regression Line v.s. Population Regression Line



| $y=\beta_{0}+\beta_{1} x$ | $y=\widehat{\beta}_{0}+\widehat{\beta}_{1} x$ |
| :---: | :---: |
| least-square regression line <br> of the population | least-square regression line <br> of the sample |
| fixed | random, changes <br> from sample to sample |
| unknown | can be calculated from sample |

## Sample Regression Line v.s. Population Regression Line



## Sample Regression Line v.s. Population Regression Line



## Sample Regression Line v.s. Population Regression Line



## How Close Is $\widehat{\beta}_{1}$ to $\beta_{1}$ ?

Under the SLR model: $y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}$, one can show that

- $\mathrm{E}\left(\widehat{\beta}_{1}\right)=\beta_{1} \ldots \ldots \ldots \ldots \ldots . \widehat{\beta}_{1}$ is an unbiased estimate of $\beta_{1}$
- $\operatorname{Var}\left(\widehat{\beta}_{1}\right)=\frac{\sigma^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}=\frac{\sigma^{2}}{(n-1) s_{x}^{2}}$.


## How Close Is $\widehat{\beta}_{1}$ to $\beta_{1}$ ?

Under the SLR model: $y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}$, one can show that

- $\mathrm{E}\left(\widehat{\beta}_{1}\right)=\beta_{1} \ldots \ldots \ldots \ldots \ldots . \widehat{\beta}_{1}$ is an unbiased estimate of $\beta_{1}$
- $\operatorname{Var}\left(\widehat{\beta}_{1}\right)=\frac{\sigma^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}=\frac{\sigma^{2}}{(n-1) s_{x}^{2}}$.
$\widehat{\beta}_{1}$ will be closer to $\beta_{1}$ if

1) the sample size $n$ is larger, or 2) $X$ has greater variability



## Proof of the Unbiasedness of $\widehat{\beta}_{1}(1)$

Recall the formula for the LS estimate for slope $\widehat{\beta}_{1}$ is

$$
\widehat{\beta}_{1}=\frac{s_{x y}}{s_{x}^{2}}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}
$$

To find the expected value of $\widehat{\beta}_{1}$, we will first show an alternative
formula for it: $\widehat{\beta}_{1}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}$.

$$
\begin{aligned}
\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right) & =\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}-\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) \bar{y} \\
& =\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}-\bar{y} \underbrace{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)}_{=0} \\
& =\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}
\end{aligned}
$$

This proves the alternative formula: $\widehat{\beta}_{1}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}$.

## Proof of the Expected Value of $\widehat{\beta}_{1}$ (2)

Under the SLR model: $y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}$, we know
$\mathrm{E}\left[y_{i}\right]=\beta_{0}+\beta_{1} x_{i}$. Hence,
$\mathrm{E}\left[\widehat{\beta}_{1}\right]=\mathrm{E}\left[\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right]=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) \mathrm{E}\left[y_{i}\right]}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(\beta_{0}+\beta_{1} x_{i}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}$
The numerator $\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(\beta_{0}+\beta_{1} x_{i}\right)$ equals

$$
\begin{aligned}
\beta_{0} \overbrace{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)}^{=0} & +\beta_{1} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) x_{i} \\
& =\beta_{1} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(x_{i}-\bar{x}\right)+\beta_{1} \bar{x} \underbrace{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)}_{=0} \\
& =\beta_{1} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}
\end{aligned}
$$

Putting the numerator back to $\mathrm{E}\left[\widehat{\beta}_{1}\right]$, we get
$\mathrm{E}\left[\widehat{\beta}_{1}\right]=\frac{\beta_{1} \sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}=\beta_{1}$. So $\widehat{\beta}_{1}$ is an unbiased estimator for $\beta_{1}$.

## Proof of Variance of $\widehat{\beta}_{1}$

For the SLR model $y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}$ as $x_{i}$ 's are regarded as fixed numbers and $\varepsilon_{i}$ 's are indep. with $\operatorname{Var}\left(\varepsilon_{i}\right)=\sigma^{2}$, we know that $y_{i}$ 's are also indep. with $\operatorname{Var}\left(y_{i}\right)=\sigma^{2}$.

Recall that for independent random variables $Y_{1}, Y_{2}, \ldots, Y_{n}$, and fixed numbers $c_{1}, c_{2}, \ldots, c_{n}$ the variance has the property:
$\operatorname{Var}\left(c_{1} Y_{1}+c_{2} Y_{2}+\ldots+c_{n} Y_{n}\right)=c_{1}^{2} \operatorname{Var}\left(Y_{1}\right)+c_{2}^{2} \operatorname{Var}\left(Y_{2}\right)+\ldots+c_{n}^{2} \operatorname{Var}\left(Y_{n}\right)$
Apply the property above to the variance of $\widehat{\beta}_{1}$ with $c_{j}=\frac{x_{j}-\bar{x}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}$, we get

$$
\begin{aligned}
\operatorname{Var}\left(\widehat{\beta}_{1}\right) & =\operatorname{Var}\left(\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right) y_{i}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right)=\operatorname{Var}\left(\sum_{i=1}^{n} c_{i} y_{i}\right)=\sum_{i=1}^{n} c_{i}^{2} \operatorname{Var}\left(y_{i}\right)=\sigma^{2} \sum_{i=1}^{n} c_{i}^{2} \\
& =\sigma^{2} \sum_{i=1}^{n}\left(\frac{\left(x_{j}-\bar{x}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right)^{2}=\sigma^{2} \frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{\left(\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}\right)^{2}}=\frac{\sigma^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}} .
\end{aligned}
$$

## Sampling Distribution of the Intercept $\widehat{\beta}_{0}$

Under the SLR model, the estimate of the intercept

$$
\widehat{\beta}_{0}=\bar{y}-\widehat{\beta}_{1} \bar{x}
$$

is also unbiased and (approx.) normal with the variance

$$
\operatorname{Var}\left(\widehat{\beta}_{0}\right)=\sigma^{2}\left(\frac{1}{n}+\frac{\bar{x}^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right)
$$

What is the intuition here?

$$
\begin{aligned}
\operatorname{Var}\left(\widehat{\beta}_{0}\right)=\operatorname{Var}\left(\bar{y}-\widehat{\beta}_{1} \bar{x}\right) & =\operatorname{Var}(\bar{y})-2 \bar{x} \overbrace{\operatorname{Cov}\left(\bar{y}, \widehat{\beta}_{1}\right)}^{=0}+\bar{x}^{2} \operatorname{Var}\left(\widehat{\beta}_{1}\right) \\
& =\frac{\sigma^{2}}{n}+0+\bar{x}^{2} \frac{\sigma^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}
\end{aligned}
$$

- $\bar{y}$ and $\widehat{\beta}_{1}$ are uncorrelated because the slope $\left(\widehat{\beta}_{1}\right)$ is invariant if you shift the response up or down $(\bar{y})$.


## Covariance of $\widehat{\beta}_{1}$ and $\widehat{\beta}_{0}$

The estimates for the slope and the intercept are negatively correlated and their covariance is

$$
\begin{aligned}
\operatorname{Cov}\left(\widehat{\beta}_{1}, \widehat{\beta}_{0}\right) & =\operatorname{Cov}\left(\widehat{\beta}_{1}, \bar{y}-\widehat{\beta}_{1} \bar{x}\right) \\
& =\underbrace{\operatorname{Cov}\left(\widehat{\beta}_{1}, \bar{y}\right)}_{=0}-\bar{x} \underbrace{\operatorname{Cov}\left(\widehat{\beta}_{1}, \widehat{\beta}_{1}\right)}_{=\operatorname{Var}\left(\widehat{\beta}_{1}\right)} \\
& =0-\bar{x} \operatorname{Var}\left(\widehat{\beta}_{1}\right)=\frac{-\sigma^{2} \bar{x}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}
\end{aligned}
$$

- Usually, if the slope estimate is too high, the intercept estimate is too low


## Estimate of $\sigma^{2}$ - Variance of the Errors $\varepsilon_{i}$.

- A naive estimate of $\sigma^{2}$ is the sample variance of the $\varepsilon_{i}$

$$
\widehat{\sigma}^{2}=\frac{\sum\left(\varepsilon_{i}-\bar{\varepsilon}\right)^{2}}{n-1} \quad \text { where } \quad \varepsilon_{i}=y_{i}-\beta_{0}-\beta_{1} x_{i}
$$

However, this is not possible as $\beta_{0}$ and $\beta_{1}$ are unknown.

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$$

However, this is not possible as $\beta_{0}$ and $\beta_{1}$ are unknown.

- We can estimate $\beta_{0}$ and $\beta_{1}$ with $\widehat{\beta}_{0}$ and $\widehat{\beta}_{1}$ and approximate the errors $\varepsilon_{i}$ with the residuals

$$
e_{i}=y_{i}-\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)=y_{i}-\widehat{y}_{i}
$$

We use the "sample variance" of the residuals $e_{i}$ to estimate $\sigma^{2}$ :

$$
\widehat{\sigma}^{2}=\frac{\sum\left(e_{i}-\bar{e}\right)^{2}}{n-2}=\frac{\sum e_{i}^{2}}{n-2}=\frac{\sum\left(y_{i}-\widehat{y}_{i}\right)^{2}}{n-2}
$$

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$$
\widehat{\sigma}^{2}=\frac{\sum\left(e_{i}-\bar{e}\right)^{2}}{n-2}=\frac{\sum e_{i}^{2}}{n-2}=\frac{\sum\left(y_{i}-\widehat{y}_{i}\right)^{2}}{n-2}
$$

- We will show in the next lecture that $\bar{e}=0$


## Estimate of $\sigma^{2}$ - Variance of the Errors $\varepsilon_{i}$.

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$$

However, this is not possible as $\beta_{0}$ and $\beta_{1}$ are unknown.

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$$

We use the "sample variance" of the residuals $e_{i}$ to estimate $\sigma^{2}$ :

$$
\widehat{\sigma}^{2}=\frac{\sum\left(e_{i}-\bar{e}\right)^{2}}{n-2}=\frac{\sum e_{i}^{2}}{n-2}=\frac{\sum\left(y_{i}-\widehat{y}_{i}\right)^{2}}{n-2}
$$

- We will show in the next lecture that $\bar{e}=0$
- We divide by $n-2$, not $n-1$ or $n$ as We are not able to estimate error unless we have at least 3 observations


## Standard Error (SE) of the Slope and the Intercept

The standard deviation (SD) of $\widehat{\beta}_{1}$ and $\widehat{\beta}_{0}$ are the square-root of their variances

$$
\mathrm{SD}\left(\widehat{\beta}_{1}\right)=\frac{\sigma}{\sqrt{\sum\left(x_{i}-\bar{x}\right)^{2}}}, \quad \mathrm{SD}\left(\widehat{\beta}_{0}\right)=\sigma \sqrt{\frac{1}{n}+\frac{\bar{x}^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}}
$$

If the unknown $\sigma$ is replaced with the estimate

$$
\widehat{\sigma}=\sqrt{\frac{\sum\left(y_{i}-\widehat{y}_{i}\right)^{2}}{n-2}},
$$

The estimated SD's are called the standard error (SE)'s:

$$
\mathrm{SE}\left(\widehat{\beta}_{1}\right)=\frac{\widehat{\sigma}}{\sqrt{\sum\left(x_{i}-\bar{x}\right)^{2}}}, \quad \mathrm{SE}\left(\widehat{\beta}_{0}\right)=\widehat{\sigma} \sqrt{\frac{1}{n}+\frac{\bar{x}^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}} .
$$

## Sampling Distributions of $\widehat{\beta}_{1}$ and $\widehat{\beta}_{0}$

The sampling distributions of $\widehat{\beta}_{1}$ and $\widehat{\beta}_{0}$ are both normal.

$$
\begin{array}{r}
\widehat{\beta}_{1} \sim N\left(\beta_{1}, \frac{\sigma^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}\right) \Rightarrow z=\frac{\widehat{\beta}_{1}-\beta_{1}}{\sigma / \sqrt{\sum\left(x_{i}-\bar{x}\right)^{2}}} \sim N(0,1) \\
\widehat{\beta}_{0} \sim N\left(\beta_{0}, \sigma^{2}\left(\frac{1}{n}+\frac{\bar{x}^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}\right)\right) \Rightarrow z=\frac{\widehat{\beta}_{0}-\beta_{0}}{\sigma \sqrt{\frac{1}{n}+\frac{\hat{x}^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}}} \sim N(0,1)
\end{array}
$$

This is (approx.) valid

- either if the errors $\varepsilon_{i}$ are i.i.d. $N\left(0, \sigma^{2}\right)$
- or if the errors $\varepsilon_{i}$ are independent and the sample size $n$ is large

If the unknown $\sigma$ is replaced by $\widehat{\sigma}, z$ become the $t$-statistic with a $t$-distribution with $\mathrm{df}=n-2$.
$T_{1}=\frac{\widehat{\beta}_{1}-\beta_{1}}{\widehat{\sigma} / \sqrt{\sum\left(x_{i}-\bar{x}\right)^{2}}}=\frac{\widehat{\beta}_{1}-\beta_{1}}{\operatorname{SE}\left(\widehat{\beta}_{1}\right)} \sim t_{n-2}, T_{0}=\frac{\widehat{\beta}_{0}-\beta_{0}}{\widehat{\sigma} \sqrt{\frac{1}{n}+\frac{\widehat{x}^{2}}{\sum\left(x_{i}-\bar{x}\right)^{2}}}}=\frac{\widehat{\beta}_{0}-\beta_{0}}{\operatorname{SE}\left(\widehat{\beta}_{0}\right)} \sim t_{n-2}$.

## Confidence Intervals for $\beta_{0}$ and $\beta_{1}$

The $(1-\alpha)$ confidence intervals for $\beta_{0}$ and $\beta_{1}$ are respectively

$$
\widehat{\beta}_{0} \pm t_{\alpha / 2, n-2} \operatorname{SE}\left(\widehat{\beta}_{0}\right) \quad \text { and } \quad \widehat{\beta}_{1} \pm t_{\alpha / 2, n-2} \operatorname{SE}\left(\widehat{\beta}_{1}\right)
$$

where $t_{\alpha / 2, n-2}$ is the value such that $P\left(|T|<t_{\alpha / 2, n-2}\right)=1-\alpha$ for $T \sim t_{n-2}$.


In R, $t_{\alpha / 2, n-2}=\mathrm{qt}($ alpha $/ 2, \mathrm{df}=\mathrm{n}-2$, lower.tail=F).

|  |  | $\begin{array}{r} 90 \% \mathrm{Cl} \\ t_{0.1 / 2, \mathrm{df}} \\ \downarrow \end{array}$ | $\begin{array}{r} 95 \% \mathrm{Cl} \\ t_{0.05 / 2, \mathrm{df}} \\ \downarrow \end{array}$ | $\begin{array}{r} 99 \% \mathrm{Cl} \\ t_{0.01 / 2, \mathrm{df}} \\ \downarrow \end{array}$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 0.1 | 0.05 | 0.025 | 0.01 | 0.005 | 0.001 | 0.0005 |
| $v$ | 3.078 | 6.314 | 12.706 | 31.821 | 63.657 | 318.309 | 636.619 |
|  | 1.886 | 2.920 | 4.303 | 6.965 | 9.925 | 22.327 | 31.599 |
|  | 1.638 | 2.353 | 3.182 | 4.541 | 5.841 | 10.215 | 12.924 |
|  | 1.533 | 2.132 | 2.776 | 3.747 | 4.604 | 7.173 | 8.610 |
|  | 1.476 | 2.015 | 2.571 | 3.365 | 4.032 | 5.893 | 6.869 |
|  | 1.440 | 1.943 | 2.447 | 3.143 | 3.707 | 5.208 | 5.959 |

## Tests for $\beta_{0}$ and $\beta_{1}$

To test the hypotheses $\mathrm{H}_{0}: \beta_{0}=c$ or $\mathrm{H}_{0}: \beta_{1}=c$ the $t$-statistic are respectively

$$
t=\frac{\widehat{\beta}_{0}-c_{0}}{\operatorname{SE}\left(\widehat{\beta}_{0}\right)} \sim t_{n-2}, \quad \text { and } \quad t=\frac{\widehat{\beta}_{1}-c_{1}}{\operatorname{SE}\left(\widehat{\beta}_{1}\right)} \sim t_{n-2}
$$

The $P$-value can be computed based on $\mathrm{H}_{a}$ :


## Example: Armor Strength

Soldiers depend on their body armor for protection. Specimens of UHMWPE body armor were shot with a 7.62 mm round at various firing velocities. The penetration areas were recorded ${ }^{a}$.
a"Testing of Body Armor Materials-Phase III", 2012, by the US Army and the National Research Council


| Velocity <br> $(\mathrm{m} / \mathrm{s})$ | Penetration <br> Area <br> $\left(\mathrm{mm}^{2}\right)$ |
| :---: | :---: |
| 670 | 66.4 |
| 675 | 64.5 |
| 679 | 63.6 |
| 681 | 72.9 |
| 694 | 79.1 |
| 699 | 76.7 |
| 699 | 65.5 |
| 708 | 68.0 |
| 726 | 57.8 |
| 732 | 72.4 |
| 738 | 78.6 |
| 740 | 87.9 |
| 762 | 92.6 |
| 762 | 83.0 |
| 768 | 79.0 |
| 780 | 75.3 |
| 792 | 83.4 |
| 786 | 100.7 |
| 790 | 106.6 |
| 787 | 112.8 |

## Least Square Regression in R

Regression in $R$ is as simple as $\operatorname{lm}(y \sim x)$, in which $\operatorname{lm}$ stands for "linear models".

```
armor = read.table(
    "http://www.stat.uchicago.edu/~yibi/s234/ArmorStrength.txt",
    header=TRUE)
lm(penetration.area ~ velocity, data=armor)
Call:
lm(formula = penetration.area ~ velocity, data = armor)
Coefficients:
(Intercept) velocity
    -107.632 0.255
```

> lmarmor = lm(penetration.area ~ velocity, data=armor)
> summary (lmarmor)

Coefficients:
Estimate Std. Error $t$ value $\operatorname{Pr}(>|t|)$
(Intercept) -107.6324 $39.7450 \quad-2.71 \quad 0.01440$
$\begin{array}{lllll}\text { velocity } & 0.2549 & 0.0541 & 4.71 & 0.00017\end{array}$

Residual standard error: 10.1 on 18 degrees of freedom Multiple R-squared: 0.552, Adjusted R-squared: 0.527 F-statistic: 22.2 on 1 and 18 DF, p-value: 0.000174
"Residual standard error: 10.1 " in the R output is the estimate for $\sigma=\mathrm{SD}\left(\varepsilon_{i}\right), \widehat{\sigma}=10.1$.

That is, the variance $\sigma^{2}=\operatorname{Var}\left(\varepsilon_{i}\right)$ for the noise term $\varepsilon_{i}$ in the SLR model: $y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}$ is estimated to be $\widehat{\sigma}^{2}=10.1^{2}$.

## The Summary Output

Coefficients:

|  | Estimate Std. Error t value $\operatorname{Pr}(>\|\mathrm{t}\|)$ |  |  |  |
| :--- | ---: | ---: | ---: | ---: |
| (Intercept) | -107.6324 | 39.7450 | -2.71 | 0.01440 |
| velocity | 0.2549 | 0.0541 | 4.71 | 0.00017 |

- The column "estimate" shows the LS estimates for the intercept $\widehat{\beta}_{0}=-107.6324$ and the slope $\widehat{\beta}_{1}=0.2549$
- The column "std. error" gives:

$$
\mathrm{SE}\left(\widehat{\beta}_{0}\right)=39.7450, \quad \mathrm{SE}\left(\widehat{\beta}_{1}\right)=0.0541
$$

## R Tests Whether $\beta_{1}$ and $\beta_{0}$ Equal 0 Automatically

Coefficients:

|  | Estimate Std. Error t value $\operatorname{Pr}(>\|\mathrm{t}\|)$ |  |  |  |
| :--- | ---: | ---: | ---: | ---: |
| (Intercept) | -107.6324 | 39.7450 | -2.71 | 0.01440 |
| velocity | 0.2549 | 0.0541 | 4.71 | 0.00017 |

- The column $\mathbf{t}$ value shows the $\mathbf{t}$-statistic for testing $\mathrm{H}_{0}: \beta_{0}=0$ and $\mathrm{H}_{0}: \beta_{1}=0$,

$$
t_{0}=\frac{\widehat{\beta}_{0}-0}{\operatorname{SE}\left(\widehat{\beta}_{0}\right)}=\frac{-107.6350}{37.7450}=-2.71, t_{1}=\frac{\widehat{\beta}_{1}-0}{\operatorname{SE}\left(\widehat{\beta}_{1}\right)}=\frac{0.2549}{0.0541}=4.71
$$

which are simply the ratios of the first two columns

- The column "p.value" shows the 2 -sided $P$-values for testing $\mathrm{H}_{0}: \beta_{0}=0$ and $\mathrm{H}_{0}: \beta_{1}=0$.
- Testing $\mathrm{H}_{0}: \beta_{1}=0$ is equivalent to testing whether the penetration area is linearly related to the velocity. The small $P$-value 0.00017 asserts the relation is significant


## Example: Testing Whether $\beta_{1}$ is a Non-Zero Value

To test whether $\beta_{1}$ equal to some non-zero value $c_{1}$, one has to calculate the $t$-statistic and $P$-value himself.

Ex. To see if the penetration area increases by $0.1 \mathrm{~mm}^{2}$ on average when the firing velocity increases by $1 \mathrm{~m} / \mathrm{s}$ i.e., $\beta_{1}=0.1$.

|  | Estimate | Std.Error | t value | $\operatorname{Pr}(>\|t\|)$ |
| :--- | ---: | ---: | ---: | ---: |
| (Intercept) | -107.6324 | 39.7450 | -2.71 | 0.01440 |
| velocity | 0.2549 | 0.0541 | 4.71 | $<0.00017$ |

To test $H_{0}: \beta_{1}=0.1$ v.s. $H_{A}: \beta_{1}>0.1$, the $t$-statistic is

$$
t_{1}=\frac{\widehat{\beta}_{1}-0.1}{\operatorname{SE}\left(\widehat{\beta}_{1}\right)}=\frac{0.2549-0.1}{0.0541} \approx 2.863 \text { with df }=20-2=18
$$

The upper one-sided $p$-value is pt(2.863, df = 20-2, lower.tail=F) $\approx 0.0052$.

Conclusion: When the firing velocity increases by $1 \mathrm{~m} / \mathrm{s}$, the penetration area increases significantly more than $0.1 \mathrm{~mm}^{2}$ on average.

## Example: Confidence Interval for $\beta_{1}$

$$
\begin{array}{lrrrr} 
& \text { Estimate } & \text { Std.Error } & \text { t value } & \operatorname{Pr}(>|t|) \\
\text { (Intercept) } & -107.6324 & 39.7450 & -2.71 & 0.01440 \\
\text { velocity } & 0.2549 & 0.0541 & 4.71 & <0.00017
\end{array}
$$

The $95 \% \mathrm{Cl}$ for the slope $\beta_{1}$ is

$$
\begin{aligned}
\widehat{\beta}_{1} \pm t_{0.05 / 2,20-2} \mathrm{SE}\left(\widehat{\beta}_{1}\right) & =0.2549 \pm 2.101 \times 0.0541 \\
& =0.2549 \pm 0.1137 \approx(0.1412,0.3686)
\end{aligned}
$$

where $t_{0.05 / 2,20-2} \approx 2.101$ for a $95 \% \mathrm{Cl}$ can be found in R or using $t$-table for $\mathrm{df}=n-2=20-2=18$.
qt( $0.05 / 2, \mathrm{df}=20-2$, lower.tail=F)
[1] 2.101
qt (1-0.05/2, df=20-2)

| $\alpha$ | 0.1 | 0.05 | 0.025 | 0.01 | 0.005 | 0.001 | 0.0005 |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $v$ | 18 | 1.330 | 1.734 | 2.101 | 2.552 | 2.878 | 3.610 |

Interpretation: With 95\% confidence, penetration area increases by 0.1412 to $0.3686 \mathrm{~mm}^{2}$ on average when firing velocity increases by 1 $\mathrm{m} / \mathrm{s}$.

## Finding Cls for Coefficients Using confint()

The confint () command can produce confidence intervals for the coefficients $\beta_{0}$ and $\beta_{1}$ for us

```
confint(lmarmor)
```

    2.5 \% 97.5 \%
    (Intercept) -191.1335 -24.1314
velocity $\quad 0.1413 \quad 0.3686$
confint (lmarmor, level $=0.95$ )
2.5 \% $97.5 \%$
(Intercept) -191.1335 -24.1314
velocity $0.1413 \quad 0.3686$
confint(lmarmor, level = 0.95, "velocity")
2.5 \% 97.5 \%
velocity 0.14130 .3686
confint(lmarmor, level = 0.95, "(Intercept)")
2.5 \% 97.5 \%
(Intercept) -191.1-24.13

Two Kinds of Conditional Predictions Problems (Section 12.4)

## Two Kinds of Conditional Predictions Problems

There are two kinds of conditional prediction problems of the response $Y$ given $X=x_{0}$ based on a SLR model $Y=\beta_{0}+\beta_{1} X+\varepsilon$ :

- when $X$ is known to be $x_{0}$, estimate the mean response $\mathrm{E}\left[Y \mid X=x_{0}\right]=\beta_{0}+\beta_{1} x_{0}$
- when $X$ is known to be $x_{0}$, predict the response for one specific observation $Y=\beta_{0}+\beta_{1} x_{0}+\varepsilon$


## Two Kinds of Conditional Predictions Problems

There are two kinds of conditional prediction problems of the response $Y$ given $X=x_{0}$ based on a SLR model $Y=\beta_{0}+\beta_{1} X+\varepsilon$ :

- when $X$ is known to be $x_{0}$, estimate the mean response

$$
\mathrm{E}\left[Y \mid X=x_{0}\right]=\beta_{0}+\beta_{1} x_{0}
$$

- when $X$ is known to be $x_{0}$, predict the response for one specific observation $Y=\beta_{0}+\beta_{1} x_{0}+\varepsilon$

For the armor strength example, one may want to

- estimate the average penetration area on the armor when shot at a firing speed of $x_{0}=700 \mathrm{~m} / \mathrm{s}$, which is $\beta_{0}+700 \beta_{1}$
- predict penetration area on the armor for one shot at a firing speed of of $x_{0}=700 \mathrm{~m} / \mathrm{s}$, which is $\beta_{0}+700 \beta_{1}+\varepsilon$.


## Estimation v.s. Prediction

The first one is an estimation problem as $\beta_{0}+\beta_{1} x_{0}$ only involve fixed parameters $\beta_{0}, \beta_{1}$, and $x_{0}$.

The second one is a prediction problem as $\beta_{0}+\beta_{1} x_{0}+\varepsilon$ involve a random number $\varepsilon$

## Estimated Value and Predicted Value

In the first one,

$$
\mathrm{E}\left[Y \mid X=x_{0}\right]=\beta_{0}+\beta_{1} x_{0} \quad \text { is estimated by } \widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0} .
$$

where the unknown $\beta_{0}$ and $\beta_{1}$ are replaced by their LS estimates.

In the second one,

$$
Y=\beta_{0}+\beta_{1} x_{0}+\varepsilon \quad \text { is predicted by } \quad \widehat{Y}=\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}+0
$$

The noise $\varepsilon$ for a future observation is predicted to be its mean 0 since it's independent of all observed $\left(x_{i}, y_{i}\right)$ 's. We cannot make a better prediction for $\varepsilon$ from the observed $\left(x_{i}, y_{i}\right)$ 's.

## The Two Prediction Problems Differ in the Uncertainty!

For estimating $\mathrm{E}\left[Y \mid X=x_{0}\right]=\beta_{0}+\beta_{1} x_{0}$, the variance for the estimate $\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}$ can be shown to be

$$
\begin{aligned}
\operatorname{Var}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}\right) & =\mathrm{E}\left[\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}-\beta_{0}-\beta_{1} x_{0}\right)^{2}\right] \\
& =\sigma^{2}\left(\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right)
\end{aligned}
$$

To predict $Y=\beta_{0}+\beta_{1} x_{0}+\varepsilon$, we need to include the extra variability from the noise $\varepsilon$.

$$
\begin{aligned}
\mathrm{E}\left[(\widehat{Y}-Y)^{2}\right] & \left.=\mathrm{E}\left[\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}-\beta_{0}-\beta_{1} x_{0}-\varepsilon\right)^{2}\right] \\
& =\operatorname{Var}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}\right)+\operatorname{Var}(\varepsilon) \\
& =\sigma^{2}\left(\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right)+\sigma^{2}
\end{aligned}
$$

As $n$ gets large, $\operatorname{Var}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0}\right)$ would go down to 0 but $\mathrm{E}\left[(\widehat{Y}-Y)^{2}\right]$ only approaches $\sigma^{2}$.

## What Affects the Accuracy of Prediction?

Recall the variances for the two prediction problems are

$$
\begin{cases}\sigma^{2}\left(\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}\right) & \text { for estimating } \mathrm{E}\left[Y \mid X=x_{0}\right]=\beta_{0}+\beta_{1} x_{0} \\ \sigma^{2}\left(1+\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\overline{x^{2}}\right.}\right) & \text { to predict } Y \text { when } X=x_{0}\end{cases}
$$

An accurate prediction (less variance) comes from

- small $\sigma^{2}$ (i.e., small noise $\varepsilon$ 's)
- large sample size $n$
- large $\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}$ (more spread in predictors)
- small $\left(x_{0}-\bar{x}\right)^{2}$


## Confidence Intervals and Prediction Intervals

The $100(1-\alpha) \%$ confidence interval for $\beta_{0}+\beta_{1} x_{0}$ is

$$
\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0} \pm t_{\alpha / 2, n-2} \widehat{\sigma} \sqrt{\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}}
$$

The $100(1-\alpha) \%$ prediction interval for $Y=\beta_{0}+\beta_{1} x_{0}+\varepsilon$ is

$$
\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{0} \pm t_{\alpha / 2, n-2} \widehat{\sigma} \sqrt{1+\frac{1}{n}+\frac{\left(x_{0}-\bar{x}\right)^{2}}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}}
$$

## Confidence Intervals and Prediction Intervals in $\mathbf{R}$

```
predict(lmarmor, data.frame(velocity=700), interval="confidence",
    level=0.95)
    fit lwr upr
1 70.83 64.73 76.92
predict(lmarmor, data.frame(velocity=700), interval="prediction",
    level=0.95)
    fit lwr upr
170.8348.67 92.98
```

- When the firing velocity is $700 \mathrm{~m} / \mathrm{s}$, the penetration area is $70.83 \mathrm{~mm}^{2}$ on average, and the $95 \%$ confidence interval is 64.73 to $76.92 \mathrm{~mm}^{2}$.
- When the firing velocity is $700 \mathrm{~m} / \mathrm{s}$, the penetration area for one shot 48.67 to $92.98 \mathrm{~mm}^{2}$ with $95 \%$ confidence.
- The prediction interval for a single shot is wider.

The plot below shows the 95\% confidence intervals and the 95\% prediction intervals at different values of $x_{0}$.


Both the confidence intervals and the prediction intervals are narrowest when $x_{0}=\bar{x}$.
geom_smooth(method='lm') in ggplot() by default includes the 95\% confidence intervals for estimating $\mathrm{E}\left(y \mid X=x_{0}\right)$.

```
ggplot(armor, aes(x=velocity, y=penetration.area)) +
    geom_point() +
    geom_smooth(method='lm') +
    xlab("Velocity (m/s)") +
    ylab("Penetration Area (mm^2)")
```



## Multiple R-Squared = Coefficient of Determination

## Properties of Residuals (1)

Recall the LS estimate ( $\left.\widehat{\beta}_{0}, \widehat{\widehat{\beta}}_{1}\right)$ that minimizes

$$
L\left(\widehat{\beta}_{0}, \widehat{\beta}_{1}\right)=\sum_{i=1}^{n}\left(y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}\right)^{2}
$$

is obtained by setting the derivatives of $L$ with respect to $\widehat{\beta}_{0}$ and $\widehat{\beta}_{1}$ to 0

$$
\begin{gathered}
\frac{\partial L}{\partial \widehat{\beta}_{0}}=\sum_{i=1}^{n}(\underbrace{y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}}_{y_{i}-\widehat{y}_{i}=e_{i}=\text { residual }})=0 \text { and } \\
\frac{\partial L}{\partial \widehat{\beta}_{1}}=\sum_{i=1}^{n} x_{i} \overbrace{y_{i}-\widehat{\beta}_{0}-\widehat{\beta}_{1} x_{i}})=0,
\end{gathered}
$$

The residuals $e_{i}$ hence have the properties

$$
\underbrace{\sum_{i=1}^{n} e_{i}=0}_{\text {Residuals add up to } 0 .}, \quad \underbrace{\sum_{i=1}^{n} x_{i} e_{i}=0}_{\text {Residuals are orthogonal to } x \text {-variable. }}
$$

## Properties of Residuals (2)

The two properties combined imply that residuals have 0 correlation with the explanatory variable $X$ since

$$
\operatorname{Cov}(X, e)=\frac{1}{n-1}(\underbrace{\sum_{i=1}^{n} x_{i} e_{i}}_{=0}-n \bar{x} \underbrace{\bar{e}}_{=0})=0
$$

## Sum of Squares

Observe that

$$
y_{i}-\bar{y}=\underbrace{\left(\hat{y}_{i}-\bar{y}\right)}_{a}+\underbrace{\left(y_{i}-\widehat{y}_{i}\right)}_{b}
$$

Squaring up both sides using the identity $(a+b)^{2}=a^{2}+b^{2}+2 a b$, we get

$$
\left(y_{i}-\bar{y}\right)^{2}=\underbrace{\left(\widehat{y}_{i}-\bar{y}\right)^{2}}_{a^{2}}+\underbrace{\left(y_{i}-\widehat{y}_{i}\right)^{2}}_{b^{2}}+\underbrace{2\left(\widehat{y}_{i}-\bar{y}\right)\left(y_{i}-\widehat{y}_{i}\right)}_{2 a b}
$$

Summing up over all the cases $i=1,2, \ldots, n$, we get

$$
\overbrace{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}^{\text {SST }}=\overbrace{\sum_{i=1}^{n}\left(\hat{y}_{i}-\bar{y}\right)^{2}}^{\text {SSR }}+\overbrace{\sum_{i=1}^{n}\left(y_{i}-\widehat{y}_{i}\right)^{2}}^{\text {SSE }}+2 \underbrace{\sum_{i=1}^{n}\left(\widehat{y}_{i}-\bar{y}\right)\left(y_{i}-\widehat{y}_{i}\right)}_{=0 \text {, see next page. }}
$$

## Why $\sum_{i=1}^{n}\left(\widehat{y}_{i}-\overline{-}\right)\left(y_{i}-\widehat{y}_{i}\right)=0$ ?

$$
\begin{aligned}
\sum_{i=1}^{n}\left(\widehat{y}_{i}-\bar{y}\right)(\underbrace{y_{i}-\widehat{y}_{i}}_{=e_{i}}) & =\sum_{i=1}^{n} \widehat{y}_{i} e_{i}-\sum_{i=1}^{n} \bar{y} e_{i} \\
& =\sum_{i=1}^{n}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right) e_{i}-\sum_{i=1}^{n} \bar{y} e_{i} \\
& =\widehat{\beta}_{0} \underbrace{\sum_{i=1}^{n} e_{i}}_{=0}+\widehat{\beta}_{1} \underbrace{\sum_{i=1}^{n} x_{i} e_{i}}_{=0}-\bar{y} \underbrace{\sum_{i=1}^{n} e_{i}}_{=0}=0
\end{aligned}
$$

in which we used the properties of residuals that $\sum_{i=1}^{n} e_{i}=0$ and $\sum_{i=1}^{n} x_{i} e_{i}=0$.

## Interpretation of Sum of Squares

$$
\underbrace{\sum_{i=1}^{n}\left(y_{i}-\bar{y}\right)^{2}}_{\text {SST }}=\underbrace{\sum_{i=1}^{n}\left(\widehat{y_{i}}-\bar{y}\right)^{2}}_{\text {SSR }}+\underbrace{\sum_{i=1}^{n}(\overbrace{y_{i}-\widehat{y}_{i}}^{=e_{i}})^{2}}_{\text {SSE }}
$$

- $\mathrm{SST}=$ total sum of squares
- total variability of $Y$
- $\operatorname{SSR}=$ regression sum of squares
- variability of $Y$ explained by $X$
- $\operatorname{SSE}=$ error (residual) sum of squares
- variability of $Y$ not explained by the $X$ 's


## Multiple $R$-Squared

Multiple $R^{2}$, also called the coefficient of determination, is defined as

$$
\begin{aligned}
R^{2} & =\frac{\mathrm{SSR}}{\mathrm{SST}}=1-\frac{\mathrm{SSE}}{\mathrm{SST}} \\
& =\text { proportion of variability in } Y \text { explained by } X
\end{aligned}
$$

which measures the strength of the linear relationship between $Y$ and the $X$ variable

- $0 \leq R^{2} \leq 1$


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which measures the strength of the linear relationship between $Y$ and the $X$ variable

- $0 \leq R^{2} \leq 1$
- For SLR, $R^{2}=r_{x y}^{2}$ is the square of the correlation between $X$ and $Y$


## Interpretation of R-squared

For the Armor Strength data, $R^{2}=r^{2}=(0.7431)^{2} \approx 0.552$, which means - $55.2 \%$ of the variability in the penetration area is explained by the firing velocity.

```
> lmarmor = lm(penetration.area ~ velocity, data=armor)
> summary(lmarmor)
```

Coefficients:

|  | Estimate Std. Error t value $\operatorname{Pr}(>\|\mathrm{t}\|)$ |  |  |  |
| :--- | ---: | ---: | ---: | ---: |
| (Intercept) | -107.6324 | 39.7450 | -2.71 | 0.01440 |
| velocity | 0.2549 | 0.0541 | 4.71 | 0.00017 |

Residual standard error: 10.1 on 18 degrees of freedom Multiple R-squared: 0.552, Adjusted R-squared: 0.527
F-statistic: 22.2 on 1 and 18 DF , p-value: 0.000174

