# STAT 513 fa 2020 Lec 07 slides 

## Simple linear regression

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These slides are an instructional aid; their sole purpose is to display, during the lecture, definitions, plots, results, etc. which take too much time to write by hand on the blackboard.

They are not intended to explain or expound on any material.

## Regression model

For data pairs $\left(Y_{1}, x_{1}\right), \ldots,\left(Y_{n}, x_{n}\right)$, suppose

$$
Y_{i}=f\left(x_{i}\right)+\varepsilon_{i}
$$

for $i=1, \ldots, n$, where

- $x_{1}, \ldots, x_{n}$ are fixed real numbers
- $Y_{1}, \ldots, Y_{n}$ are independent random variables
- $f: \mathbb{R} \rightarrow \mathbb{R}$ is an unknown function
- $\varepsilon_{1}, \ldots, \varepsilon_{n}$ are iid rvs called errors with
- $\mathbb{E} \varepsilon_{i}=0$
- $\operatorname{Var} \varepsilon_{i}=\sigma^{2}$ for $i=1, \ldots, n$.

Goal: Estimate the unknown function $f$ and the error variance $\sigma^{2}$.

We observe a function plus noise:




## Simple linear regression model

For data pairs $\left(Y_{1}, x_{1}\right), \ldots,\left(Y_{n}, x_{n}\right)$, suppose

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

for $i=1, \ldots, n$, where

- $x_{1}, \ldots, x_{n}$ are fixed real numbers
- $Y_{1}, \ldots, Y_{n}$ are independent random variables
- $\beta_{0}$ and $\beta_{1}$ are unknown constants
- $\varepsilon_{1}, \ldots, \varepsilon_{n}$ are iid errors with
- $\mathbb{E} \varepsilon_{i}=0$
- $\operatorname{Var} \varepsilon_{i}=\sigma^{2}$ for $i=1, \ldots, n$.

Goal: Estimate the unknown constants $\beta_{0}$ and $\beta_{1}$ and the error variance $\sigma^{2}$.

## Topics:

(1) Estimation of $\beta_{0}, \beta_{1}$, and $\sigma^{2}$ as well as of $\beta_{0}+\beta_{1} x_{\text {new }}$.
(2) Inference about $\beta_{0}$ and $\beta_{1}$, e.g. testing $H_{0}: \beta_{1}=0$ versus $H_{1}: \beta_{1} \neq 0$. Also confidence intervals for $\beta_{0}+\beta_{1} x_{\text {new }}$.
(0) Prediction of $Y_{\text {new }}$ of a "new" obs. ( $x_{\text {new }}, Y_{\text {new }}$ ) with a prediction interval.

- Likelihood approach under Normal errors.

Least-squares estimators of simple linear regression coefficients Provided $\sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right)^{2}>0$, the function

$$
Q_{n}\left(\beta_{0}, \beta_{1}\right):=\sum_{i=1}^{n}\left[Y_{i}-\left(\beta_{0}+\beta_{1} x_{i}\right)\right]^{2}
$$

is (uniquely) minimized at

$$
\begin{aligned}
& \hat{\beta}_{0}=\bar{Y}_{n}-\hat{\beta}_{1} \bar{x}_{n} \\
& \hat{\beta}_{1}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right)\left(Y_{i}-\bar{Y}_{n}\right)}{\sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right)^{2}}
\end{aligned}
$$

Exercise: Derive this result.


Define some new quantities:

$$
\begin{gathered}
S_{X Y}=\sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right)\left(Y_{i}-\bar{Y}_{n}\right), \quad S_{X X}=\sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right)^{2}, \quad S_{Y Y}=\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}_{n}\right)^{2}, \\
r_{X Y}=\frac{S_{X Y}}{\sqrt{S_{X X} S_{Y Y}}}, \quad s_{Y}=\frac{S_{Y Y}}{n-1}, \quad s_{X}=\frac{S_{X X}}{n-1} .
\end{gathered}
$$

Then we have the following simpler expressions for $\hat{\beta}_{1}$ :

$$
\hat{\beta}_{1}=\frac{S_{X Y}}{S_{X x}} \quad \text { or } \quad \hat{\beta}_{1}=r_{X Y}\left(\frac{S_{Y Y}}{S_{X x}}\right)^{1 / 2} \quad \text { or } \quad \hat{\beta}_{1}=r_{X Y}\left(s_{Y} / s_{X}\right) .
$$

Exercise: Generate a toy data set in R and plot the least-squares line.

- The fitted values are

$$
\hat{Y}_{i}=\hat{\beta}_{0}+\hat{\beta}_{1} x_{i} \quad \text { for } i=1, \ldots, n .
$$

- The residuals are

$$
\hat{\varepsilon}_{i}=Y_{i}-\hat{Y}_{i} \quad \text { for } i=1, \ldots, n .
$$

Log of beryllium abundance versus temperature of 38 stars with least-squares line.


Data from [1].

Some moments of the least-squares estimators
We have $\mathbb{E} \hat{\beta}_{0}=\beta_{0}$ and $\mathbb{E} \hat{\beta}_{1}=\beta_{1}$ as well as

$$
\begin{aligned}
\operatorname{Var} \hat{\beta}_{0} & =\left(n^{-1}+\bar{x}_{n}^{2} S_{x x}^{-1}\right) \sigma^{2} \\
\operatorname{Var} \hat{\beta}_{1} & =S_{x x}^{-1} \sigma^{2} \\
\operatorname{Cov}\left(\hat{\beta}_{0}, \hat{\beta}_{1}\right) & =-\bar{x}_{n} S_{x x}^{-1} \sigma^{2} .
\end{aligned}
$$

Exercise: Derive these, beginning by showing that $\hat{\beta}_{0}$ and $\hat{\beta}_{1}$ can be written as

$$
\begin{aligned}
& \hat{\beta}_{0}=\beta_{0}+\frac{\bar{x}_{n}}{S_{x x}} \sum_{i=1}^{n}\left[\frac{S_{x x}}{n \bar{x}_{n}}-\left(x_{i}-\bar{x}_{n}\right)\right] \varepsilon_{i} \\
& \hat{\beta}_{1}=\beta_{1}+\frac{1}{S_{x x}} \sum_{i=1}^{n}\left(x_{i}-\bar{x}_{n}\right) \varepsilon_{i} .
\end{aligned}
$$

## Unbiased estimator of $\sigma^{2}$

The estimator

$$
\hat{\sigma}^{2}=\frac{1}{n-2} \sum_{i=1}^{n} \hat{\varepsilon}_{i}^{2}
$$

is unbiased for $\sigma^{2}$.

The proof is omitted. The best way to prove this is with matrix algebra.

Mean and variance of estimated function at a point
We have

$$
\begin{aligned}
\mathbb{E}\left(\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }}\right) & =\beta_{0}+\beta_{1} x_{\text {new }} \\
\operatorname{Var}\left(\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }}\right) & =\left[\frac{1}{n}+\frac{\left(x_{\text {new }}-\bar{x}_{n}\right)^{2}}{S_{x x}}\right] \sigma^{2}
\end{aligned}
$$

Exercise: Derive the above.

## Sampling distribution results under Normal errors

If $\varepsilon_{1}, \ldots, \varepsilon_{n} \stackrel{\text { ind }}{\sim} \operatorname{Normal}\left(0, \sigma^{2}\right)$, then

$$
\begin{aligned}
\hat{\beta}_{0} & \sim \operatorname{Normal}\left(\beta_{0},\left(n^{-1}+\bar{x}_{n}^{2} S_{x x}^{-1}\right) \sigma^{2}\right) \\
\hat{\beta}_{1} & \sim \operatorname{Normal}\left(\beta_{1}, S_{x x}^{-1} \sigma^{2}\right) \\
\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }} & \sim \operatorname{Normal}\left(\beta_{0}+\beta_{1} x_{\text {new }},\left[n^{-1}+S_{x x}^{-1}\left(x_{\text {new }}-\bar{x}_{n}\right)^{2}\right] \sigma^{2}\right) \\
(n-2) \hat{\sigma}^{2} / \sigma^{2} & \sim \chi_{n-2}^{2}
\end{aligned}
$$

Moreover, the above gives

$$
\begin{aligned}
& \frac{\hat{\beta}_{0}-\beta_{0}}{\hat{\sigma} \sqrt{n^{-1}+\bar{x}_{n}^{2} S_{x x}^{-1}}} \sim t_{n-2}, \quad \frac{\hat{\beta}_{1}-\beta_{1}}{\hat{\sigma} \sqrt{S_{x x}^{-1}}} \sim t_{n-2} \\
& \text { and } \quad \frac{\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }}-\left(\beta_{0}+\beta_{1} x_{\text {new }}\right)}{\hat{\sigma} \sqrt{n^{-1}+S_{x x}^{-1}\left(x_{\text {new }}-\bar{x}_{n}\right)^{2}}} \sim t_{n-2}
\end{aligned}
$$

## Confidence intervals

We may construct $(1-\alpha) 100 \%$ CIs for $\beta_{0}, \beta_{1}$, and $\beta_{0}+\beta_{1} x_{\text {new }}$ as

$$
\begin{gathered}
\hat{\beta}_{0} \pm t_{n-2, \alpha / 2} \hat{\sigma} \sqrt{n^{-1}+\bar{x}_{n}^{2} S_{x x}^{-1}} \\
\hat{\beta}_{1} \pm t_{n-2, \alpha / 2} \hat{\sigma} \sqrt{S_{x x}^{-1}} \\
\left(\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }}\right) \pm t_{n-2, \alpha / 2} \hat{\sigma} \sqrt{n^{-1}+S_{x x}^{-1}\left(x_{\text {new }}-\bar{x}_{n}\right)^{2}}
\end{gathered}
$$

Exercise: Get the beryllium data and under $\alpha=0.05$ :
(9) Build CIs for $\beta_{0}$ and $\beta_{1}$.
(2) Build Cls for $\beta_{0}+\beta_{1} x_{\text {new }}$ across a range of $x_{\text {new }}$ values and plot them.

## Testing hypotheses about $\beta_{1}$

Consider testing hypotheses about $\beta_{1}$ with respect to a null value $\beta_{1}^{*}$, and define

$$
T_{1, n}=\frac{\hat{\beta}_{1}-\beta_{1}^{*}}{\hat{\sigma} \sqrt{S_{x x}^{-1}}} .
$$

We have the following:

| $H_{0}$ | $H_{1}$ | Reject $H_{0}$ at $\alpha$ iff | $p$-value |
| :--- | :--- | :--- | :--- |
| $\beta_{1} \leq \beta_{1}^{*}$ | $\beta_{1}>\beta_{1}^{*}$ | $T_{1, n}>t_{n-2, \alpha}$ | $1-F_{t_{n-2}}\left(T_{1, n}\right)$ |
| $\beta_{1} \geq \beta_{1}^{*}$ | $\beta_{1}<\beta_{1}^{*}$ | $T_{1, n}<-t_{n-2, \alpha}$ | $F_{t_{n-2}}\left(T_{1, n}\right)$ |
| $\beta_{1}=\beta_{1}^{*}$ | $\beta_{1} \neq \beta_{1}^{*}$ | $\left\|T_{1, n}\right\|>t_{n-2, \alpha / 2}$ | $2\left[1-F_{t_{n-2}}\left(\left\|T_{1, n}\right\|\right)\right]$ |

Exercise: Get the $p$-value for testing $H_{0}: \beta_{1}=0$ for the beryllium data.

## Prediction interval for a new observation

A $(1-\alpha) \times 100 \%$ prediction interval for $Y_{\text {new }}$ of a new obs. $\left(Y_{\text {new }}, x_{\text {new }}\right)$ is given by

$$
\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }} \pm t_{n-2, \alpha / 2} \hat{\sigma} \sqrt{1+n^{-1}+S_{x x}^{-1}\left(x_{\text {new }}-\bar{x}_{n}\right)^{2}}
$$

Exercise: Derive the above using the distribution of $\hat{\varepsilon}_{\text {new }}=Y_{\text {new }}-\left(\hat{\beta}_{0}+\hat{\beta}_{1} x_{\text {new }}\right)$.
Exercise: With the Beryllium data, construct Pls over a range of $x_{\text {new }}$ values.

Cls for the height of the regression function as well as Pls for new obs.


Data from [1].

## Exercise: Let

$$
Y_{i}=\beta_{0}+\beta_{1} x_{i}+\varepsilon_{i}, \quad i=1, \ldots, n,
$$

where $\varepsilon_{1}, \ldots, \varepsilon_{n} \stackrel{\text { ind }}{\sim} \operatorname{Normal}\left(0, \sigma^{2}\right)$.
(1) Give the likelihood function for $\beta_{0}, \beta_{1}$, and $\sigma^{2}$.
(2) Give the log-likelihood function for $\beta_{0}, \beta_{1}$, and $\sigma^{2}$.
(0) Show that the size- $\alpha$ LRT for $H_{0}: \beta_{1}=0$ vs $H_{1}: \beta_{1} \neq 0$ is

$$
\text { Reject } H_{0} \text { iff } S_{x x}^{1 / 2}\left|\hat{\beta}_{1}\right| / \hat{\sigma}>t_{n-2, \alpha / 2} .
$$

圊 Nuno C Santos, G Israelian, RJ García López, M Mayor, R Rebolo, S Randich, A Ecuvillon, and C Domínguez Cerdeña. Are beryllium abundances anomalous in stars with giant planets? Astronomy \& Astrophysics, 427(3):1085-1096, 2004.

