

Lecture 02

Simple Linear Models: OLS

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STAT 312/612

The Yale University logo, featuring the word "Yale" in a blue, serif font.

OFFICE HOURS

- Taylor Arnold:
 - 24 Hillhouse, Office # 206
 - Wednesdays 13:30-15:00, or by appointment
 - Short one-on-one meetings (or small groups)
- Jason Klusowski:
 - 24 Hillhouse, Main Classroom
 - Tuesdays 19:00-20:30
 - Group Q&A style

WEBSITE

<http://euler.stat.yale.edu/~tba3/stat612>

Goals for today

1. calculate the MLE for simple linear regression
2. derive basic properties of the simple linear model MLE
3. introduction to R for simulations and data analysis

SIMPLE LINEAR MODELS: MLEs

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$$y_i = x_i\beta + \epsilon_i, \quad i = 1, \dots, n.$$

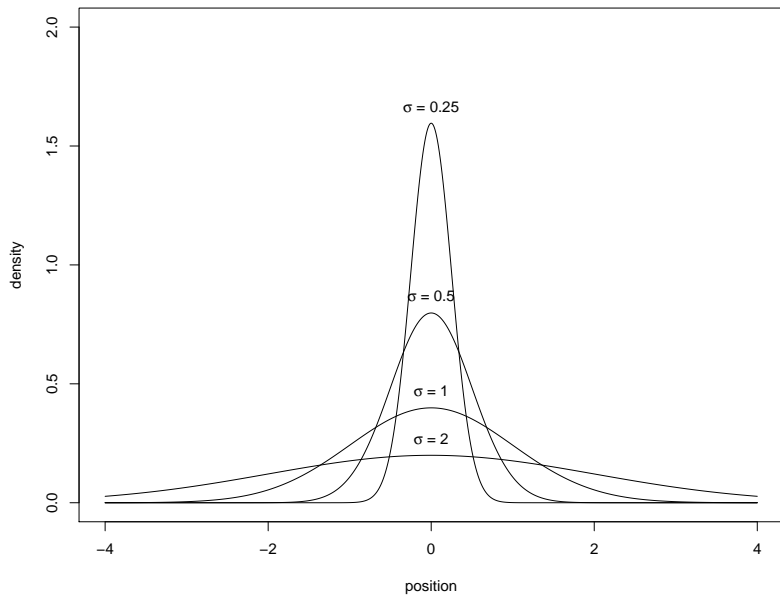
This is, perhaps, the simplest linear model.

For today, we will assume that the x_i 's are fixed and known quantities. This is called a **fixed design**, compared to a **random design**.

The error terms are assumed to be independent and identically distributed random variables with a normal density function:

$$\epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

For some unknown variance $\sigma^2 > 0$.



The density function of a normally distributed random variable with mean μ and variance σ^2 is given by:

$$f(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \times \exp \left\{ -\frac{1}{2\sigma^2} (z - \mu)^2 \right\}$$

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Conceptually, the front term is just a normalization to make the density sum to 1. The important part is:

$$f(z) \propto \exp \left\{ -\frac{1}{2\sigma^2}(z - \mu)^2 \right\}$$

Which you have probably seen rewritten as:

$$f(z) \propto \exp \left\{ -0.5 \cdot \left(\frac{z - \mu}{\sigma} \right)^2 \right\}$$

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Notice that the **mean** μ from the general case has been replaced by βx_i , which should be the mean of $y_i|x_i$.

We can bring the product up into the the exponent as a sum:

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Let's highlight the slope parameter β :

$$\mathcal{L}(\beta, \sigma | x, y) = (2\pi\sigma^2)^{-n/2} \times \exp \left\{ -\frac{1}{2\sigma^2} \cdot \sum_i (y_i - \beta x_i)^2 \right\}$$

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What is the MLE for β ?

Without resorting to any fancy math, we can see that:

$$\hat{\beta}_{MLE} = \arg \min_{b \in \mathbb{R}} \left\{ \sum_i (y_i - b \cdot x_i)^2 \right\} \quad (1)$$

The least squares estimator.

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Now the minimum of this corresponds with the maximum likelihood estimators.

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And we can again see without resorting to derivatives that the maximum likelihood estimator is that one that minimizes the sum of squares:

$$\hat{\beta}_{mle} = \arg \min_{b \in \mathbb{R}} \left\{ \sum_i (y_i - bx_i)^2 \right\}$$

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Taking the derivative of the sum of squares with respect to β we get:

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If you have seen the standard simple least squares solution (that is, with an intercept) this should look familiar.

There are many ways of thinking about the maximum likelihood estimator, one of which is as a weighted sum of the data points y_i :

$$\begin{aligned}\hat{\beta} &= \frac{\sum_i y_i x_i}{\sum_i x_i^2} \\ &= \sum_i \left(y_i \cdot \frac{x_i}{\sum_j x_j^2} \right) \\ &= \sum_i y_i w_i\end{aligned}$$

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One thing that the weighted form of the estimator makes obvious is that the estimator is distributed normally:

$$\hat{\beta} \sim \mathcal{N}(\cdot, \cdot)$$

As it is the sum of normally distributed variables (y_i).

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And so we see the estimator is unbiased.

A normally distributed random variable is entirely characterised by its mean and variance. So let us compute the variance of our MLE estimator:

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If $\sum_i x_i^2$ diverges, we will get a consistent estimator.

So we now know that the MLE is distributed as:

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Does this make sense? What if $x_i = 1$ for all i ?

The MLE is weighting the data y_i according to:

$$w_i \propto x_i$$

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Does this make sense? **Why?**

SIMULATIONS

We will be using the R programming language for data analysis and simulations



- Open source software, available at:
<https://www.r-project.org/>
- An implementation of the S programming language
- Designed for interactive data analysis
- For pros/cons, check out the many lengthy internet articles & arguments



Things to know

- everything in R is an object
- indexing starts at 1
- no scalar type, numeric objects are all vectors
- mostly functional language, with some OO features

GAUß-MARKOV THEOREM

Many of the nice properties of the MLE estimator result from being unbiased and normally distributed. A natural question is whether another weighted sum of the data points y_i would yield a better estimator.

Formally, if we define:

$$\hat{\beta}_{BLUE} = \sum_i y_i \cdot a_i$$

What values of a_i will minimise the variance of the estimator assuming that we force it to be unbiased? BLUE stands for the Best Linear Unbiased Estimator.

To force unbiasedness, we must have:

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As we cannot change σ^2 , minimising the variance amounts to minimising $\sum_i a_i^2$.

So we have reduced the problem to solving the following:

$$\arg \min_{a \in \mathbb{R}^n} \left\{ \sum_i a_i^2 \quad \text{s.t.} \quad \sum_i a_i x_i = 1 \right\}$$

Lagrange multiplier

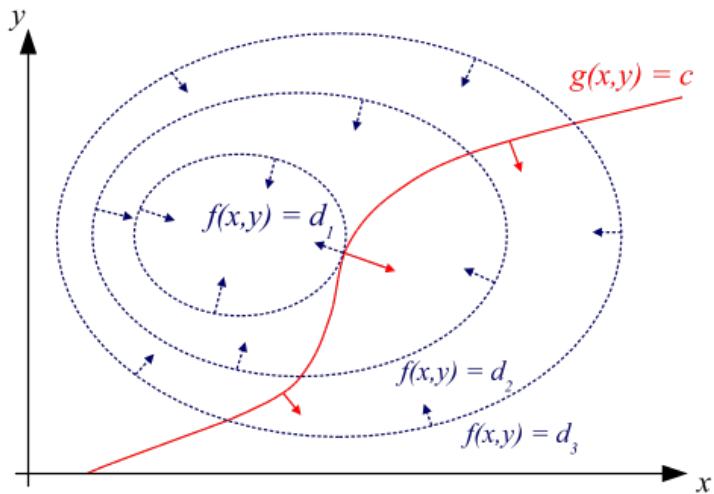
To solve the constrained problem:

$$\arg \min_{x \in \mathbb{R}^p} \{f(x) \quad \text{s.t.} \quad g(x) = k\}$$

Find stationary points (zero partial derivatives) of:

$$L(x, \lambda) = f(x) + \lambda \cdot (g(x) - k)$$

This will give the set of possible minimisers to the original constrained problem.



For our problem we have:

$$L(a, \lambda) = \sum_i a_i^2 + \lambda \cdot \left(1 - \sum_i a_i x_i \right)$$

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Which gives:

$$\frac{\partial}{\partial a_k} L(a, \lambda) = 2a_k - \lambda x_k$$

$$2a_k - \lambda x_k = 0$$

$$a_k = \frac{1}{2} \cdot \lambda \cdot x_k$$

The lambda derivative, which is just the constraint, shows the specific value of λ that we need:

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Plugging our previous version of a_i :

$$\sum_i \frac{1}{2} \cdot \lambda \cdot x_i \cdot x_i = 1$$
$$\lambda \cdot \sum_i \frac{1}{2} \cdot x_i^2 = 1$$
$$\lambda = \frac{2}{\sum_i x_i^2}$$

Finally, plugging this back in:

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And this gives:

$$\hat{\beta}_{BLUE} = \sum_i y_i \cdot \frac{x_i}{\sum_j x_j^2}$$
$$= \hat{\beta}_{MLE}$$

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- has an analytic solution

The more common formulation of simple linear models includes an unknown intercept term α .

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$$y_i = \alpha + x_i\beta + \epsilon_i, \quad i = 1, \dots, n.$$

The likelihood function for this revised model is almost the same as before

$$\mathcal{L}(\beta, \sigma|x, y) = (2\pi\sigma^2)^{-n/2} \times \exp\left\{-\frac{1}{2\sigma^2} \cdot \sum_i (y_i - \alpha - x_i\beta)^2\right\}$$

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Clearly, by the same logic the MLE is given by minimizing the sum of squared residuals.

Solving the least squares problem is only slightly more difficult because now we have two parameters and need to use partial derivatives to solve them. Otherwise the process is the same with a few more terms floating around.

The estimators in this case become:

$$\hat{\beta} = \frac{\sum_i (y_i - \bar{y})(x_i - \bar{x})}{\sum_i (x_i - \bar{x})^2}$$
$$\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x}$$

Where $\bar{x} = n^{-1} \sum_i x_i$ and $\bar{y} = n^{-1} \sum_i y_i$.

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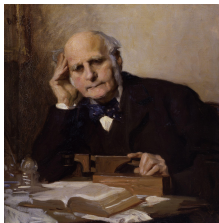
Notice what happens when both means are zero.

All of these properties are maintained jointly for $(\hat{\alpha}, \hat{\beta})$

- unbiased
- consistent as long as $\sum_i (x_i - \bar{x})^2$ diverges
- normally distributed
- is the BLUE estimator
- achieves the Cramér–Rao bound
- has an analytic solution

APPLICATIONS

Sir Francis Galton & Regression



- ‘Co-relations and their measurement, chiefly from anthropometric data’ (1888).
- further ideas in *Natural Inheritance*
 - sweet peas and regression to the mean
 - extinction of surnames (Galton–Watson stochastic processes)
 - ‘Good and Bad Temper in English Families’

Some parting words from Sir Francis Galton

as any other quality. Also, that although it exerts an immense influence for good or ill on domestic happiness, it seems that good temper has not been especially looked for, nor ill temper especially shunned, as it ought to be in marriage-selection.