

# MS&E 125: Intro to Applied Statistics

## Linear regression

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May 3, 2023

## Announcements

- ▶ section today
- ▶ hw5 out today, due next Tuesday
- ▶ not sure if you're on the right track on hw? come to OH!

# Outline

Linear models

Prediction

Fitting linear regression

Maximum likelihood

Multiple regression

## Motivation: linear models

Linear models can be used for

- ▶ **prediction:** given a set of input variables, predict a value for the output variable
- ▶ **understanding:** how are the input variables related to the output variable, and to each other?
- ▶ **inference:** how much do the input variables affect the output variable?
- ▶ **counterfactuals:** what would happen if we changed the input variables?
- ▶ **control:** how can we change the input variables to achieve a desired output?

## Prediction examples

- ▶ **House Price Prediction:**

- ▶ Input variables ( $x$ ): square footage, number of bedrooms, age of the house, location, etc.
- ▶ Output variable ( $y$ ): price of the house

- ▶ **Sales Forecasting:**

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### ▶ **Energy Consumption Forecasting:**

- ▶ Input variables ( $x$ ): temperature, humidity, time of day, day of the week, etc.
- ▶ Output variable ( $y$ ): energy consumption of a building or household



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## Regression setup

we want to predict output given inputs

- ▶ input variables  $x \in \mathbf{R}^p$ 
  - ▶ also called “predictors”, “independent variables”, “covariates”
  - ▶ a row of a data table
- ▶ output variable  $y \in \mathbf{R}$ 
  - ▶ also called “outcome”, “response”, “dependent variable”, “label”, “target” ...

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example: to predict the cost of an insurance claim,

- ▶  $y$  is the cost of an insurance claim.
- ▶ entries of  $x$  are the properties of the insured and his/her vehicle, e.g., credit score, age of the vehicle, ...

## Demo: simple linear regression

`https://colab.research.google.com/github/  
stanford-mse-125/demos/blob/main/regression.ipynb`

## Simple linear regression

simple linear regression:  $p = 1$

- ▶ predict

$$\hat{y} = \beta_0 + \beta_1 x$$

- ▶  $\beta_0, \beta_1 \in \mathbf{R}$  are called **regression coefficients**
- ▶  $\hat{y}$  is called the **prediction** for input  $x$

## Predictions: example

In the fathers and sons dataset, we found

$$\hat{y} = 34 + 0.5x$$

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where  $x$  is the height of the father in inches.

**Q:** What do the numbers 34 and .5 mean?

**A:** A father with height 0 inches has a son with height 34 inches. For each inch of height, the son is expected to be 0.5 inches taller.



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## Residuals

look at **residual**  $r$  to understand how well the model fits the data

$$r = y - \hat{y} = y - \beta_0 - \beta_1 x_1$$

pick  $\beta$  so the residuals are small

# Dataset

to find the best line, we need a dataset! suppose we have

- ▶  $n$  data points  $(x_1, y_1), \dots, (x_n, y_n)$ 
  - ▶ also called **dataset**, **examples**, **observations**, **samples** or **measurements**
- ▶ each  $x_i \in \mathbf{R}^p$  is a vector of  $p$  input variables
  - ▶ a row from the data table
- ▶ each  $y_i \in \mathbf{R}$  is a scalar output variable

## Linear regression: two perspectives

how to choose  $\beta$ ?

- ▶ **optimization perspective:** find  $\beta$  to minimize the sum of squared errors

$$\text{minimize} \quad \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_1)^2$$

- ▶ **statistical perspective:** find the line that maximizes the likelihood of the data

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- ▶ **statistical perspective:** find the line that maximizes the likelihood of the data

theorem: for appropriate assumptions, the two perspectives give the same answer

(coming in a few slides, or see All of Statistics ch. 14)

## Least squares fitting

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**Q:** Given  $x_i \in \mathbf{R}$ , what is  $\beta_1$ ?

**A:** Set derivative to zero; solution is slope of the line of best fit.

## Solve for $\beta_0$

$$\text{minimize} \quad \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

take derivative wrt  $\beta_0$  and set to zero:

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

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

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

$\implies$  the model goes through the point of averages

## Solve for $\beta_1$

$$\text{minimize} \quad \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

take derivative wrt  $\beta_1$  and set to zero:

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

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

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

interpretation:

- ▶ suppose  $x$  and  $y$  have been standardized so that  $\sum_{i=1}^n x_i = \sum_{i=1}^n y_i = 0$  and  $\frac{1}{n} \sum_{i=1}^n x_i^2 = \frac{1}{n} \sum_{i=1}^n y_i^2 = 1$ .
- ▶ then  $\beta_1 = \frac{1}{n} \sum_{i=1}^n x_i y_i$  is the **correlation** between  $x$  and  $y$

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## Linear regression model

### **probabilistic model for linear regression:**

suppose the  $x$ s are fixed, and  $y$ s are generated by

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$

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under the model, the likelihood of observing residual  $r = y - \hat{y}$  is

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

## Demo: are errors iid normal?

`https://colab.research.google.com/github/  
stanford-mse-125/demos/blob/main/regression.ipynb`



## Maximum likelihood

**likelihood function:** probability of data given parameters

$$\ell(\beta_0, \beta_1) = \prod_{i=1}^n (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2}\right)$$

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**maximum likelihood estimation (MLE):**

choose  $\beta_0$  and  $\beta_1$  to maximize the likelihood function

$$\hat{\beta}_0, \hat{\beta}_1 = \underset{\beta_0, \beta_1}{\operatorname{argmax}} \ell(\beta_0, \beta_1) = \underset{\beta_0, \beta_1}{\operatorname{argmax}} \log \ell(\beta_0, \beta_1)$$

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**maximum likelihood estimation (MLE):**

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## Maximum likelihood

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**maximum likelihood estimation (MLE):**

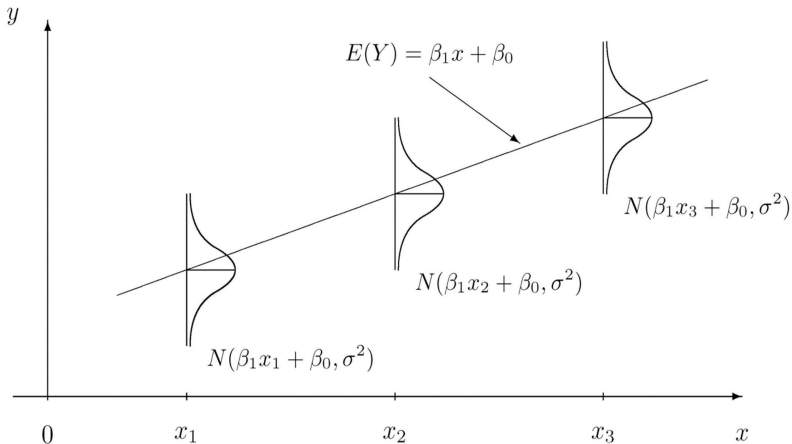
choose  $\beta_0$  and  $\beta_1$  to maximize the likelihood function

$$\begin{aligned}\hat{\beta}_0, \hat{\beta}_1 &= \operatorname{argmax}_{\beta_0, \beta_1} \ell(\beta_0, \beta_1) = \operatorname{argmax}_{\beta_0, \beta_1} \log \ell(\beta_0, \beta_1) \\ &= \operatorname{argmax}_{\beta_0, \beta_1} \sum_{i=1}^n \log \left( (2\pi\sigma^2)^{-1/2} \exp \left( -\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right) \right) \\ &= \operatorname{argmax}_{\beta_0, \beta_1} \left[ -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \right] \\ &= \operatorname{argmin}_{\beta_0, \beta_1} \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2\end{aligned}$$

$\implies$  least squares finds the maximum likelihood estimate!

## Probabilistic interpretation

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$



## Estimation puts a hat on it

statisticians use hats to denote estimates:

- ▶  $\hat{\beta}_0$  is the estimate of  $\beta_0$
- ▶  $\hat{y}$  is the estimate of  $y$

these estimates are **random quantities** that depend on the data

```
https://colab.research.google.com/github/  
stanford-mse-125/demos/blob/main/  
regression-uncertainty.ipynb
```

## Properties of the estimator

putting it together, we have found:

$$\hat{\beta}_1 = \rho(x, y) \hat{\sigma}_y / \hat{\sigma}_x, \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

where

- ▶  $\rho(x, y)$  is the correlation between  $x$  and  $y$
- ▶  $\hat{\sigma}_x$  and  $\hat{\sigma}_y$  are the sample standard deviations of  $x$  and  $y$
- ▶  $\bar{x}$  and  $\bar{y}$  are the sample means of  $x$  and  $y$

under the normal model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

these estimates are unbiased:

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

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All of Statistics ch 14 derives the variance of the estimates



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## Matrix notation

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

rewrite using linear algebra:

- ▶ form **response vector**  $y \in \mathbf{R}^n$ : each outcome  $y_i$  is an entry of  $y$ 
  - ▶ also called **target vector**
- ▶ form **design matrix**  $X \in \mathbf{R}^{n \times p}$ : each example  $x^{(i)}$  is a row of  $X$ 
  - ▶ also called **feature matrix**
  - ▶ if the model includes a constant term, the 0th column of  $X \in \mathbf{R}^{n \times p+1}$  is all ones

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} X_{11} & \cdots & X_{1p} \\ \vdots & \vdots & \vdots \\ X_{n1} & \cdots & X_{np} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

## Least squares in matrix notation

rewrite error:

$$\sum_{i=1}^n (y_i - \hat{y}_i)^2 = \|y - X\beta\|^2$$

interpretation:

- ▶  $X\beta$  is a linear combination of the columns of  $X$
- ▶ we seek the linear combination that best matches  $y$

## Linear regression: model

we can rewrite the model as

$$y_i = \beta_0 + \beta_1 X_{i,1} + \beta_2 X_{i,2} + \cdots + \beta_p X_{i,p} + \varepsilon_i$$

- ▶ notice that  $\beta_0, \beta_1, \dots, \beta_p$  do not depend on  $i$
- ▶ the columns of the data table are  $Y_i, X_{i,1}, \dots, X_{i,p}$

$i$	$y_i$	$X_{i,1}$	$X_{i,2}$	$\dots$	$X_{i,p}$
1	2.3	1.1	6.2	$\dots$	5.9
2	12.7	2.4	5.4	$\dots$	9.6
3	6.3	0.9	6.9	$\dots$	1.5

## Example: electricity usage

- ▶ We are managing a large complex of apartments in the Northeast.
- ▶ We pay for the electricity used by our residents.
- ▶ We would like to predict electricity usage so that we can estimate how much money should be set aside.

## Demo: multiple linear regression

`https://colab.research.google.com/github/  
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