22.01.2019

Statistical Methods in AI (CSE/ECE 471)

Lecture-7:

- A short detour back to NB
- Linear Regression
- Logistic Regression

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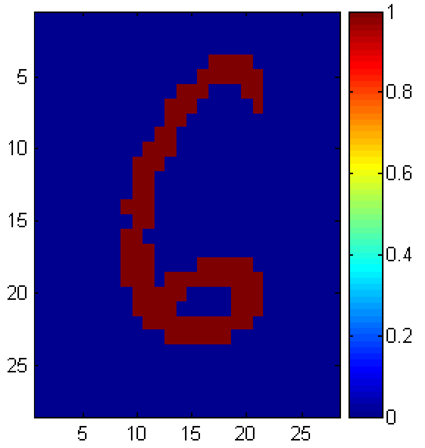
Center for Visual Information Technology (CVIT), IIIT Hyderabad

Announcements

- A2 is due Feb 2, 11.59 pm
- SMAI Mid-1 will be on Feb 7 (Thursday)
  - Syllabus: Lec 1 – Lec 8 (this week's Friday lecture)

A short detour back to Naïve Bayes

$$\arg\max_{Y} P(Y|X_1,\ldots,X_n)$$

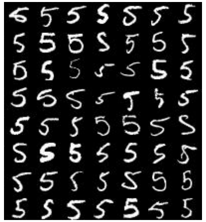


Likelihood

Prior

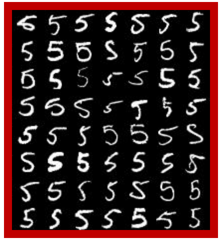
$$P(Y|X_1,\ldots,X_n) = \frac{P(X_1,\ldots,X_n|Y)P(Y)}{P(X_1,\ldots,X_n)}$$

Normalization Constant



$$P(X_1,\ldots,X_n|Y) = \prod_{i=1}^{n} P(X_i|Y)$$

Generative v/s Discriminative Models



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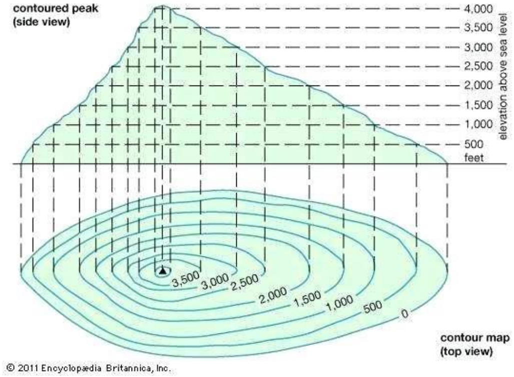
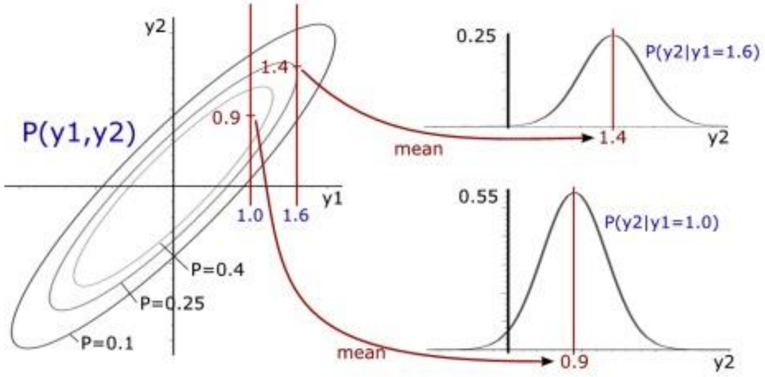
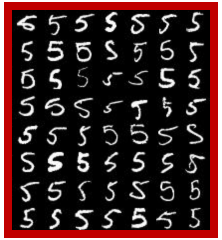




Generative v/s Discriminative Models



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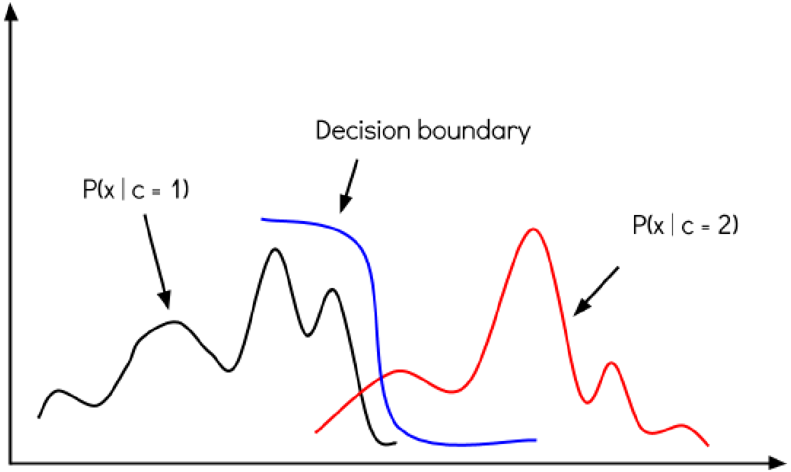
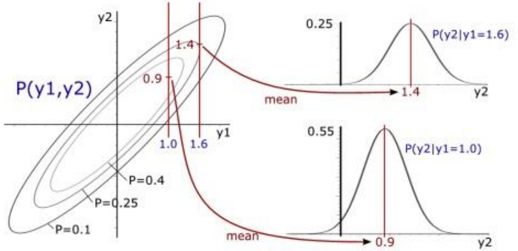
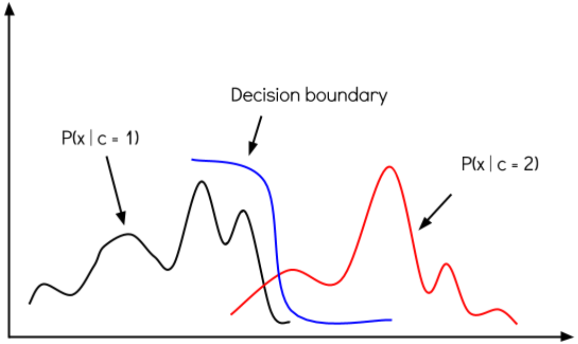


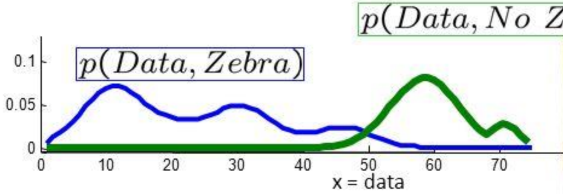


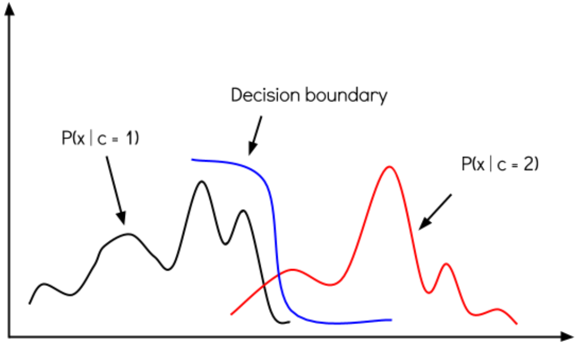


Discriminative vs. generative

- Generative model

(*The artist*)





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- Generative model

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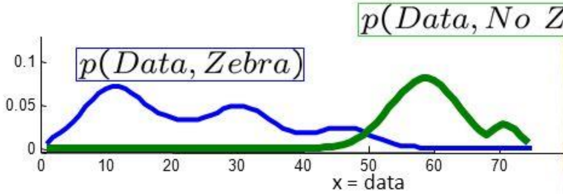
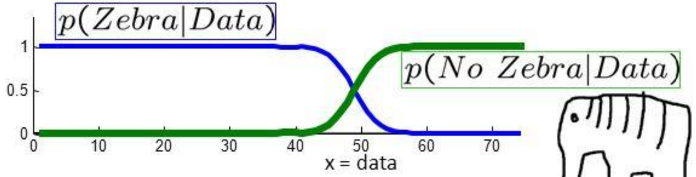
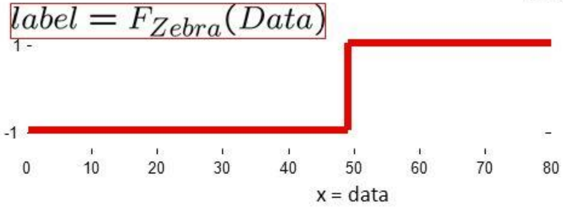


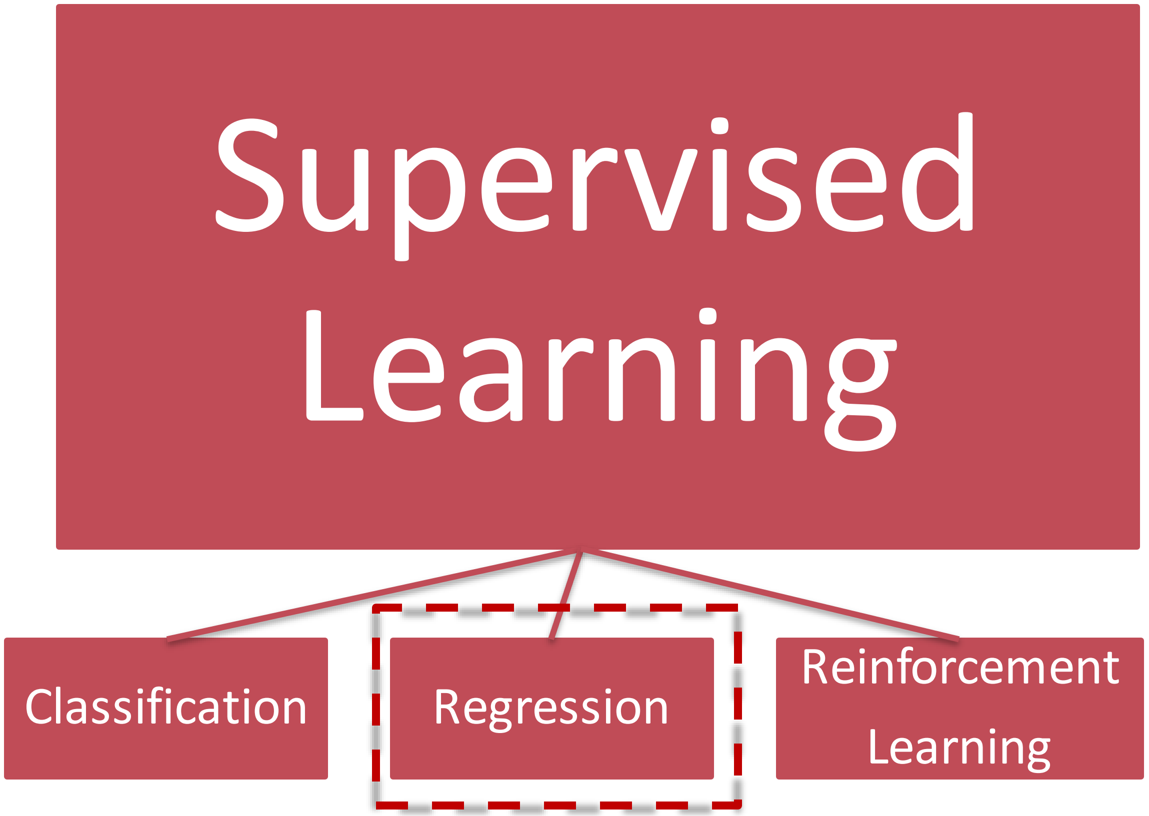
- Discriminative model

(The lousy painter)



- Classification function




Supervised Learning
Classification
Regression
Reinforcement Learning

Linear Regression Model

- 1. Relationship Between Variables Is a Linear Function

Population Y-Intercept

Population Slope

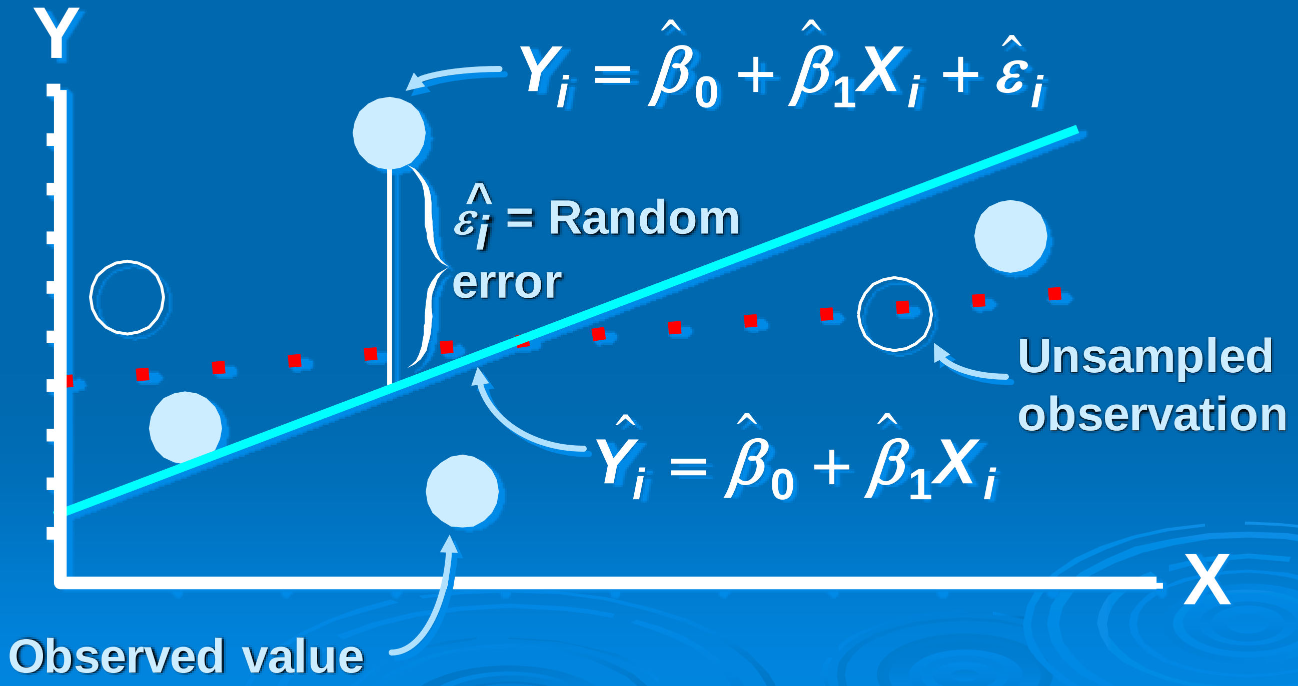
Random Error

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

Dependent (Response) Variable (e.g. Salary)

Independent (Explanatory) Variable (e.g. Yrs of experience)

Sample Linear Regression Model



Least Squares

- 1. 'Best Fit' Means Difference Between Actual Y Values & Predicted Y Values is a Minimum. *But* Positive Differences Off-Set Negative ones. So square errors!

$$\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2 = \sum_{i=1}^{n}\hat{\varepsilon}_i^2$$

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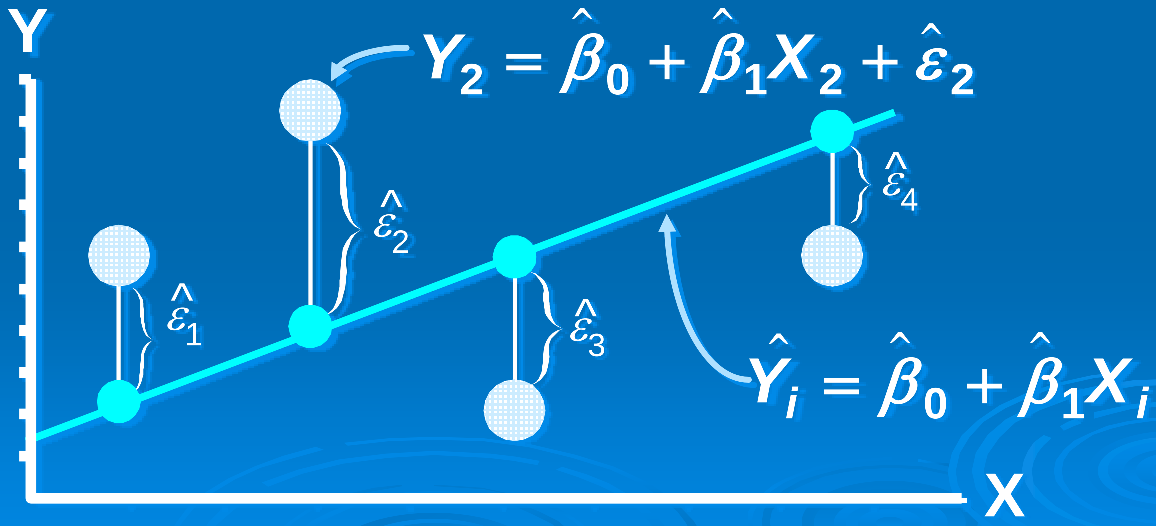
$$\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2 = \sum_{i=1}^{n}\hat{\varepsilon}_i^2$$

- 2. LS Minimizes the Sum of the Squared Differences (errors) (SSE)

Least Squares Graphically

LS minimizes $\sum_{i=1}^{n} \hat{\varepsilon}_i^2 = \hat{\varepsilon}_1^2 + \hat{\varepsilon}_2^2 + \hat{\varepsilon}_3^2 + \hat{\varepsilon}_4^2$



Coefficient Equations

- Prediction equation

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- Sample slope

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2}$$

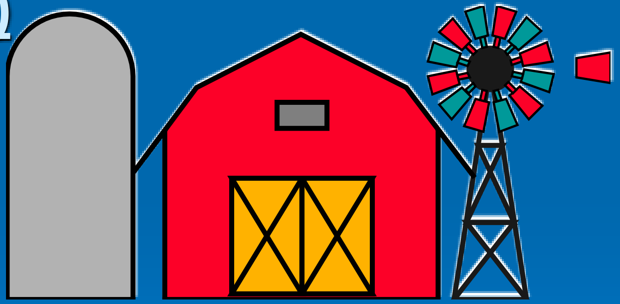
- Sample Y - intercept

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

Parameter Estimation Thinking Challenge

- You’re a Vet epidemiologist for the county cooperative. You gather the following data:
- **Food (lb.)** / **Milk yield (lb.)**

Food (lb.)	Milk yield (lb.)
4	3.0
6	5.5
10	6.5
12	9.0



- What is the **relationship** between cows’ food intake and milk yield?

Coefficient Interpretation Solution*

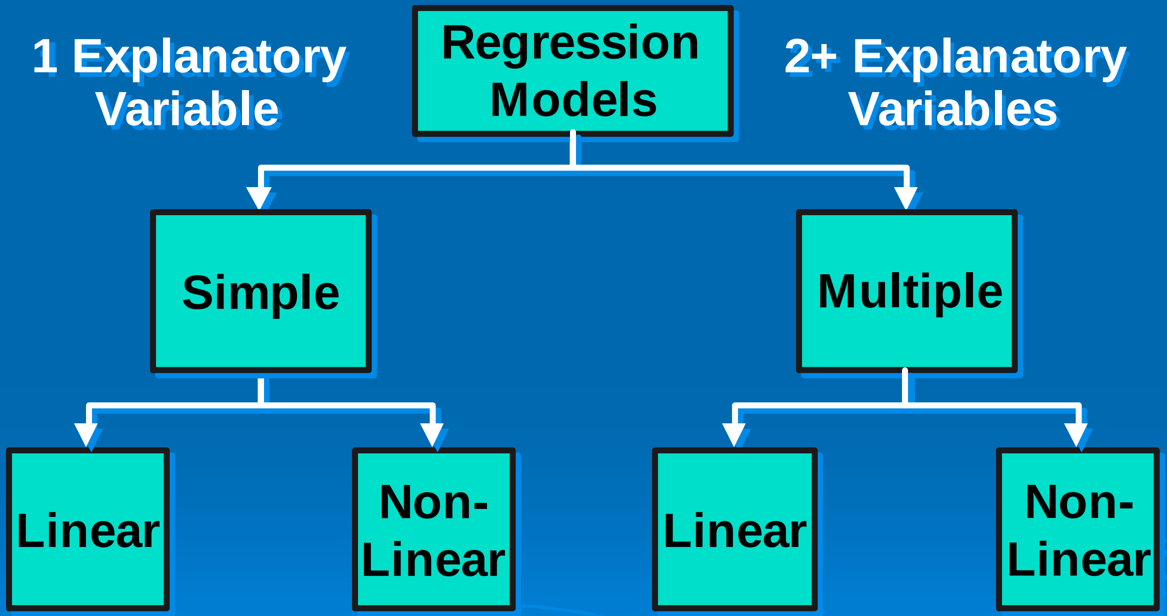
- 1. Slope ($\hat{\beta}_1$)
  - Milk Yield (*Y*) Is Expected to Increase by .65 lb. for Each 1 lb. Increase in Food intake (*X*)

Coefficient Interpretation Solution*

- 1. Slope ($\hat{\beta}_1$)
  - Milk Yield (Y) Is Expected to Increase by .65 lb. for Each 1 lb. Increase in Food intake (X)

- 2. Y-Intercept ($\hat{\beta}_0$)
  - Average Milk yield (Y) Is Expected to Be 0.8 lb. When Food intake (X) Is 0

Types of Regression Models

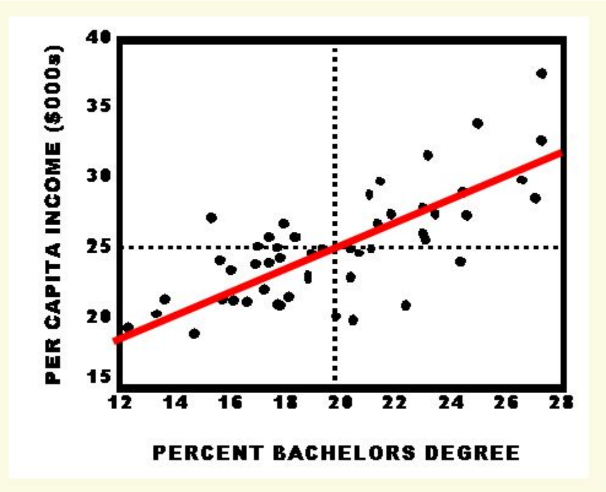


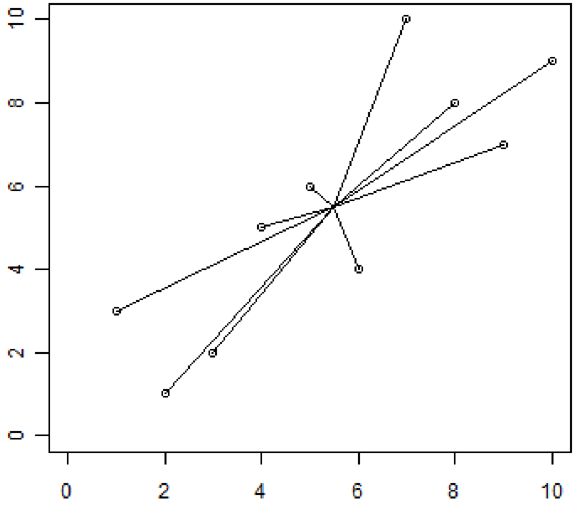
Interpretation of coefficients

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

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

$$\hat{\beta}_1 = \frac{SS_{xy}}{SS_{xx}} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$$





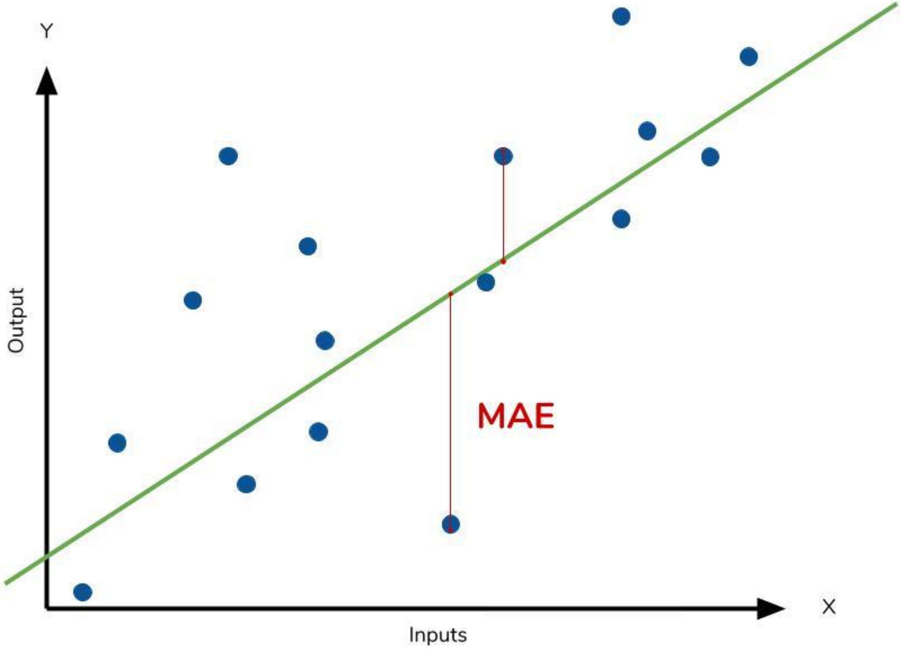
Regression – Error measures

Divide by the total number of data points

Predicted output value

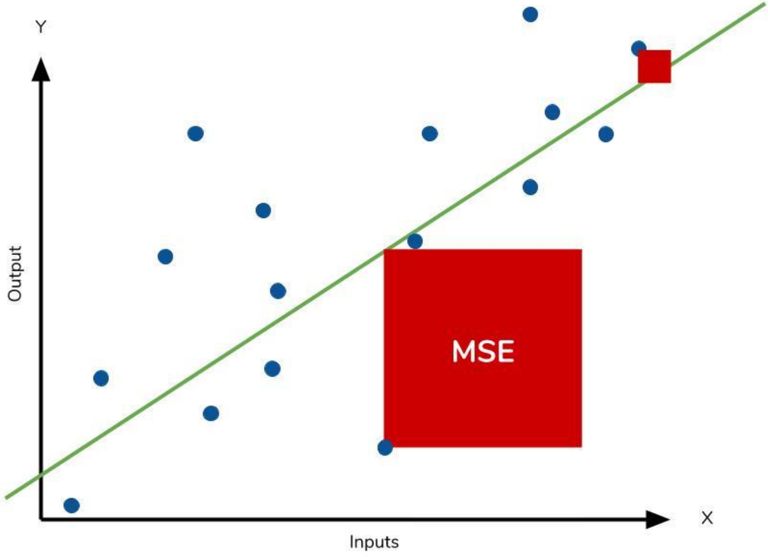
Actual output value

$$MAE = \boxed{\frac{1}{n}}\underset{\text{Sum of}}{\sum}\underbrace{\left|\boxed{y}-\boxed{\hat{y}}\right|}_{\text{The absolute value of the residual}}$$

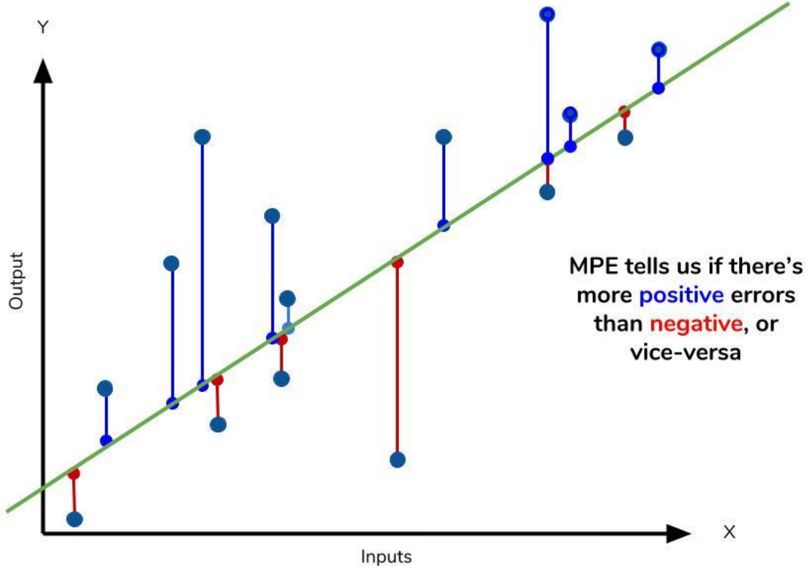


Regression – Error measures

$$MSE = \frac{1}{n}\Sigma\left(\underbrace{y - \widehat{y}}_{\substack{\text{The square of the difference}\\ \text{between actual and}\\ \text{predicted}}}\right)^2$$



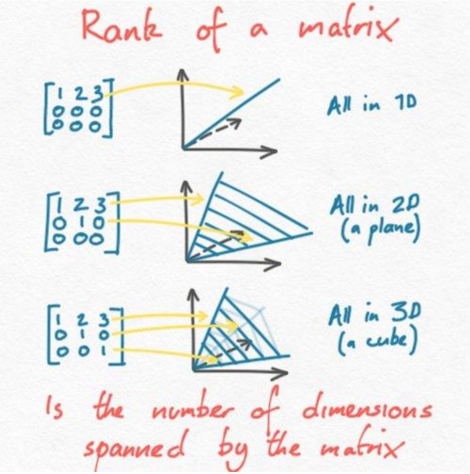
$$MPE = \frac{100\%}{n} \Sigma \left(\frac{y - \widehat{y}}{y} \right)$$



MPE tells us if there's more positive errors than negative, or vice-versa

Linear Algebra in 1 slide

- Matrices – Square, Rectangular
- Matrix ops – Transpose, Inverse
- Rank of a matrix



Linear Regression – Matrix Form

Linear Regression – Matrix Form

Consider the model

$$Y = X\beta + \epsilon$$

where $Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$ $\quad X = \begin{pmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \\ 1 & X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{pmatrix}$ $\quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$ $\quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$

Based on this model we get the following expansion for the first subject:

$$Y_1 = \beta_0 + \beta_1 X_{11} + \beta_2 X_{12} + \ldots + \beta_p X_{1p} + \epsilon_1$$

Then using matrix calculus we find that the least squares estimate for β is given by

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

Linear Regression – Matrix Form - Issues

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

- N samples, p-dimensional (what if p > N ?)
- Complexity of matrix inversion (what if N very large ?)
- Collinearity

- Linear Regression ➔ Linear in coefficients and NOT variables

  - A second-order model (quadratic model):

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

  - β_1: Linear effect parameter.
  - β_2: Quadratic effect parameter.

kth order polynomial model in one variable

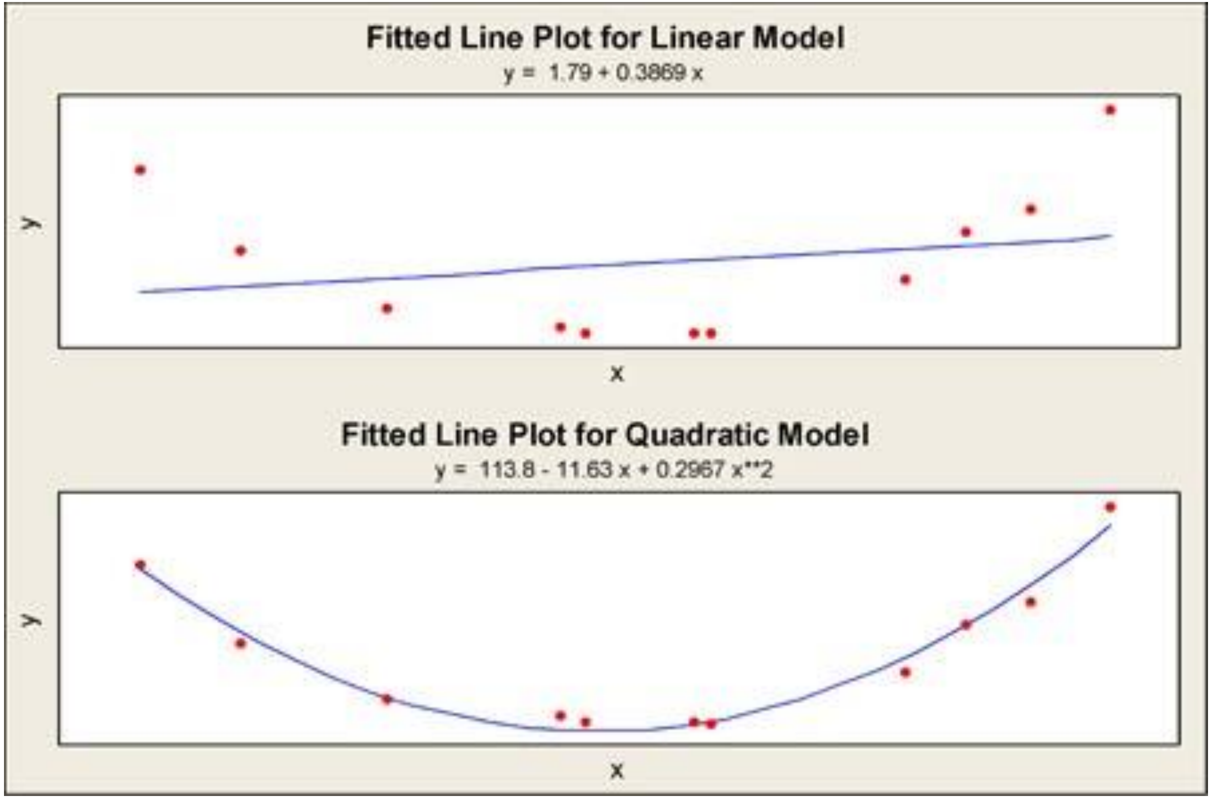
$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_k x^k + \epsilon$$

A quadratic polynomial regression function

$$Y_i = \beta_0 + \beta_1 X_i + \beta_{11} X_i^2 + \varepsilon_i$$

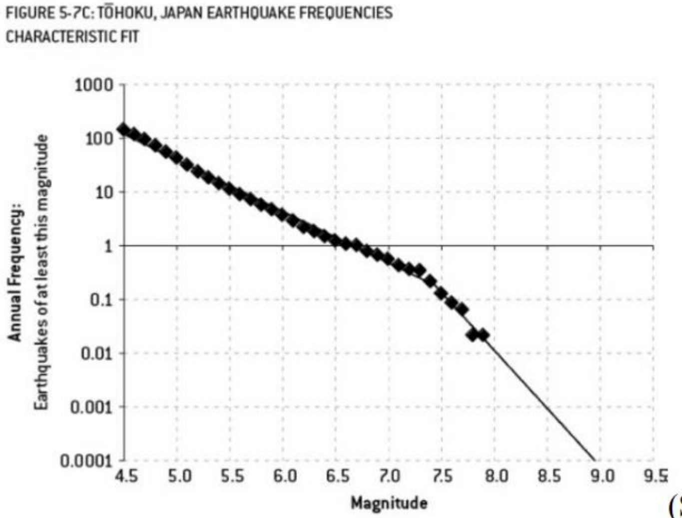
where:

- Y_i = amount of immunoglobin in blood (mg)
- X_i = maximal oxygen uptake (ml/kg)
- typical assumptions about error terms ("INE")

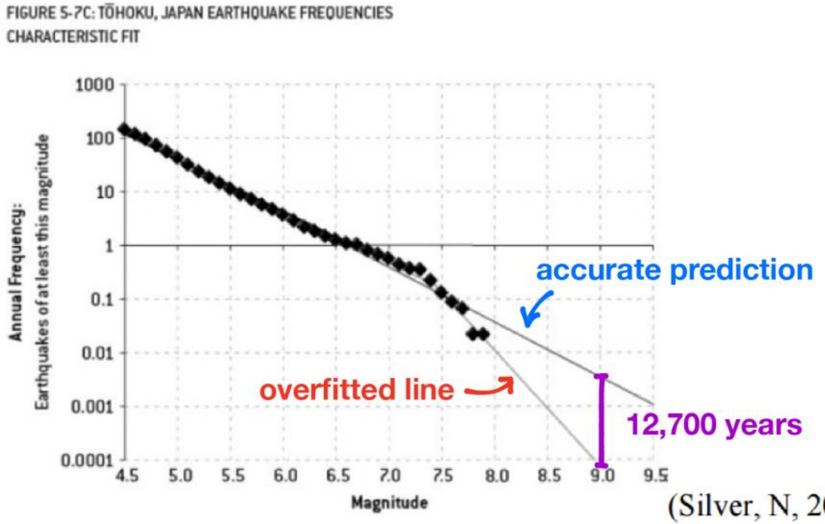

Fitted Line Plot for Linear Model
y = 1.79 + 0.3869 x
y
x
Fitted Line Plot for Quadratic Model
y = 113.8 - 11.63 x + 0.2967 x**2
y
x

- Linear Regression → Linear in coefficients and NOT variables

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^m \\ 1 & x_2 & x_2^2 & \dots & x_2^m \\ 1 & x_3 & x_3^2 & \dots & x_3^m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^m \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_m \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \\ \varepsilon_n \end{bmatrix},$$

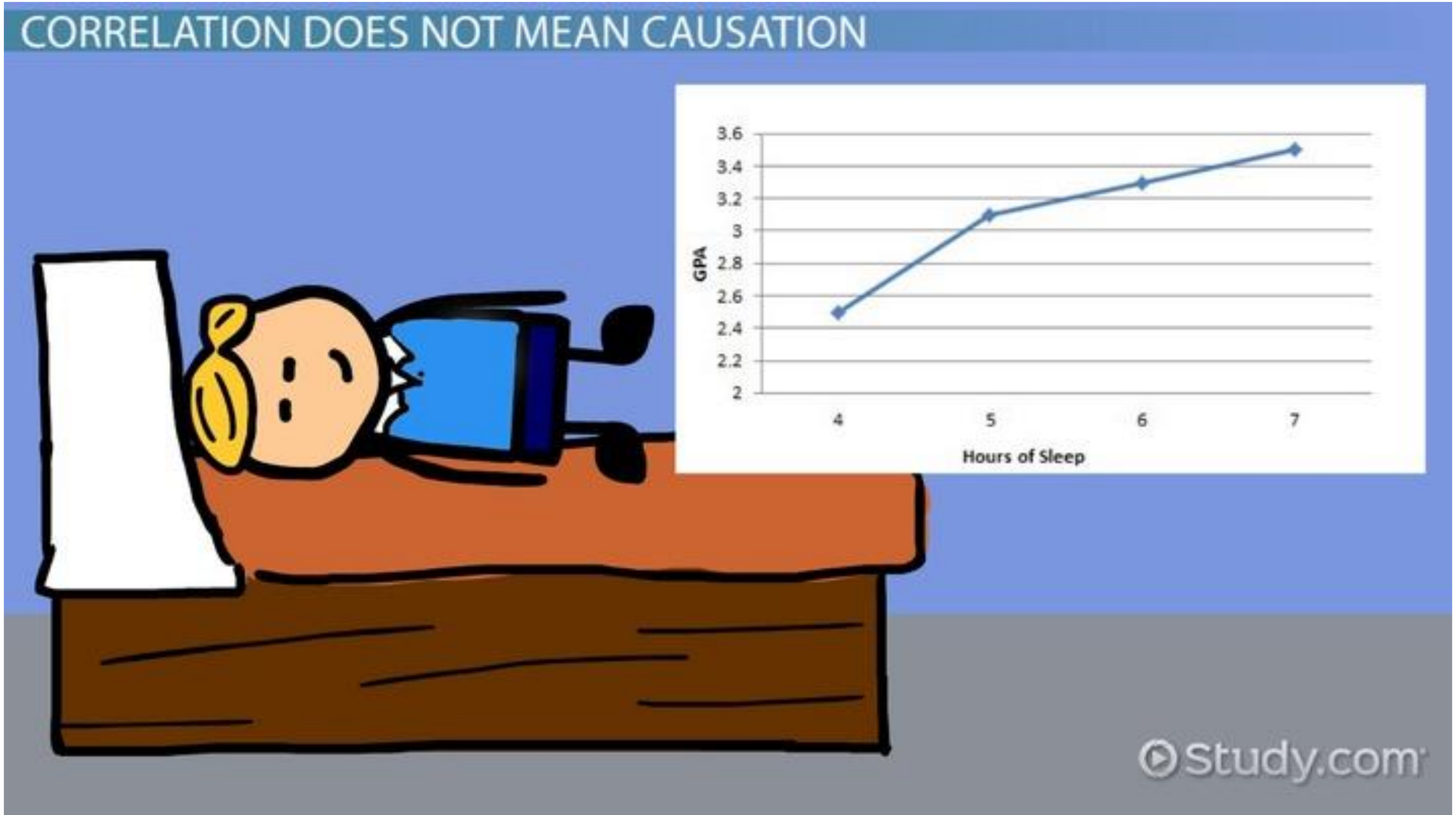


(Silver, N, 2012)

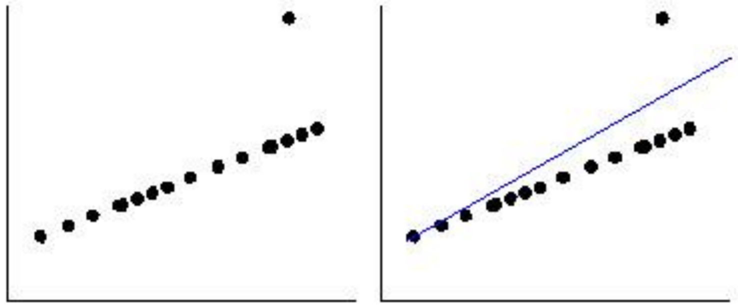


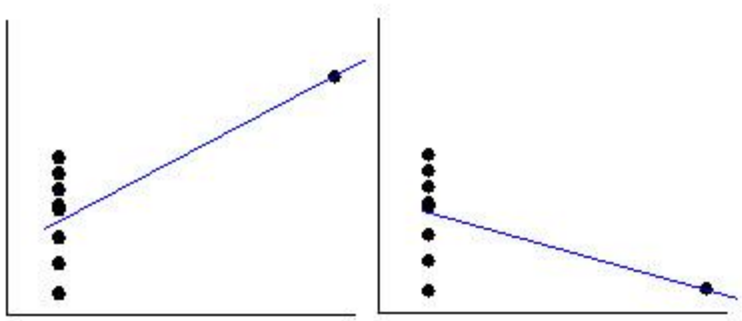
(Silver, N, 2012)

Careful: X may not be causing y !

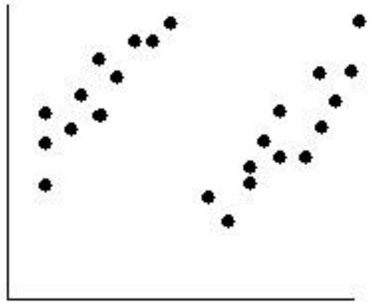


Linear Regression – Outliers





Linear Regression is problematic in many other cases



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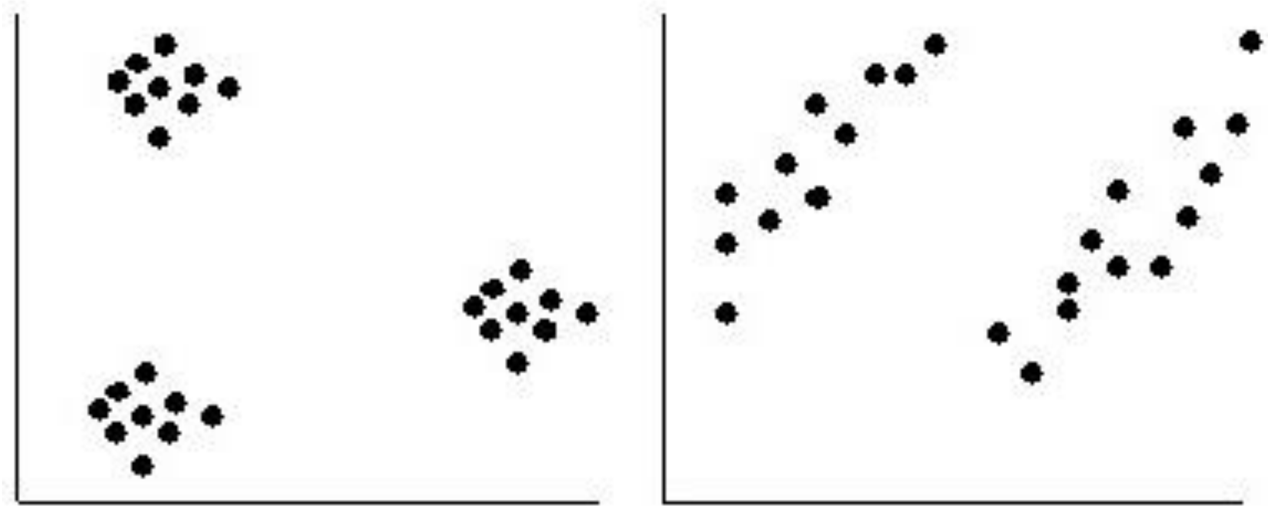

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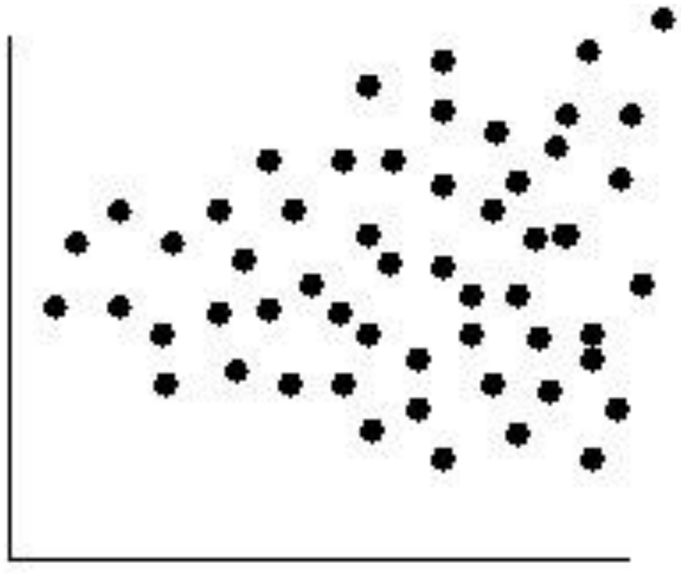

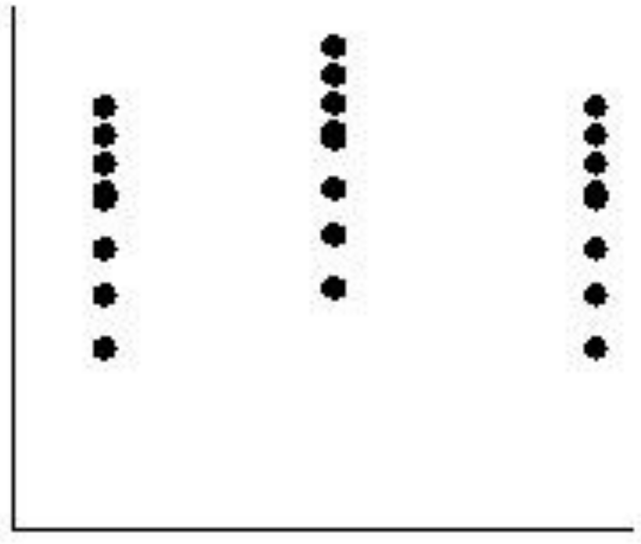

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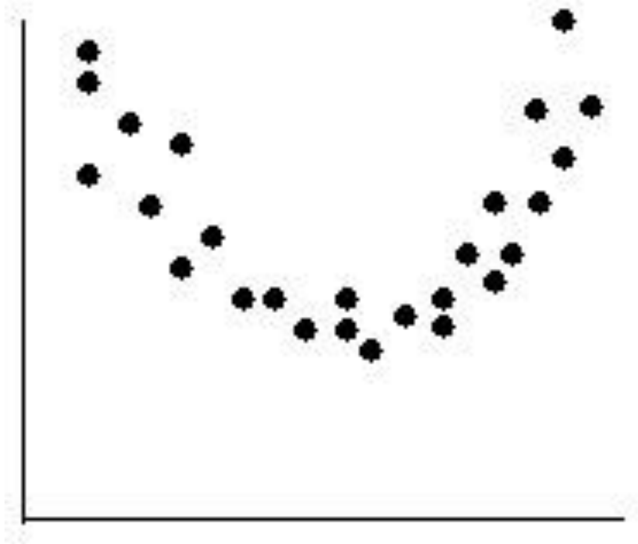
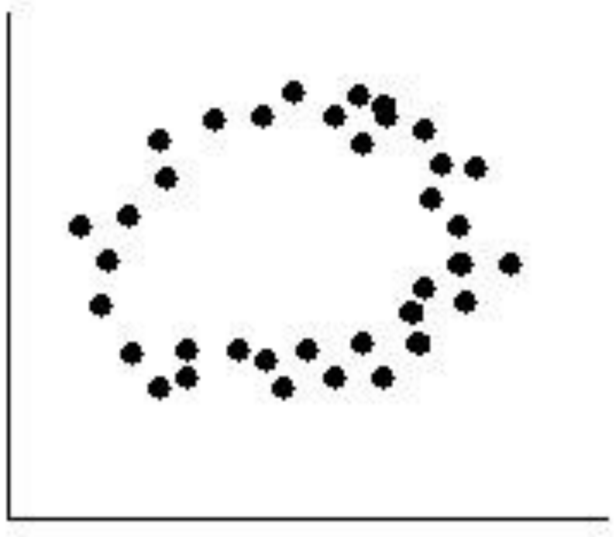
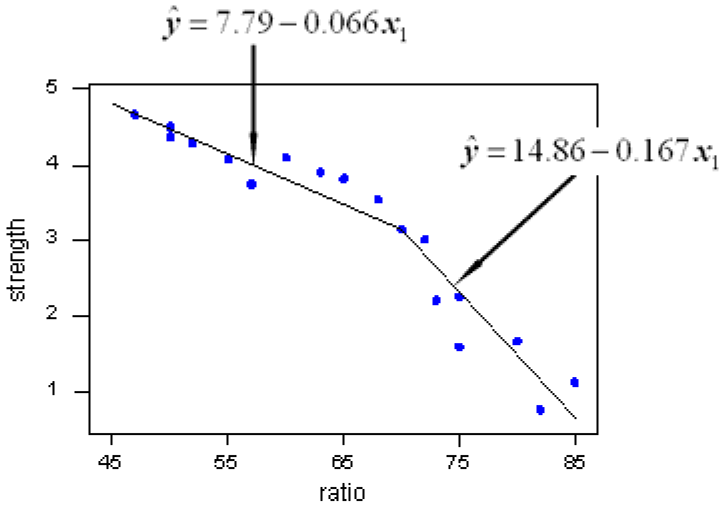
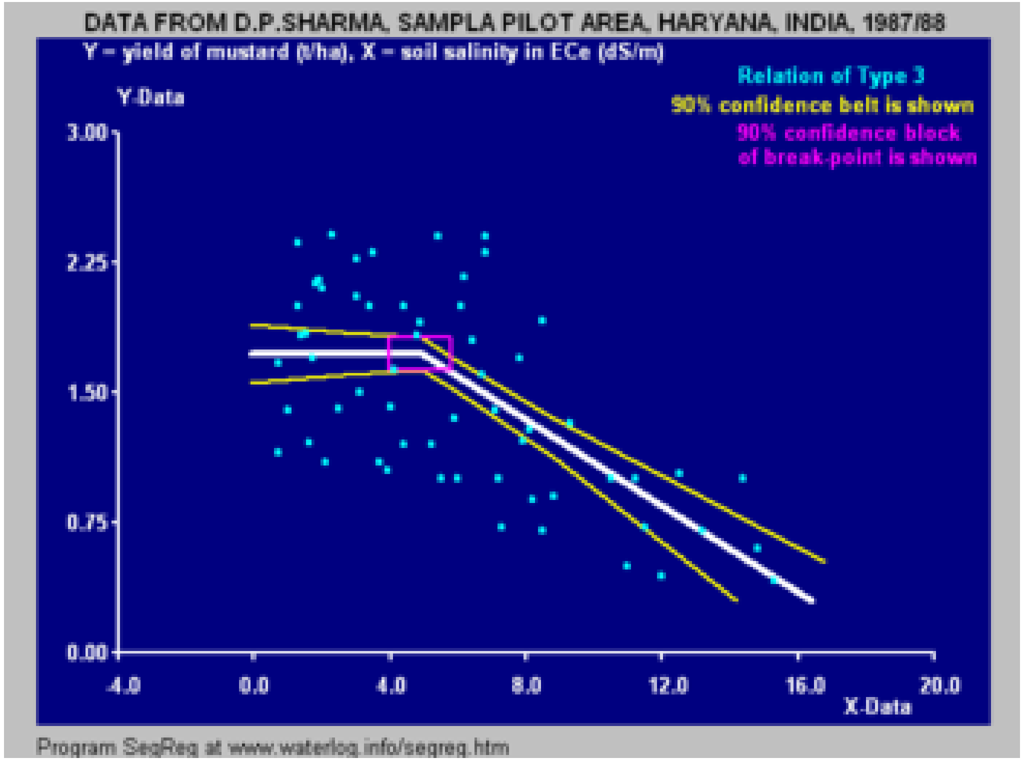


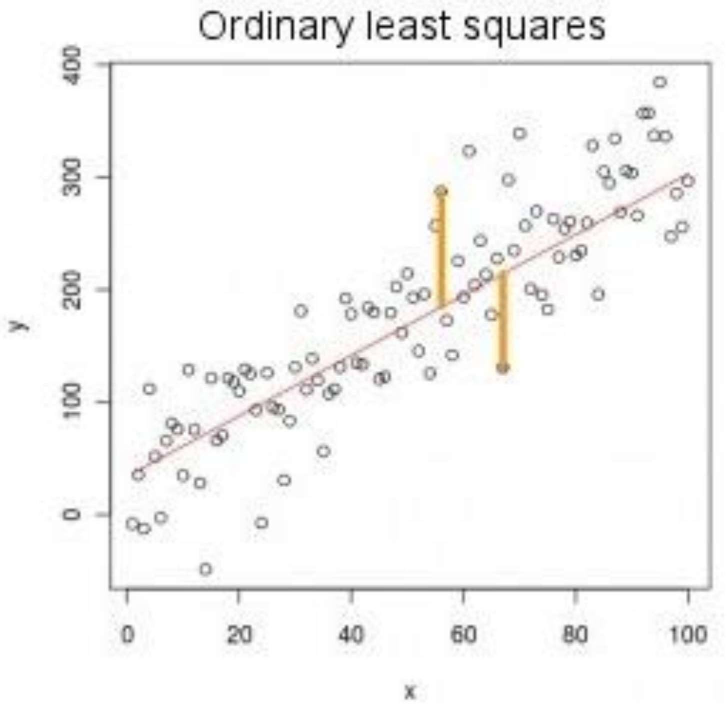


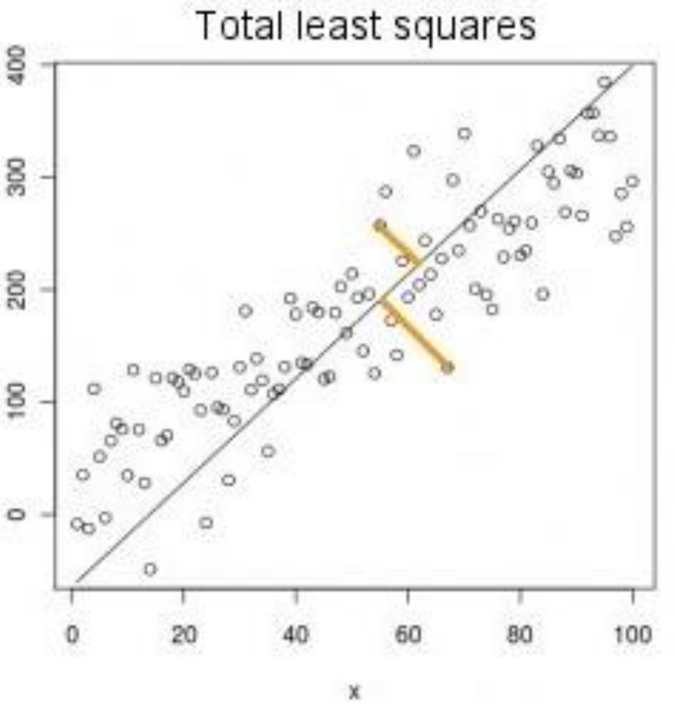
Piecewise Linear Regression



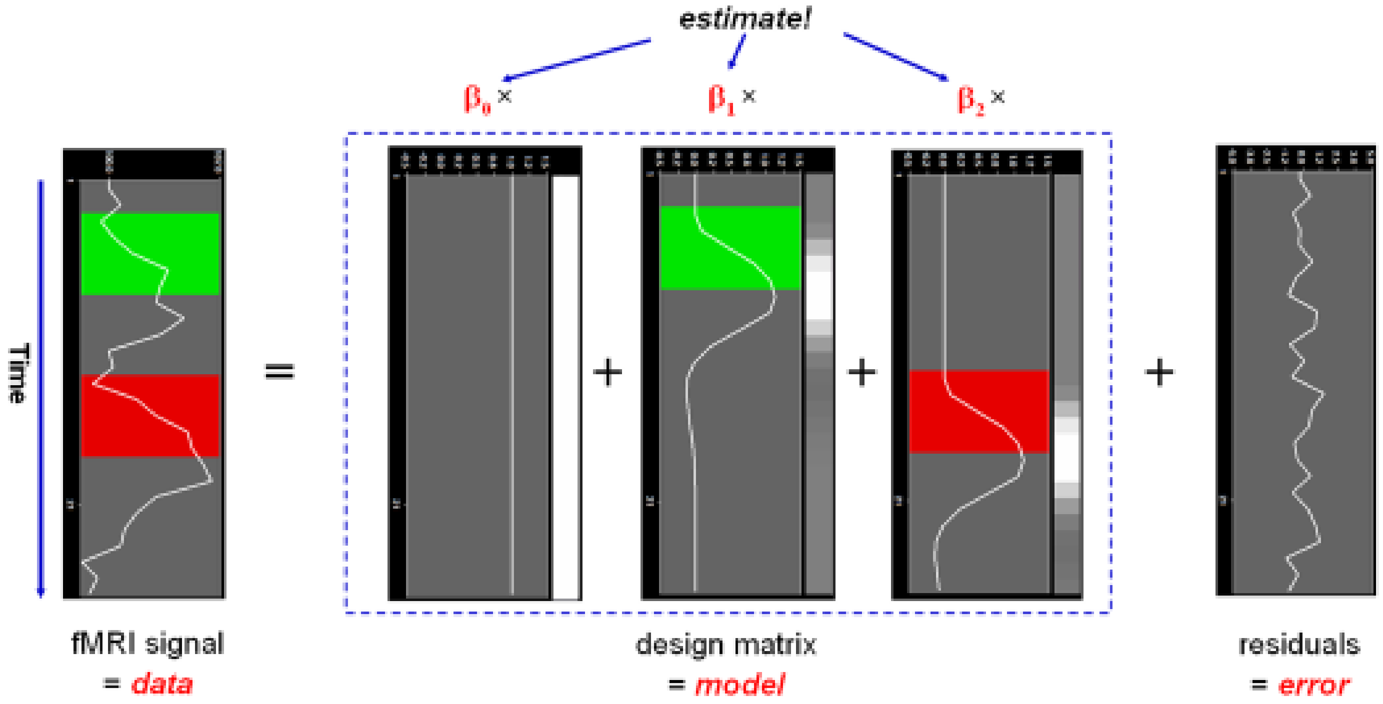


Total Least Squares ("Errors-in-variables" model)





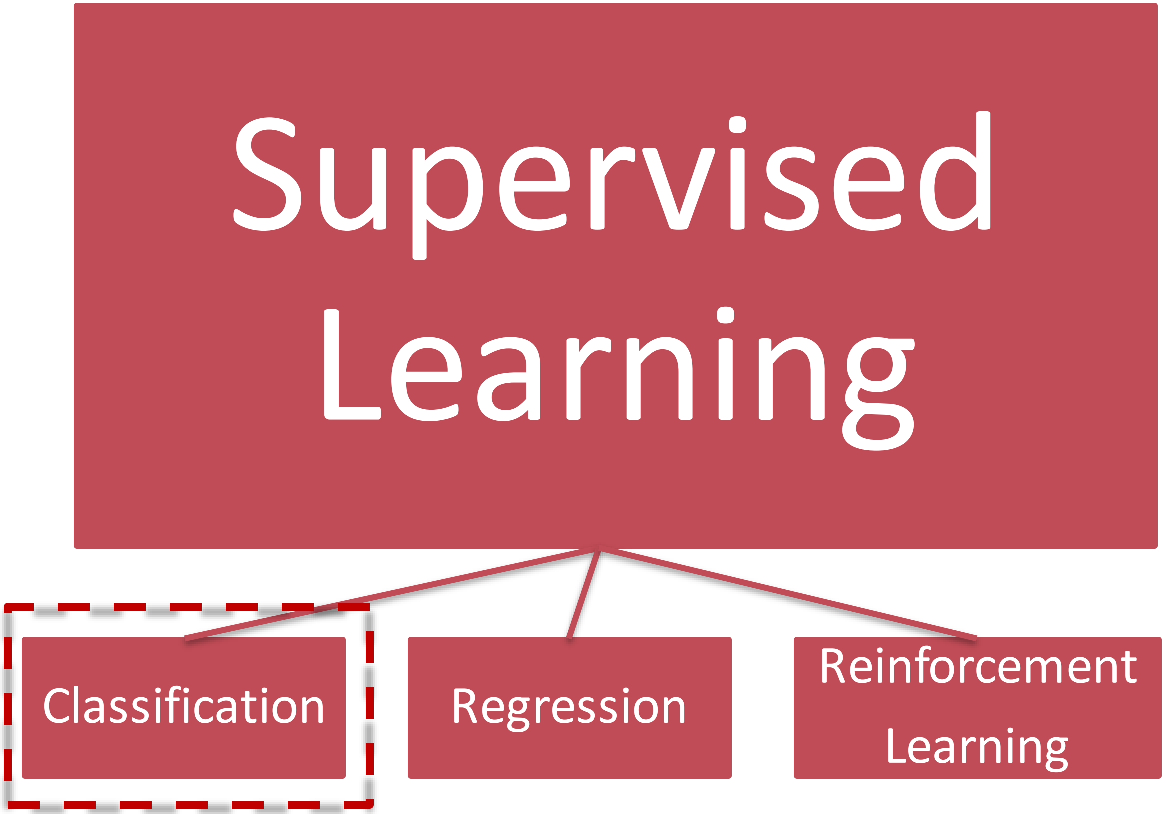
General Linear Models

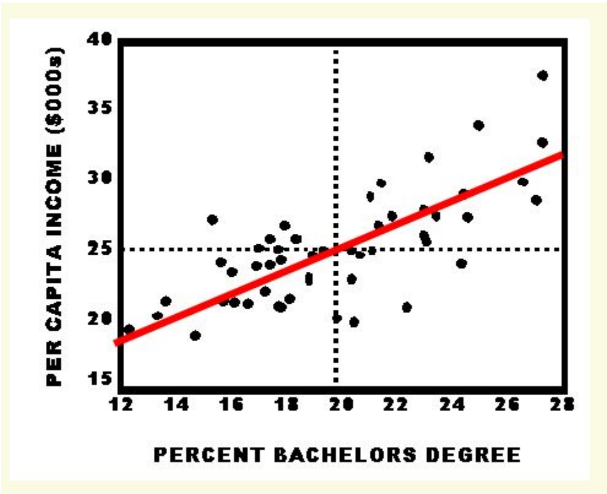


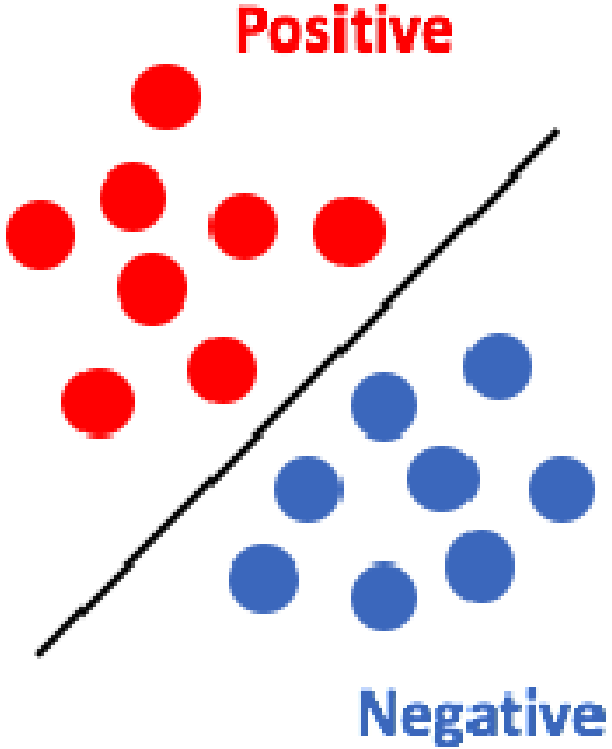
https://en.wikipedia.org/wiki/General_linear_model

Generalized Linear Models

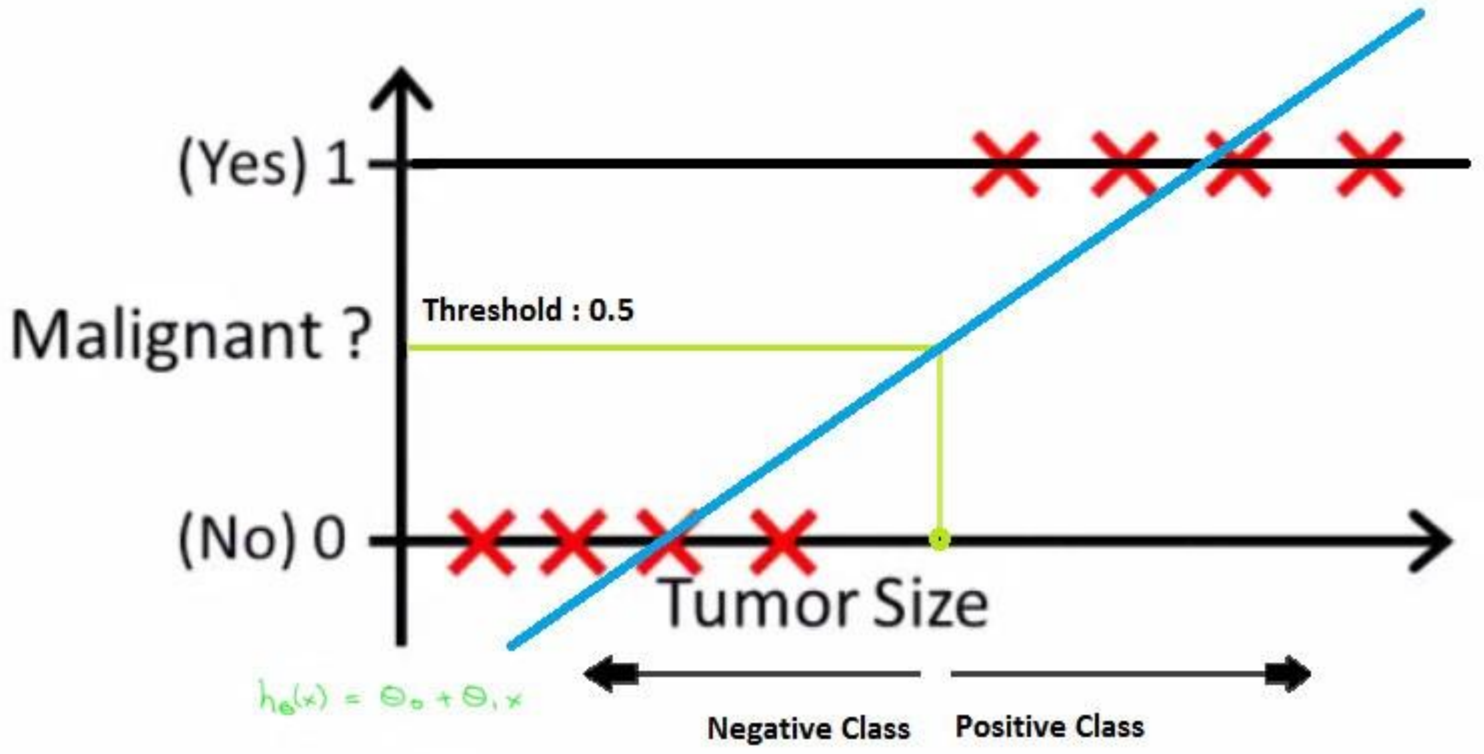
- For bounded or discrete data
  - Positive quantities (e.g. prices, populations)
  - Varying over a large scale (log-normal, Poisson distribution)
  - Categorical data (Bernoulli / Binomial / Multinomial)
  - Ordinal data (e.g. ratings – Ordered logit)


Supervised Learning
Classification
Regression
Reinforcement Learning

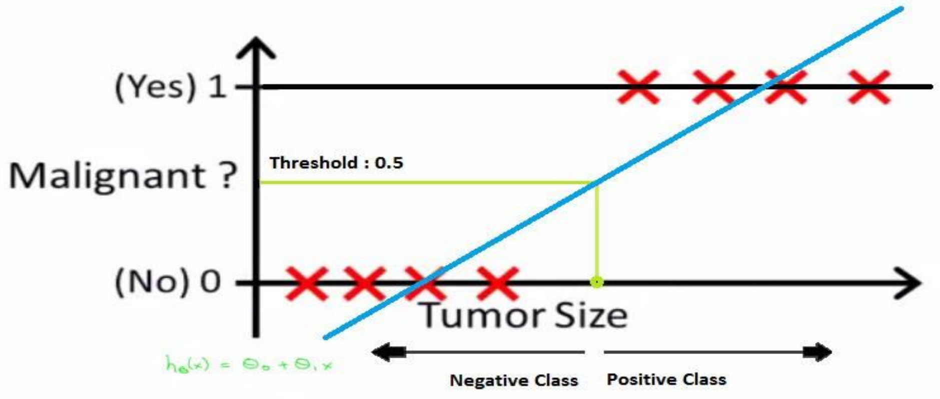

PER CAPITA INCOME ($000s)
40
35
30
25
20
15
12
14
16
18
20
22
24
26
28
PERCENT BACHELORS DEGREE


Positive
Negative

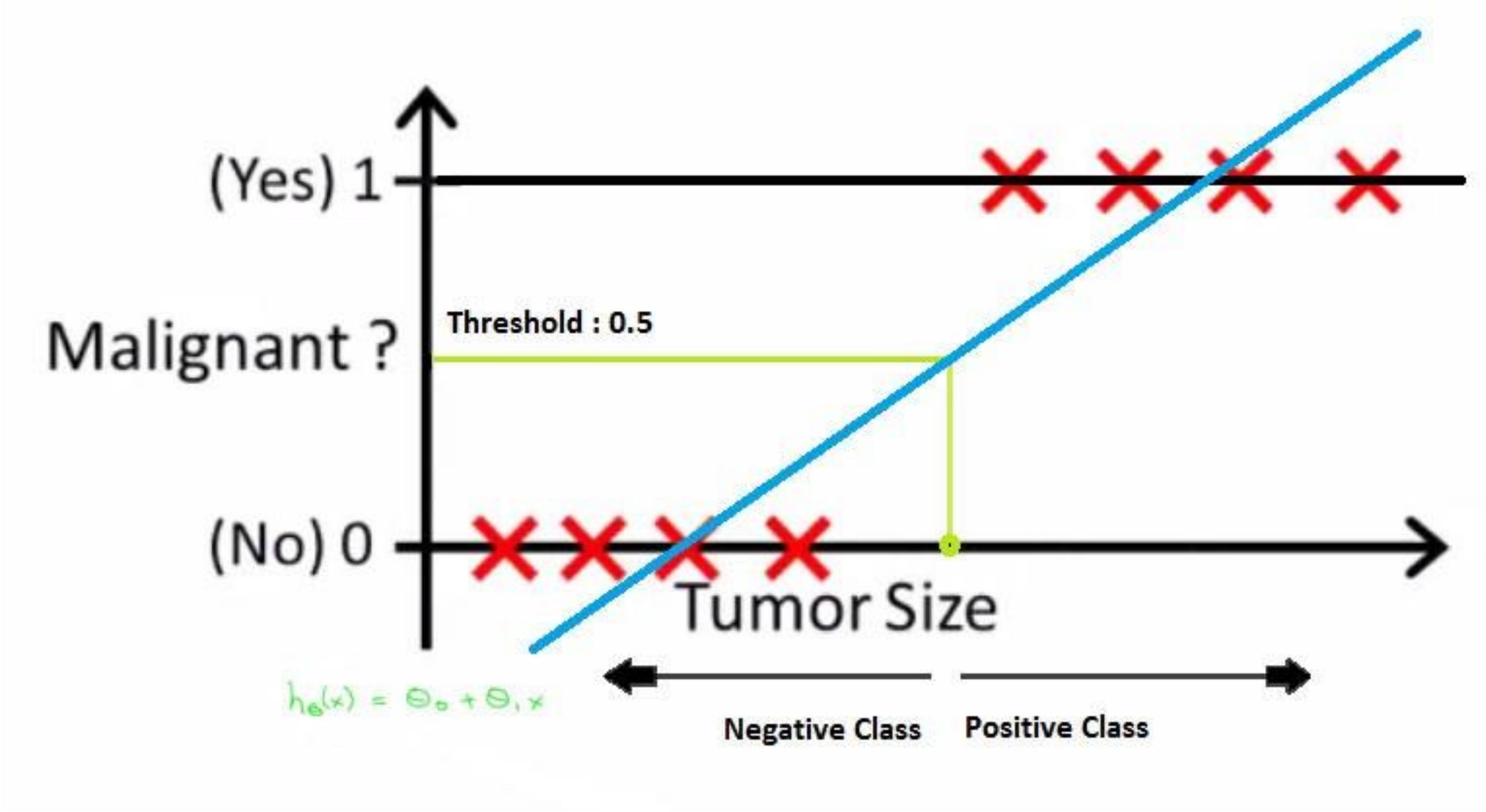
Re-using linear regression ?



Re-using linear regression ?

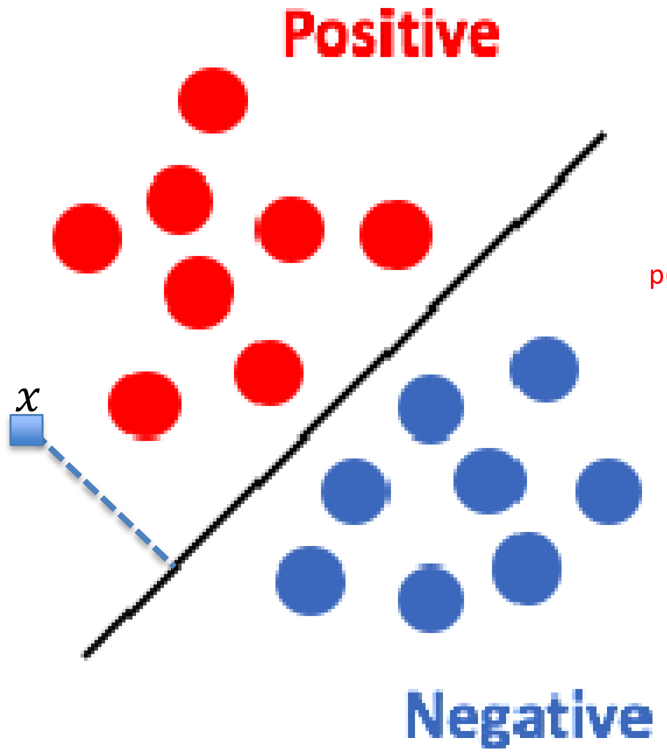


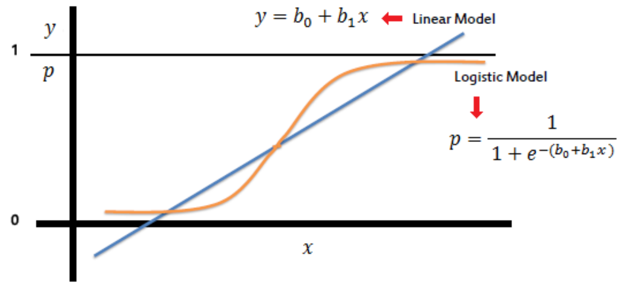
What we really want – a step function !



- We want a step-function like behavior
  - But with nicer mathematical properties (e.g. like linear regression)!
- Probabilistic classification is also nice (Naïve Bayes)
- Combine all of these ?

Logistic Regression - Intuition





p(X) = p(Y=1|x) = probability that x belongs to positive class

$$\implies p(X) = \frac{e^{(\beta_o + \beta_1 x)}}{e^{(\beta_o + \beta_1 x)} + 1}$$

$$\implies p(e^{(\beta_o + \beta_1 x)} + 1) = e^{(\beta_o + \beta_1 x)}$$

$$\implies p.e^{(\beta_o + \beta_1 x)} + p = e^{(\beta_o + \beta_1 x)}$$

$$\implies p = e^{(\beta_o + \beta_1 x)} - p.e^{(\beta_o + \beta_1 x)}$$

$$\implies p = e^{(\beta_o + \beta_1 x)}(1 - p)$$

$$\implies \frac{p}{1-p} = e^{(\beta_o + \beta_1 x)}$$

$$\implies \ln(\tfrac{p}{1-p}) = \beta_0 + \beta_1 x$$

Distance of x from boundary

Maximum Likelihood

- The likelihood function is the simultaneous density of the observation, as a function of the model parameters.

$$L(\Theta) = \Pr(Data|\Theta)$$

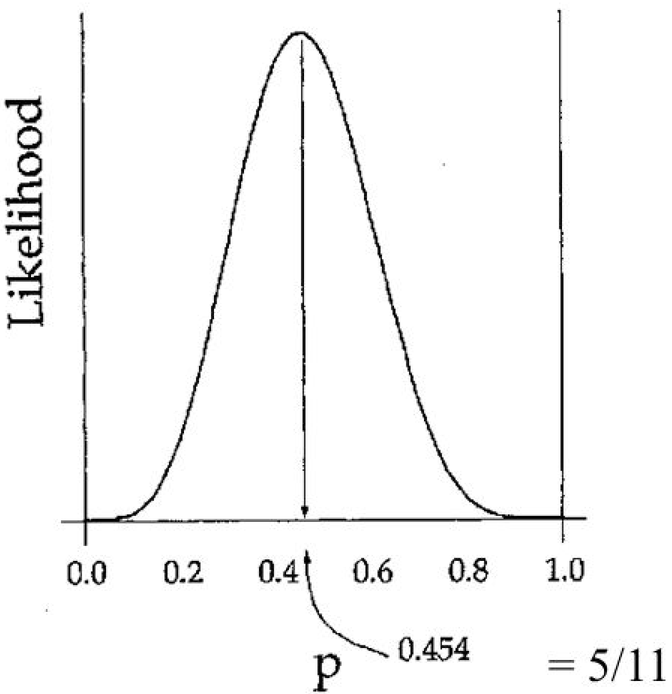
- If the observations are independent, we can decompose the term into

$$\Pr(Data \mid \Theta) = \prod_{i=1}^{n} \Pr(X_i \mid \Theta)$$

An example

- Consider the estimation of heads probability of a coin tossed *n* times
- Heads probability p
- Data = HHTTHTHHTTT
- $L(p) = \Pr(D|p) = pp(1-p)(1-p)p(1-p)pp(1-p)(1-p)(1-p) = p^5(1-p)^6$

$$L(p) = p^5(1-p)^6$$



Maximum Likelihood

$L(p) = p^5(1-p)^6$

Take the derivative of L with respect to p:

$$\frac{dL}{dp} = 5p^4(1-p)^6 - 6p^5(1-p)^5$$

Equate it to zero and solve:

$$\hat{p} = 5/11$$

Log Likelihood

$L(p) = p^5(1-p)^6$

- For computational reasons, we maximise the logarithm

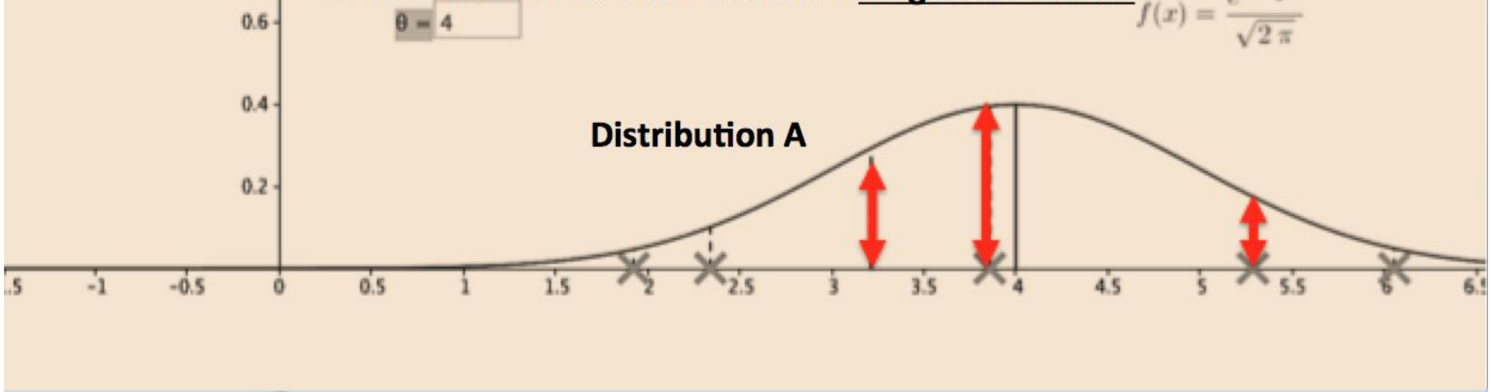
$\ln L = 5 \ln p + 6 \ln(1-p)$

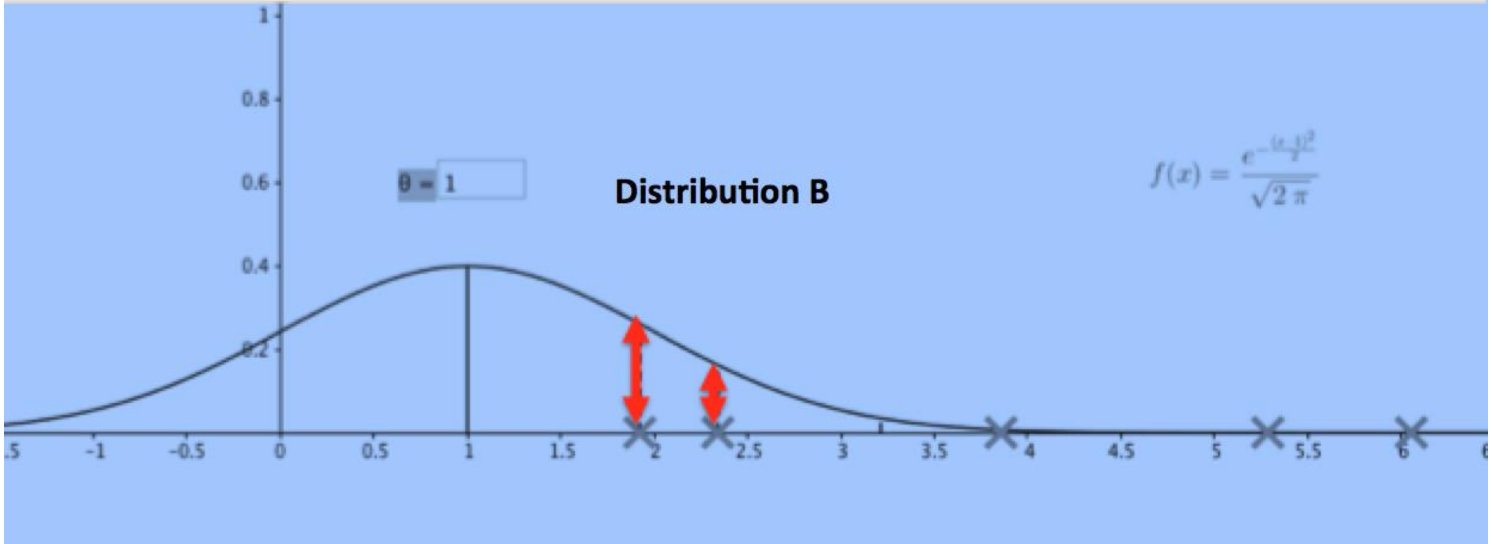
with derivative

$$\frac{d(\ln L)}{dp} = \frac{5}{p} - \frac{6}{(1-p)} = 0$$

$\hat{p} = 5/11$

Maximum Likelihood Estimator will maximize p(x1)p(x2)p(x3)…
-> called the Likelihood function
Pick value of theta that results in a **longer red arrows**





Logistic Regression - Learning parameters

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1+e^{-\theta^T x}}$$

$$p(y \mid x;\theta) = (h_\theta(x))^y \, (1 - h_\theta(x))^{1-y}$$

$$\begin{aligned} L(\theta) &= p(\vec{y} \mid X;\theta) \\ &= \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)};\theta) \\ &= \prod_{i=1}^{m} \left(h_\theta(x^{(i)})\right)^{y^{(i)}} \left(1 - h_\theta(x^{(i)})\right)^{1-y^{(i)}} \end{aligned}$$

$$\begin{aligned} \ell(\theta) &= \log L(\theta) \\ &= \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)})) \end{aligned}$$

References and Reading

- Linear Regression
  - https://en.wikipedia.org/wiki/Linear_regression
  - http://www.stat.purdue.edu/~boli/stat512/lectures/topic3.pdf (up to page 7)
- Logistic Regression
  - https://en.wikipedia.org/wiki/Logistic_regression (up to Section 6)