DS203: Programming in Data Science

Linear Regression

Manjesh K. Hanawal

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Classification vs Regression

Learning setup:

- $S = \{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}$ is a set of data points
- $x_i \in \mathcal{X}$ for all $i = 1, 2, \ldots, m$ are drawn iid
- $y_i \in \mathcal{Y}$ is the label of x_i. $y_i = f_i(y_i)$ (f is unknown)

(Supervised) Learning problem: Given S (dataset) find 'best' label for a new sample $x \in \mathcal{X}$ drawn from the same distribution.

- when $|\mathcal{Y}|$ is finite, learning classification problem
- When $|\mathcal{Y}|$ is not finite, learning is a regression problem

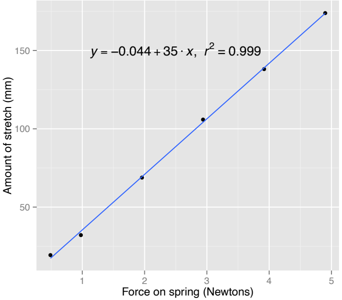
Regression

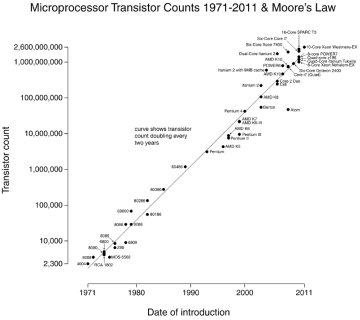
- Example 1:Health
  x=(age, height, weight), y=BMI
- Example 2: Housing
  x=(carpet area, no. of rooms, distance to city center), y= cost of house
- Example 3: Weather
  x=(temperature, wind speed, humidity level), y=amount of rain fall

How are the features/attributes related to the label?
Goal: Find a relation that best explains labels of each sample in the dataset

Linear Regression

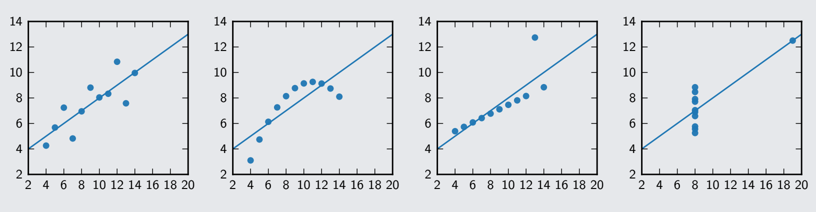
We will focus on simple type of relations: **Linear**





- Amount of stretch when force is applied on a spring (spring constant!)
- Number of transistor on the silicon area doubles 18 months (Moore's Law!)

Everything is not linear!



- Data with similar quantitative (mean) may look very different
- Visualization of data is reveals patterns that are hidden in pure numerical analysis

Simple Linear Regression

- Assume: Each sample has one feature/attribute ($x_i \in \mathcal{R}$)
- We will fit line of the from $y = \beta_1 x + \beta_0$

- x is called the independent/predictor variable
- y is called the dependent/response variable
- β_1 is the slope and β_0 is the intercept
- We will get different lines for different choice of (β_0, β_1)

- How to quantify how good is a line?
- Choose the best line!

Probabilistic Model for Linearly Related Data

- Instead of $y_i = \beta_1 x_i + \beta_0$ assume data is perturbed by noise
- $y_i = \beta_1 x_i + \beta_0 + \epsilon_i$, where ϵ_i is random perturbation (noise)
- perturbation denotes that data won't be fit the model perfectly
- We assume that $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, where σ^2 is known

Quantify goodness of a line: Mean Squared Error

- Minimize the distance between the line and points
- distance of point (x_i, y_i) from line (β_0, β_1) (error)

$$y_i - (\beta_1 x_i + \beta_0)$$

- As staying above or below line are equally bad we can take

$$|y_i - (\beta_1 x_i + \beta_0)| \text{ absolute error}$$

$$(y_i - (\beta_1 x_i + \beta_0))^2 \text{ squared error}$$

- We take goodness of line (β_0, β_1) as sum of the squared errors

$$\frac{1}{m} \sum_{=1}^{n} (y_i - (\beta_1 x_i + \beta_0))^2$$

Mean Squared Error (MSE)

The best line: Least Squared Regression

$$\min_{(\beta_0,\beta_1)} \frac{1}{m} \sum_{=1}^{n} (y_i - (\beta_1 x_i + \beta_0))^2$$

Alternate derviation from MLE

- $y_i = \beta_1 x_i + \beta_0 + \epsilon_i \implies y_i \sim \mathcal{N}(\beta_1 x_i + \beta_0, \sigma^2)$
- $(\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$ are iid hence $(y_1, y_2, \ldots, y_n)$ are iid.
- Likelihood of $y = (y_1, y_2, \ldots, y_m)$ under the parameters $\beta = (\beta_0, \beta_1)$ is

$$L(y|\beta) = \prod_{i=1}^{m} f(y_i|\beta) = \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-(y_i - \beta_1 x_i \beta_0)^2 / 2\sigma^2\right\}$$

$$= \frac{1}{(2\pi\sigma^2)^{m/2}} \exp\left\{-\sum_{i=1}^{m} (y_i - \beta x_i - \beta_0)^2 / 2\sigma^2\right\}$$

$$\max_{\beta} L(y|\beta) = \min_{\beta} \sum_{i=1}^{m} (y_i - \beta x_i - \beta_0)^2$$

Least Squared Solution

$$(\hat{\beta}_0, \hat{\beta}_1) = \arg \min_{(\beta_0,\beta_1)} \frac{1}{m} \sum_{=1}^{n} (y_i - (\beta_1 x_i + \beta_0))^2$$

$$\hat{\beta}_1 = \frac{\frac{1}{m}\left(\sum_{i=1}^{m} x_i y_i\right) - \left(\frac{1}{m}\sum_{i=1}^{m} x_i\right)\left(\frac{1}{m}\sum_{i=1}^{m} y_i\right)}{\frac{1}{m}\left(\sum_{i=1}^{m} x_i^2\right) - \left(\frac{1}{m}\sum_{i=1}^{m} x_i\right)^2}$$

$$\beta_0 = \left(\frac{1}{m}\sum_{i=1}^{m} y_i\right) - \hat{\beta}_1 \left(\frac{1}{m}\sum_{i=1}^{m} x_i\right)$$

Expressing the solutions in terms of statistics

Given a random sample $(X_1, X_2, \ldots, X_m)$

- Sample mean: $\bar{X} = \frac{1}{m}\left(\sum_{i=1}^{m} X_i\right)$
- Sample variance: $S_X^2 = \frac{1}{m-1}\left(\sum_{i=1}^{m}(X_i - \bar{X})^2\right)$
- Sample standard deviations: $S_X = \sqrt{S_X^2}$.

For give data $S = \{(x_1, y_1), (x_2, y_2), \ldots (x_m, y_m)\}$

$$\bar{x} = \frac{1}{m}\left(\sum_{i=1}^{m} x_i\right) \qquad s_x = \frac{1}{m-1}\left(\sum_{i=1}^{m}(x_i - \bar{x})^2\right)$$

$$\bar{y} = \frac{1}{m}\left(\sum_{i=1}^{m} y_i\right) \qquad s_y = \frac{1}{m-1}\left(\sum_{i=1}^{m}(y_i - \bar{y})^2\right)$$

$$r = \frac{1}{m-1}\sum_{i=1}^{m}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right) \text{ Correlation coefficient}$$

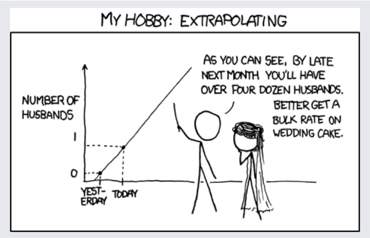
Prediction

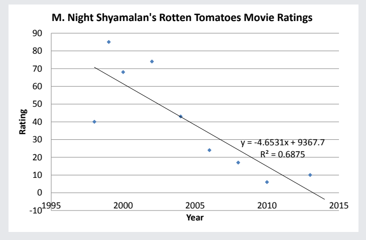
$$\hat{\beta}_1 = r\frac{s_y}{s_x} \text{ and } \hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x}$$

Given any sample x, its predicted label is

$$y = \hat{\beta}_1 x + \hat{\beta}_0$$

For what all x we can get prediction?

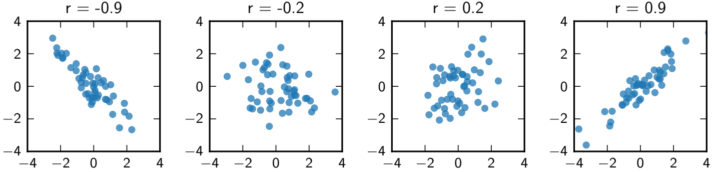




Correlation coefficient

$$r = \frac{1}{m-1}\sum_{i=1}^{m}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right)$$

- $-1 \leq r \leq 1$. Measure how much y is related to x
- if r is positive y increases in x
- if r is negative y decreases in x



- r^2 is called coefficient of determination (explains how well data is fit).

Multiple Linear Regression

$S = \{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}, x_i \in \mathcal{R}^d$, where $d > 1$.
Each sample point $x_i = (x_{i1}, x_{i2}, \ldots, x_{id})$.

- We can write linear relation: $y_i = \sum_{j=1}^{d} x_{ij}\beta_j + \beta_0$
- $y_i = \sum_{j=0}^{d} x_{ij}\beta_j$, where $x_{i0} = 1$ for all $i = 1, 2 \ldots, m$
- set $\beta = (\beta_0, \beta_1, \beta_2, \ldots, \beta_d)$ and $x_i = (1, x_{i1}, x_{i2}, \ldots, x_{id})$
- Compactly $y_i = x_i\beta^T$ for all $i = 1, 2, \ldots, m$
- The probabilistic model is $y_i = x_i\beta^T + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \ldots x_{1d} \\ 1 & x_{21} & x_{22} & \ldots x_{2d} \\ \vdots & & & \\ 1 & x_{m1} & x_{m2} & \ldots x_{md} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_m \end{bmatrix}$$

$$y = X\beta^T \text{ where } X \text{ is data matrix}$$

The probabilistic model is then

$$y = X\beta^T + \epsilon$$

Solution of Multiple Linear Regression

$$\hat{\beta} = \arg\min_{\beta} \sum_{i1=1}^{m} (y_i - x_i \beta^T)^2$$

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