CS70: Jean Walrand: Lecture 30.

Linear Regression

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Linear Regression: Preamble

The best guess about Y, if we know only the distribution of Y, is $E[Y]$.

More precisely, the value of a that minimizes $E[(Y-a)^2]$ is $a = E[Y]$.

Proof:

Let $\hat{Y} := Y - E[Y]$. Then, $E[\hat{Y}] = 0$. So, $E[\hat{Y}c] = 0, \forall c$. Now,

$$\begin{aligned} E[(Y-a)^2] &= E[(Y-E[Y]+E[Y]-a)^2] \\ &= E[(\hat{Y}+c)^2] \text{ with } c = E[Y]-a \\ &= E[\hat{Y}^2 + 2\hat{Y}c + c^2] = E[\hat{Y}^2] + 2E[\hat{Y}c] + c^2 \\ &= E[\hat{Y}^2] + 0 + c^2 \geq E[\hat{Y}^2]. \end{aligned}$$

Hence, $E[(Y-a)^2] \geq E[(Y-E[Y])^2], \forall a$. $\square$

Linear Regression: Preamble

Thus, if we want to guess the value of Y, we choose $E[Y]$.

Now assume we make some observation X related to Y.

How do we use that observation to improve our guess about Y?

The idea is to use a function $g(X)$ of the observation to estimate Y.

The simplest function $g(X)$ is a constant that does not depend of X.

The next simplest function is linear: $g(X) = a + bX$.

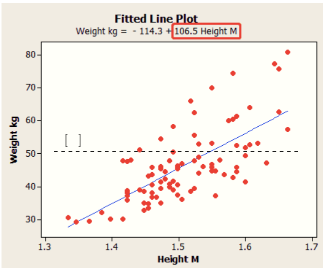
What is the best linear function? That is our next topic.

A bit later, we will consider a general function $g(X)$.

Linear Regression: Motivation

Example 1: 100 people.

Let (X_n, Y_n) = (height, weight) of person n, for $n = 1, \ldots, 100$:



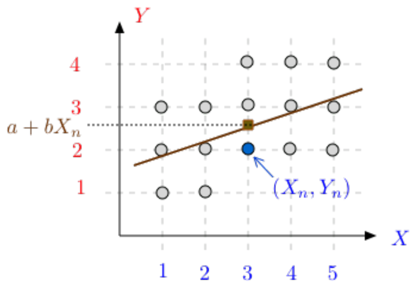
The blue line is $Y = -114.3 + 106.5X$. (X in meters, Y in kg.)

Best linear fit: Linear Regression.

Motivation

Example 2: 15 people.

We look at two attributes: (X_n, Y_n) of person n, for $n = 1, \ldots, 15$:



The line $Y = a + bX$ is the linear regression.

Covariance

Definition The covariance of X and Y is

$$cov(X,Y) := E[(X-E[X])(Y-E[Y])].$$

Fact

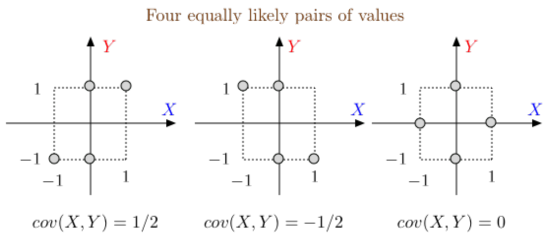
$$cov(X,Y) = E[XY] - E[X]E[Y].$$

Proof:

$$\begin{aligned} E[(X-E[X])(Y-E[Y])] &= E[XY - E[X]Y - XE[Y] + E[X]E[Y]] \\ &= E[XY] - E[X]E[Y] - E[X]E[Y] + E[X]E[Y] \\ &= E[XY] - E[X]E[Y]. \end{aligned}$$

$\square$

Examples of Covariance



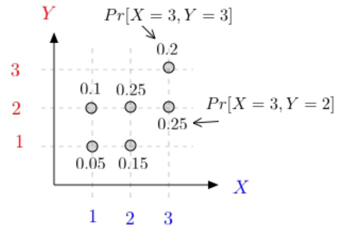
Note that $E[X] = 0$ and $E[Y] = 0$ in these examples. Then $cov(X,Y) = E[XY]$.

When $cov(X,Y) > 0$, the RVs X and Y tend to be large or small together. X and Y are said to be positively correlated.

When $cov(X,Y) < 0$, when X is larger, Y tends to be smaller. X and Y are said to be negatively correlated.

When $cov(X,Y) = 0$, we say that X and Y are uncorrelated.

Examples of Covariance



$$E[X] = 1\times 0.15 + 2\times 0.4 + 3\times 0.45 = 1.9$$
$$E[X^2] = 1^2\times 0.15 + 2^2\times 0.4 + 3^2\times 0.45 = 5.8$$
$$E[Y] = 1\times 0.2 + 2\times 0.6 + 3\times 0.2 = 2$$
$$E[XY] = 1\times 0.05 + 1\times 2\times 0.1 + \cdots + 3\times 3\times 0.2 = 4.85$$
$$cov(X,Y) = E[XY] - E[X]E[Y] = 1.05$$
$$var[X] = E[X^2] - E[X]^2 = 2.19.$$

Properties of Covariance

$$cov(X,Y) = E[(X - E[X])(Y - E[Y])] = E[XY] - E[X]E[Y].$$

Fact

(a) $var[X] = cov(X,X)$
(b) X,Y independent $\Rightarrow cov(X,Y) = 0$
(c) $cov(a + X, b + Y) = cov(X,Y)$
(d) $cov(aX + bY, cU + dV) = ac.cov(X,U) + ad.cov(X,V) + bc.cov(Y,U) + bd.cov(Y,V)$.

Proof:

(a)-(b)-(c) are obvious.
(d) In view of (c), one can subtract the means and assume that the RVs are zero-mean. Then,

$$\begin{aligned} cov(aX + bY, cU + dV) &= E[(aX + bY)(cU + dV)] \\ &= ac.E[XU] + ad.E[XV] + bc.E[YU] + bd.E[YV] \\ &= ac.cov(X,U) + ad.cov(X,V) + bc.cov(Y,U) + bd.cov(Y,V). \end{aligned}$$

□

Linear Regression: Non-Bayesian

Definition

Given the samples $\{(X_n, Y_n), n = 1,\ldots,N\}$, the Linear Regression of Y over X is

$$\hat{Y} = a + bX$$

where (a,b) minimize

$$\sum_{n=1}^{N}(Y_n - a - bX_n)^2.$$

Thus, $\hat{Y}_n = a + bX_n$ is our guess about Y_n given X_n. The squared error is $(Y_n - \hat{Y}_n)^2$. The LR minimizes the sum of the squared errors.

Why the squares and not the absolute values? Main justification: much easier!

Note: This is a non-Bayesian formulation: there is no prior.

Linear Least Squares Estimate

Definition

Given two RVs X and Y with known distribution $Pr[X = x, Y = y]$, the Linear Least Squares Estimate of Y given X is

$$\hat{Y} = a + bX =: L[Y|X]$$

where (a,b) minimize

$$g(a,b) := E[(Y - a - bX)^2].$$

Thus, $\hat{Y} = a + bX$ is our guess about Y given X. The squared error is $(Y - \hat{Y})^2$. The LLSE minimizes the expected value of the squared error.

Why the squares and not the absolute values? Main justification: much easier!

Note: This is a Bayesian formulation: there is a prior.

LR: Non-Bayesian or Uniform?

Observe that

$$\frac{1}{N}\sum_{n=1}^{N}(Y_n - a - bX_n)^2 = E[(Y - a - bX)^2]$$

where one assumes that

$$(X,Y) = (X_n, Y_n), \text{ w.p. } \frac{1}{N} \text{ for } n = 1,\ldots,N.$$

That is, the non-Bayesian LR is equivalent to the Bayesian LLSE that assumes that (X,Y) is uniform on the set of observed samples.

Thus, we can study the two cases LR and LLSE in one shot.

However, the interpretations are different!

LLSE

Theorem
Consider two RVs X, Y with a given distribution $Pr[X = x, Y = y]$. Then,

$$L[Y|X] = \hat{Y} = E[Y] + \frac{cov(X,Y)}{var(X)}(X - E[X]).$$

Proof 1:
$Y - \hat{Y} = (Y - E[Y]) - \frac{cov(X,Y)}{var[X]}(X - E[X])$. Hence, $E[Y - \hat{Y}] = 0$.

Also, $E[(Y - \hat{Y})X] = 0$, after a bit of algebra. (See next slide.)

Hence, by combining the two brown equalities, $E[(Y - \hat{Y})(c + dX)] = 0$. Then, $E[(Y - \hat{Y})(\hat{Y} - a - bX)] = 0, \forall a, b$.
Indeed: $\hat{Y} = \alpha + \beta X$ for some α, β, so that $\hat{Y} - a - bX = c + dX$ for some c, d. Now,

$$E[(Y - a - bX)^2] = E[(Y - \hat{Y} + \hat{Y} - a - bX)^2]$$
$$= E[(Y - \hat{Y})^2] + E[(\hat{Y} - a - bX)^2] + 0 \geq E[(Y - \hat{Y})^2].$$

This shows that $E[(Y - \hat{Y})^2] \leq E[(Y - a - bX)^2]$, for all (a, b).
Thus $\hat{Y}$ is the LLSE. $\square$

A Bit of Algebra

$Y - \hat{Y} = (Y - E[Y]) - \frac{cov(X,Y)}{var[X]}(X - E[X])$.

Hence, $E[Y - \hat{Y}] = 0$. We want to show that $E[(Y - \hat{Y})X] = 0$.

Note that

$$E[(Y - \hat{Y})X] = E[(Y - \hat{Y})(X - E[X])],$$

because $E[(Y - \hat{Y})E[X]] = 0$.

Now,

$$E[(Y - \hat{Y})(X - E[X])]$$
$$= E[(Y - E[Y])(X - E[X])] - \frac{cov(X,Y)}{var[X]} E[(X - E[X])(X - E[X])]$$
$$=^{(*)} cov(X,Y) - \frac{cov(X,Y)}{var[X]} var[X] = 0. \quad \square$$

$^{(*)}$ Recall that $cov(X,Y) = E[(X - E[X])(Y - E[Y])]$ and $var[X] = E[(X - E[X])^2]$.

Estimation Error

We saw that the LLSE of Y given X is

$$L[Y|X] = \hat{Y} = E[Y] + \frac{cov(X,Y)}{var(X)}(X - E[X]).$$

How good is this estimator? That is, what is the mean squared estimation error?

We find

$$E[|Y - L[Y|X]|^2] = E[(Y - E[Y] - (cov(X,Y)/var(X))(X - E[X]))^2]$$
$$= E[(Y - E[Y])^2] - 2(cov(X,Y)/var(X))E[(Y - E[Y])(X - E[X])]$$
$$+ (cov(X,Y)/var(X))^2 E[(X - E[X])^2]$$
$$= var(Y) - \frac{cov(X,Y)^2}{var(X)}.$$

Without observations, the estimate is $E[Y] = 0$. The error is $var(Y)$. Observing X reduces the error.

Estimation Error: A Picture

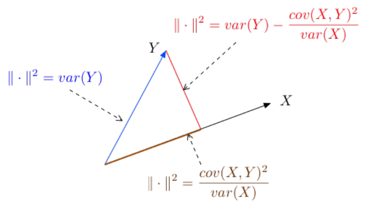
We saw that

$$L[Y|X] = \hat{Y} = E[Y] + \frac{cov(X,Y)}{var(X)}(X - E[X])$$

and

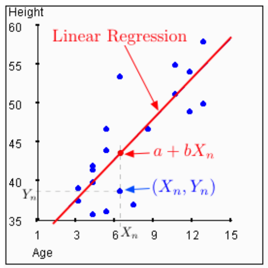
$$E[|Y - L[Y|X]|^2] = var(Y) - \frac{cov(X,Y)^2}{var(X)}.$$

Here is a picture when $E[X] = 0, E[Y] = 0$:



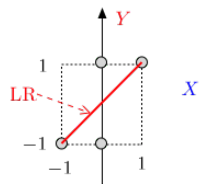
Linear Regression Examples

Example 1:



Linear Regression Examples

Example 2:

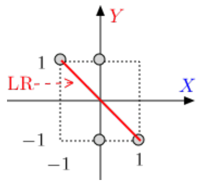


We find:

$E[X] = 0; E[Y] = 0; E[X^2] = 1/2; E[XY] = 1/2;$
$var[X] = E[X^2] - E[X]^2 = 1/2; cov(X,Y) = E[XY] - E[X]E[Y] = 1/2;$
LR: $\hat{Y} = E[Y] + \frac{cov(X,Y)}{var[X]}(X - E[X]) = X.$

Linear Regression Examples

Example 3:



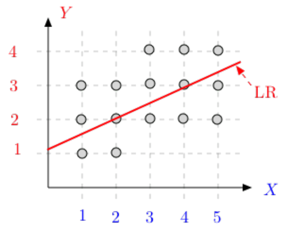
We find:

$E[X] = 0; E[Y] = 0; E[X^2] = 1/2; E[XY] = -1/2;$
$var[X] = E[X^2] - E[X]^2 = 1/2; cov(X,Y) = E[XY] - E[X]E[Y] = -1/2;$

LR: $\hat{Y} = E[Y] + \frac{cov(X,Y)}{var[X]}(X - E[X]) = -X.$

Linear Regression Examples

Example 4:

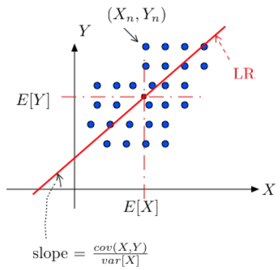


We find:

$E[X] = 3; E[Y] = 2.5; E[X^2] = (3/15)(1 + 2^2 + 3^2 + 4^2 + 5^2) = 11;$
$E[XY] = (1/15)(1 \times 1 + 1 \times 2 + \cdots + 5 \times 4) = 8.4;$
$var[X] = 11 - 9 = 2; cov(X,Y) = 8.4 - 3 \times 2.5 = 0.9;$

LR: $\hat{Y} = 2.5 + \frac{0.9}{2}(X - 3) = 1.15 + 0.45X.$

LR: Another Figure



Note that

- the LR line goes through $(E[X], E[Y])$
- its slope is $\frac{cov(X,Y)}{var(X)}$.

Summary

Linear Regression

1. Linear Regression: $L[Y|X] = E[Y] + \frac{cov(X,Y)}{var(X)}(X - E[X])$
2. Non-Bayesian: minimize $\sum_n (Y_n - a - bX_n)^2$
3. Bayesian: minimize $E[(Y - a - bX)^2]$