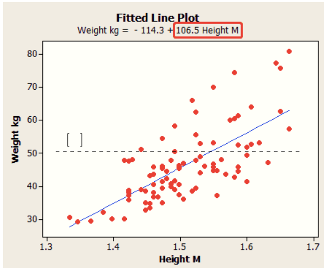
CS70: Lecture 35.

Regression (contd.): Linear and Beyond

1. Review: Linear Regression (LR), LLSE
2. LR: Examples
3. Beyond LR: Quadratic Regression
4. Conditional Expectation (CE) and properties
5. Non-linear Regression: CE = Minimum Mean-Squared Error (MMSE)

Review: Linear Regression – Motivation

Example: 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.

Review: Covariance

Definition

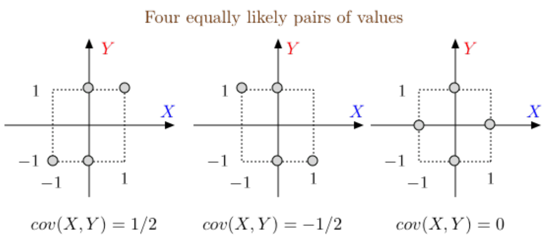
The covariance of X and Y is

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

Fact

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

Review: 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.

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

Review: Linear Least Squares Estimate (LLSE)

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

Review: 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!

Review: LLSE

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

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

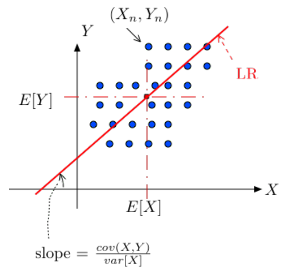
Non-Bayesian setting:

$$E[X] = \frac{1}{N}\sum_{n=1}^{N} X_n; \qquad E[Y] = \frac{1}{N}\sum_{n=1}^{N} Y_n$$

$$Var[X] = E[X^2] - (E[X])^2 = \frac{1}{N}\sum_{n=1}^{N}(X_n)^2 - (\frac{1}{N}\sum_{n=1}^{N}(X_n))^2$$

$$Cov(X,Y) = E[XY] - E[X]E[Y] = \frac{1}{N}\sum_{n=1}^{N}(X_nY_n) - (\frac{1}{N}\sum_{n=1}^{N}X_n)(\frac{1}{N}\sum_{n=1}^{N}Y_n)$$

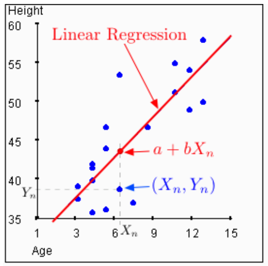
LR: Illustration



Note that

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

Linear Regression: Examples



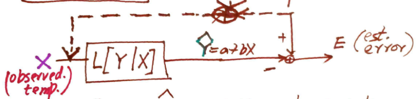
Example: "Removing noise or de-noising"

Y: temp. in a room (quantity of interest)
$[Y = \mathcal{N}(\mu_Y, \sigma_Y^2)]$

Z: thermal noise of temp. sensor
$[Z = \mathcal{N}(0, \sigma_Z^2)]$

X: observed (noisy) temp. measurement @ sensor

$\boxed{X = Y + Z}$



$L[Y|X] = \hat{Y} = a + bX$, where a, b chosen to min $\mathbb{E}[(\text{est. error})^2] = \mathbb{E}[(Y - \hat{Y})^2]$

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

- $\mathbb{E}[X] = \mathbb{E}[Y + Z] = \underbrace{\mathbb{E}[Y]}_{\mu_Y} + \underbrace{\mathbb{E}[Z]}_{0} = \mu_Y$
- $cov(X,Y) = \mathbb{E}[XY] - \mathbb{E}[X]\cdot\mathbb{E}[Y]$

$$= \underbrace{\mathbb{E}[(Y+Z)Y]}_{\underbrace{\mathbb{E}[Y^2] + \mathbb{E}[YZ]}_{\sigma_Y^2 + \mu_Y^2 + \underbrace{\mathbb{E}[Y]}_{\mu_Y}\cdot\underbrace{\mathbb{E}[Z]}_{0}}} - \underbrace{\mathbb{E}[Y+Z]}_{\mu_Y}\cdot\underbrace{\mathbb{E}[Y]}_{\mu_Y}$$

$$\Rightarrow cov(X,Y) = \sigma_Y^2 + \mu_Y^2 - \mu_Y^2 = \boxed{\sigma_Y^2}$$

- $var(X) = \underbrace{var(Y)}_{\sigma_Y^2} + \underbrace{var(Z)}_{\sigma_Z^2} = \boxed{\sigma_Y^2 + \sigma_Z^2}$

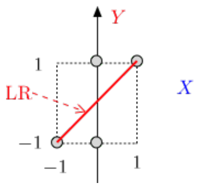
$$\boxed{\hat{Y} = L[Y|X] = \mu_Y + \left(\frac{\sigma_Y^2}{\sigma_Y^2 + \sigma_Z^2}\right)(X - \mu_Y)}$$

Remarks: (1) If $\sigma_Z^2 \approx 0$ (no noise) $\Rightarrow \hat{Y} \cong X$ ("believe the obs.")

(2) If $\sigma_Z^2 >> \sigma_Y^2$ (v. noisy) $\Rightarrow \hat{Y} \cong \mu_Y = \mathbb{E}[Y]$ ("believe the model & not the obs. data")

(3) If $\mu_Y = 70^0F$, $\sigma_Y^2 = 5$, $\sigma_Z^2 = 2$
$\hat{Y} = 70 + \frac{5}{7}(X - 70)$

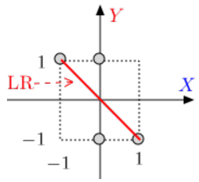
Linear Regression: Example 2



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

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

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

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

Wrap-up of Linear Regression

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 $E[(Y - a - bX)^2]$

Beyond Linear Regression: Discussion

Goal: guess the value of Y in the expected squared error sense. We know nothing about Y other than its distribution. Our best guess is? $E[Y]$.

Now assume we make some observation X related to Y.

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

Idea: use a function $g(X)$ of the observation to estimate Y.

LR: Restriction to linear functions: $g(X) = a + bX$.

With no such constraints, what is the best $g(X)$?

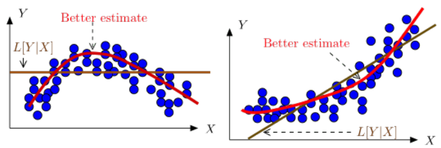
Answer: $E[Y|X]$.

This is called the Conditional Expectation (CE).

Nonlinear Regression: Motivation

There are many situations where a good guess about Y given X is not linear.

E.g., (diameter of object, weight), (school years, income), (PSA level, cancer risk).



Our goal: explore estimates $\hat{Y} = g(X)$ for nonlinear functions $g(\cdot)$.

Quadratic Regression

Let X, Y be two random variables defined on the same probability space.

Definition: The quadratic regression of Y over X is the random variable

$$Q[Y|X] = a + bX + cX^2$$

where a, b, c are chosen to minimize $E[(Y - a - bX - cX^2)^2]$.

Derivation: We set to zero the derivatives w.r.t. a, b, c. We get

$$\begin{aligned} 0 &= E[Y - a - bX - cX^2] \\ 0 &= E[(Y - a - bX - cX^2)X] \\ 0 &= E[(Y - a - bX - cX^2)X^2] \end{aligned}$$

We solve these three equations in the three unknowns (a, b, c).

Conditional Expectation

Definition Let X and Y be RVs on Ω. The conditional expectation of Y given X is defined as

$$E[Y|X] = g(X)$$

where

$$g(x) := E[Y|X = x] := \sum_y yPr[Y = y|X = x].$$

Deja vu, all over again?

Have we seen this before? Yes.

Is anything new? Yes.

The idea of defining $g(x) = E[Y|X = x]$ and then $E[Y|X] = g(X)$.

Big deal? Quite! Simple but most convenient.

Recall that $L[Y|X] = a + bX$ is a function of X.

This is similar: $E[Y|X] = g(X)$ for some function $g(\cdot)$.

In general, $g(X)$ is not linear, i.e., not $a + bX$. It could be that $g(X) = a + bX + cX^2$. Or that $g(X) = 2\sin(4X) + \exp\{-3X\}$. Or something else.

Properties of CE

$$E[Y|X = x] = \sum_y yPr[Y = y|X = x]$$

Theorem

(a) X, Y independent $\Rightarrow E[Y|X] = E[Y]$;

(b) $E[aY + bZ|X] = aE[Y|X] + bE[Z|X]$;

(c) $E[Yh(X)|X] = h(X)E[Y|X], \forall h(\cdot)$;

(d) $E[E[Y|X]] = E[Y]$.

Calculating $E[Y|X]$

Let X, Y, Z be i.i.d. with mean 0 and variance 1. We want to calculate

$$E[2 + 5X + 7XY + 11X^2 + 13X^3Z^2|X].$$

We find

$$\begin{aligned} &E[2 + 5X + 7XY + 11X^2 + 13X^3Z^2|X] \\ &= 2 + 5X + 7XE[Y|X] + 11X^2 + 13X^3E[Z^2|X] \\ &= 2 + 5X + 7XE[Y] + 11X^2 + 13X^3E[Z^2] \\ &= 2 + 5X + 11X^2 + 13X^3(var[Z] + E[Z]^2) \\ &= 2 + 5X + 11X^2 + 13X^3. \end{aligned}$$

CE = MMSE

(Conditional Expectation = Minimum Mean Squared Error)

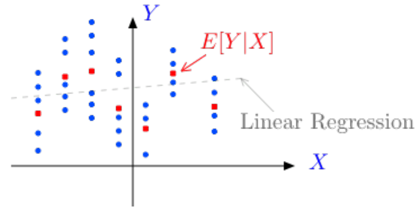
Theorem

$g(X) := E[Y|X]$ is the function of X that minimizes $E[(Y - g(X))^2]$.

That is, $E[Y|X]$ is the 'best' guess about Y based on X.

Specifically, it is the function $g(X)$ of X that

minimizes $E[(Y - g(X))^2]$.



Summary

Linear and Non-Linear Regression: Conditional Expectation

- Linear Regression: $L[Y|X] = E[Y] + \frac{cov(X,Y)}{var(X)}(X - E[X])$
- Non-linear Regression: MMSE: $E[Y|X]$ minimizes $E[(Y - g(X))^2]$ over all $g(\cdot)$
- Definition: $E[Y|X] := \sum_y yPr[Y = y|X = x]$