

## Nonlinear Regression

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## 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

$$0 = E[Y - a - bX - cX^{2}]$$
  

$$0 = E[(Y - a - bX - cX^{2})X]$$
  

$$0 = E[(Y - a - bX - cX^{2})X^{2}]$$

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

**Note:** These equations imply that E[(Y - Q[Y|X])h(X)] = 0 for any  $h(X) = d + eX + tX^2$ . That is, the estimation error is orthogonal to all the quadratic functions of *X*. Hence, Q[Y|X] is the projection of *Y* onto the space of quadratic functions of *X*.

## Review

**Definitions** Let X and Y be RVs on  $\Omega$ .

- ► Joint Distribution: Pr[X = x, Y = y]
- Marginal Distribution:  $Pr[X = x] = \sum_{y} Pr[X = x, Y = y]$
- ► Conditional Distribution:  $Pr[Y = y | X = x] = \frac{Pr[X = x, Y = y]}{Pr[X = x]}$
- ► LLSE: L[Y|X] = a + bX where a, b minimize  $E[(Y a bX)^2]$ .

We saw that

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

Recall the non-Bayesian and Bayesian viewpoints.

# **Conditional Expectation**

**Definition** Let X and Y be RVs on  $\Omega$ . The conditional expectation of Y given X is defined as

E[Y|X] = g(X)

where

Fact

$$g(x) := E[Y|X = x] := \sum_{y} yPr[Y = y|X = x].$$
$$E[Y|X = x] = \sum_{\omega} Y(\omega)Pr[\omega|X = x].$$

**Proof:** E[Y|X = x] = E[Y|A] with  $A = \{\omega : X(\omega) = x\}$ .

## 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  $g(\cdot)$ .

# 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**

$$E[Y|X=x] = \sum_{y} y Pr[Y=y|X=x]$$

## 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)  $E[h(X)E[Y|X]] = E[h(X)Y], \forall h(\cdot);$ (e) E[E[Y|X]] = E[Y]. **Proof:** (a),(b) Obvious

(a), (b) Excludes (c)  $E[Yh(X)|X = x] = \sum_{\omega} Y(\omega)h(X(\omega)Pr[\omega|X = x])$  $= \sum_{\omega} Y(\omega)h(x)Pr[\omega|X = x] = h(x)E[Y|X = x]$ 

# Properties of CE

## Theorem

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Note that (d) says that

E[(Y - E[Y|X])h(X)] = 0.

We say that the estimation error Y - E[Y|X] is orthogonal to every function h(X) of X.

We call this the projection property. More about this later.

## **Properties of CE**

$$E[Y|X=x] = \sum_{y} y Pr[Y=y|X=x]$$

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

## Proof: (continued)

(d) 
$$E[h(X)E[Y|X]] = \sum_{x} h(x)E[Y|X = x]Pr[X = x]$$
$$= \sum_{x} h(x)\sum_{y} yPr[Y = y|X = x]Pr[X = x]$$
$$= \sum_{x} h(x)\sum_{y} yPr[X = x, y = y]$$
$$= \sum_{x,y} h(x)yPr[X = x, y = y] = E[h(X)Y]$$

# Application: 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

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

# **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) $E[h(X)E[Y|X]] = E[h(X)Y], \forall h(\cdot);$ (e) E[E[Y|X]] = E[Y]. Proof: (continued) (e) Let h(X) = 1 in (d). **Application: Diluting** $X_1 = N$ $X_2 = N - 1$ $X_3 = N - 2$ $X_4 = N - 2$ red balls At each step, pick a ball from a well-mixed urn. Replace it with a blue ball. Let $X_n$ be the number of red balls in the urn at step *n*. What is $E[X_n]$ ? Given $X_n = m$ , $X_{n+1} = m - 1$ w.p. m/N (if you pick a red ball) and $X_{n+1} = m$ otherwise. Hence,

 $E[X_{n+1}|X_n = m] = m - (m/N) = m(N-1)/N = X_n \rho,$ 

with  $\rho := (N-1)/N$ . Consequently,

$$E[X_{n+1}] = E[E[X_{n+1}|X_n]] = \rho E[X_n], n \ge 1.$$
  
$$\implies E[X_n] = \rho^{n-1} E[X_1] = N(\frac{N-1}{N})^{n-1}, n \ge 1.$$



## Diluting

By analyzing  $E[X_{n+1}|X_n]$ , we found that  $E[X_n] = N(\frac{N-1}{N})^{n-1}, n \ge 1$ .

Here is another argument for that result.

Consider one particular red ball, say ball *k*. At each step, it remains red w.p. (N-1)/N, when another ball is picked. Thus, the probability that it is still red at step *n* is  $[(N-1)/N]^{n-1}$ . Let

 $Y_n(k) = 1$ {ball k is red at step n}.

Then,  $X_n = Y_n(1) + \cdots + Y_n(N)$ . Hence,

 $E[X_n] = E[Y_n(1) + \dots + Y_n(N)] = NE[Y_n(1)]$ = NPr[Y\_n(1) = 1] = N[(N-1)/N]^{n-1}.

# Application: Mixing





## **Application:** Mixing



At each step, pick a ball from each well-mixed urn. We transfer them to the other urn. Let  $X_n$  be the number of red balls in the bottom urn at step n. What is  $E[X_n]$ ?

Given  $X_n = m$ ,  $X_{n+1} = m+1$  w.p. *p* and  $X_{n+1} = m-1$  w.p. *q* 

where  $p = (1 - m/N)^2$  (B goes up, R down) and  $q = (m/N)^2$  (R goes up, B down).

Thus,  $E[X_{n+1}|X_n] = X_n + p - q = X_n + 1 - 2X_n/N = 1 + \rho X_n, \rho := (1 - 2/N).$ 

## Application: Going Viral

Consider a social network (e.g., Twitter). You start a rumor (e.g., Walrand is really weird). You have *d* friends. Each of your friend retweets w.p. *p*. Each of your friends has *d* friends, etc. Does the rumor spread? Does it die out (mercifully)?





# CE = MMSE

Theorem E[Y|X] is the 'best' guess about Y based on X. Specifically, it is the function g(X) of X that

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





To see this, note that given  $X_n = k$ , and given the numbers of friends  $D_1 = d_1, \ldots, D_k = d_k$  of these  $X_n$  people, one has

 $X_{n+1} = B(d_1 + \dots + d_k, p)$ . Hence,

 $E[X_{n+1}|X_n = k, D_1 = d_1, \dots, D_k = d_k] = p(d_1 + \dots + d_k).$ 

Thus,  $E[X_{n+1}|X_n = k, D_1, \dots, D_k] = p(D_1 + \dots + D_k).$ Consequently,  $E[X_{n+1}|X_n = k] = E[p(D_1 + \cdots + D_k)] = pdk$ . Finally,  $E[X_{n+1}|X_n] = pdX_n$ , and  $E[X_{n+1}] = pdE[X_n]$ . We conclude as before.

# CE = MMSE

Theorem CE = MMSE g(X) := E[Y|X] is the function of X that minimizes  $E[(Y-g(X))^2].$ Proof: Let h(X) be any function of X. Then

 $E[(Y-h(X))^2] = E[(Y-g(X)+g(X)-h(X))^2]$  $= E[(Y - g(X))^{2}] + E[(g(X) - h(X))^{2}]$ +2E[(Y-g(X))(g(X)-h(X))].

## But,

E[(Y-g(X))(g(X)-h(X))] = 0 by the projection property.

Thus,  $E[(Y - h(X))^2] > E[(Y - q(X))^2].$ 

## Application: Wald's Identity

Here is an extension of an identity we used in the last slide. Theorem Wald's Identity Assume that  $X_1, X_2, \ldots$  and Z are independent, where Z takes values in  $\{0, 1, 2, \ldots\}$ and  $E[X_n] = \mu$  for all  $n \ge 1$ . Then.  $E[X_1 + \cdots + X_Z] = \mu E[Z].$ 

## Proof:

 $E[X_1 + \dots + X_Z | Z = k] = \mu k.$ Thus,  $E[X_1 + \cdots$ Hence,  $E[X_1 +$ 

# E[Y|X] and L[Y|X] as projections



L[Y|X] is the projection of Y on  $\{a+bX, a, b \in \Re\}$ : LLSE E[Y|X] is the projection of Y on  $\{g(X), g(\cdot) : \Re \to \Re\}$ : MMSE.

$$\dots + X_Z[Z] = \mu Z.$$
  
$$\dots + X_Z[Z] = E[\mu Z] = \mu E[Z]$$

