CS70: Jean Walrand: Lecture 31.

Nonlinear Regression

1. Review: joint distribution, LLSE
2. Quadratic Regression
3. Definition of Conditional expectation
4. Properties of CE
5. Applications: Diluting, Mixing, Rumors
6. $C E=$ MMSE

## 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

$$
Q[Y \mid X]=a+b X+c X^{2}
$$

where $a, b, c$ are chosen to minimize $E\left[\left(Y-a-b X-c X^{2}\right)^{2}\right]$.
Derivation: We set to zero the derivatives w.r.t. $a, b, c$. We get

$$
\begin{aligned}
& 0=E\left[Y-a-b X-c X^{2}\right] \\
& 0=E\left[\left(Y-a-b X-c X^{2}\right) X\right] \\
& 0=E\left[\left(Y-a-b X-c X^{2}\right) X^{2}\right]
\end{aligned}
$$

We solve these three equations in the three unknowns $(a, b, c)$.
Note: These equations imply that $E[(Y-Q[Y \mid X]) h(X)]=0$ for any $h(X)=d+e X+f X^{2}$. That is, the estimation error is orthogonal to all the quadratic functions of $X$. Hence, $Q[Y \mid X]$ 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: $\operatorname{Pr}[X=x, Y=y]$
- Marginal Distribution: $\operatorname{Pr}[X=x]=\sum_{y} \operatorname{Pr}[X=x, Y=y]$
- Conditional Distribution: $\operatorname{Pr}[Y=y \mid X=x]=\frac{\operatorname{Pr}[X=x, Y=y]}{\operatorname{Pr}[X=x]}$
- LLSE: $L[Y \mid X]=a+b X$ where $a, b$ minimize $E\left[(Y-a-b X)^{2}\right]$.

We saw that

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

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

$$
E[Y \mid X]=g(X)
$$

where

$$
g(x):=E[Y \mid X=x]:=\sum_{y} y \operatorname{Pr}[Y=y \mid X=x] .
$$

Fact

$$
E[Y \mid X=x]=\sum_{\omega} Y(\omega) \operatorname{Pr}[\omega \mid X=x] .
$$

Proof: $E[Y \mid X=x]=E[Y \mid A]$ 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 $g(x)=E[Y \mid X=x]$ and then $E[Y \mid X]=g(X)$
Big deal? Quite! Simple but most convenient.
Recall that $L[Y \mid X]=a+b X$ is a function of $X$.
This is similar: $E[Y \mid X]=g(X)$ for some function $g(\cdot)$.
In general, $g(X)$ is not linear, i.e., not $a+b X$. It could be that $g(X)=a+b X+c X^{2}$. Or that $g(X)=2 \sin (4 X)+\exp \{-3 X\}$. Or something else.

## Properties of CE

$$
E[Y \mid X=x]=\sum_{y} y P r[Y=y \mid X=x]
$$

## Theorem

(a) $X, Y$ independent $\Rightarrow E[Y \mid X]=E[Y]$;
(b) $E[a Y+b Z \mid X]=a E[Y \mid X]+b E[Z \mid X]$;
(c) $E[Y h(X) \mid X]=h(X) E[Y \mid X], \forall h(\cdot)$;
(d) $E[h(X) E[Y \mid X]]=E[h(X) Y], \forall h(\cdot) ;$
(e) $E[E[Y \mid X]]=E[Y]$.

Proof:
(a),(b) Obvious
(c) $E[Y h(X) \mid X=x]=\sum_{\omega} Y(\omega) h(X(\omega) \operatorname{Pr}[\omega \mid X=x]$
$=\sum_{\omega} Y(\omega) h(x) \operatorname{Pr}[\omega \mid X=x]=h(x) E[Y \mid X=x]$

## Properties of CE

## Theorem

(a) $X, Y$ independent $\Rightarrow E[Y \mid X]=E[Y]$
(b) $E[a Y+b Z \mid X]=a E[Y \mid X]+b E[Z \mid X]$
(c) $E[Y h(X) \mid X]=h(X) E[Y \mid X], \forall h(\cdot)$;
(d) $E[h(X) E[Y \mid X]]=E[h(X) Y], \forall h(\cdot) ;$
(e) $E[E[Y \mid X]]=E[Y]$.

Note that (d) says that
$E[(Y-E[Y \mid X]) h(X)]=0$.
We say that the estimation error $Y-E[Y \mid X]$ is orthogonal to every function $h(X)$ of $X$.
We call this the projection property. More about this later.

## Properties of CE

$$
E[Y \mid X=x]=\sum_{y} y P r[Y=y \mid X=x]
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## Theorem

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(b) $E[a Y+b Z \mid X]=a E[Y \mid X]+b E[Z \mid X]$
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(d) $E[h(X) E[Y \mid X]]=E[h(X) Y], \forall h(\cdot)$
(e) $E[E[Y \mid X]]=E[Y]$

Proof: (continued)
(d) $E[h(X) E[Y \mid X]]=\sum h(x) E[Y \mid X=x] \operatorname{Pr}[X=x]$

$$
\begin{aligned}
& =\sum_{x} h(x) \sum_{y}^{x} y \operatorname{Pr}[Y=y \mid X=x] \operatorname{Pr}[X=x] \\
& =\sum_{x} h(x) \sum_{y} y \operatorname{Pr}[X=x, y=y] \\
& =\sum_{x, y} h(x) y \operatorname{Pr}[X=x, y=y]=E[h(X) Y] .
\end{aligned}
$$

Application: Calculating $E[Y \mid X]$
Let $X, Y, Z$ be i.i.d. with mean 0 and variance 1 . We want to calculate

$$
E\left[2+5 X+7 X Y+11 X^{2}+13 X^{3} Z^{2} \mid X\right]
$$

We find
$E\left[2+5 X+7 X Y+11 X^{2}+13 X^{3} Z^{2} \mid X\right]$
$=2+5 X+7 X E[Y \mid X]+11 X^{2}+13 X^{3} E\left[Z^{2} \mid X\right]$
$=2+5 X+7 X E[Y]+11 X^{2}+13 X^{3} E\left[Z^{2}\right]$
$=2+5 X+11 X^{2}+13 X^{3}\left(\operatorname{var}[Z]+E[Z]^{2}\right)$
$=2+5 X+11 X^{2}+13 X^{3}$.

## Properties of CE

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

## heorem

(a) $X, Y$ independent $\Rightarrow E[Y \mid X]=E[Y]$;
(b) $E[a Y+b Z \mid X]=a E[Y \mid X]+b E[Z \mid X]$;
c) $E[Y h(X) \mid X]=h(X) E[Y \mid X], \forall h(\cdot)$;
(d) $E[h(X) E[Y \mid X]]=E[h(X) Y], \forall h(\cdot)$;
(e) $E[E[Y \mid X]]=E[Y]$.

Proof: (continued)
(e) Let $h(X)=1$ in (d).

## Application: Diluting


$X_{1}=N \quad X_{2}=N-1 \quad X_{3}=N-2 \quad X_{4}=N-2$ 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 $E\left[X_{n}\right]$ ?
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,

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

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

$$
\begin{gathered}
E\left[X_{n+1}\right]=E\left[E\left[X_{n+1} \mid X_{n}\right]\right]=\rho E\left[X_{n}\right], n \geq 1 . \\
\Longrightarrow E\left[X_{n}\right]=\rho^{n-1} E\left[X_{1}\right]=N\left(\frac{N-1}{N}\right)^{n-1}, n \geq 1 .
\end{gathered}
$$

## Diluting

Here is a plot:


Mixing

We saw that $E\left[X_{n+1} \mid X_{n}\right]=1+\rho X_{n}, \rho:=(1-2 / N)$. Hence,

$$
\begin{aligned}
& E\left[X_{n+1}\right]=1+\rho E\left[X_{n}\right] \\
& E\left[X_{2}\right]=1+\rho N ; E\left[X_{3}\right]=1+\rho(1+\rho N)=1+\rho+\rho^{2} N \\
& E\left[X_{4}\right]=1+\rho\left(1+\rho+\rho^{2} N\right)=1+\rho+\rho^{2}+\rho^{3} N \\
& E\left[X_{n}\right]=1+\rho+\cdots+\rho^{n-2}+\rho^{n-1} N .
\end{aligned}
$$

Hence,

$$
E\left[X_{n}\right]=\frac{1-\rho^{n-1}}{1-\rho}+\rho^{n-1} N, n \geq 1
$$

## Diluting

By analyzing $E\left[X_{n+1} \mid X_{n}\right]$, we found that $E\left[X_{n}\right]=N\left(\frac{N-1}{N}\right)^{n-1}, n \geq 1$.
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

$$
Y_{n}(k)=1\{\text { ball } k \text { is red at step } n\} .
$$

Then, $X_{n}=Y_{n}(1)+\cdots+Y_{n}(N)$. Hence,

$$
\begin{aligned}
E\left[X_{n}\right] & =E\left[Y_{n}(1)+\cdots+Y_{n}(N)\right]=N E\left[Y_{n}(1)\right] \\
& =\operatorname{NPr}\left[Y_{n}(1)=1\right]=N[(N-1) / N]^{n-1} .
\end{aligned}
$$

## Application: Mixing

Here is the plot.


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 $E\left[X_{n}\right]$ ?
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,
$E\left[X_{n+1} \mid X_{n}\right]=X_{n}+p-q=X_{n}+1-2 X_{n} / N=1+\rho X_{n}, \rho:=(1-2 / N)$.

## 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)?


In this example, $d=4$.

## Application: Going Viral



Fact: Let $X=\sum_{n=1}^{\infty} X_{n}$. Then, $E[X]<\infty$ iff $p d<1$.
Proof:
Given $X_{n}=k, X_{n+1}=B(k d, p)$. Hence, $E\left[X_{n+1} \mid X_{n}=k\right]=k p d$.
Thus, $E\left[X_{n+1} \mid X_{n}\right]=p d X_{n}$. Consequently, $E\left[X_{n}\right]=(p d)^{n-1}, n \geq 1$.
If $p d<1$, then $E\left[X_{1}+\cdots+X_{n}\right] \leq(1-p d)^{-1} \Longrightarrow E[X] \leq(1-p d)^{-1}$
If $p d \geq 1$, then for all $C$ one can find $n$ s.t.
$E[X] \geq E\left[X_{1}+\cdots+X_{n}\right] \geq C$.
In fact, one can show that $p d \geq 1 \Longrightarrow \operatorname{Pr}[X=\infty]>0$.

## $C E=$ MMSE

Theorem
$E[Y \mid X]$ is the 'best' guess about $Y$ based on $X$.
Specifically, it is the function $g(X)$ of $X$ that
minimizes $E\left[(Y-g(X))^{2}\right]$.


## Application: Going Vira



An easy extension: Assume that everyone has an independent An easy extension: Assume that everyone has an independent
number $D_{i}$ of friends with $E\left[D_{i}\right]=d$. Then, the same fact holds.
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
$X_{n+1}=B\left(d_{1}+\cdots+d_{k}, p\right)$. Hence,
$E\left[X_{n+1} \mid X_{n}=k, D_{1}=d_{1}, \ldots, D_{k}=d_{k}\right]=p\left(d_{1}+\cdots+d_{k}\right)$.
Thus, $E\left[X_{n+1} \mid X_{n}=k, D_{1}, \ldots, D_{k}\right]=p\left(D_{1}+\cdots+D_{k}\right)$.
Consequently, $E\left[X_{n+1} \mid X_{n}=k\right]=E\left[p\left(D_{1}+\cdots+D_{k}\right)\right]=p d k$.
Finally, $E\left[X_{n+1} \mid X_{n}\right]=p d X_{n}$, and $E\left[X_{n+1}\right]=p d E\left[X_{n}\right]$.
We conclude as before

## CE = MMSE

## Theorem CE = MMSE

$g(X):=E[Y \mid X]$ is the function of $X$ that minimizes
$E\left[(Y-g(X))^{2}\right]$.
Proof:
Let $h(X)$ be any function of $X$. Then

$$
\begin{aligned}
E\left[(Y-h(X))^{2}\right]= & E\left[(Y-g(X)+g(X)-h(X))^{2}\right] \\
= & E\left[(Y-g(X))^{2}\right]+E\left[(g(X)-h(X))^{2}\right] \\
& \quad+2 E[(Y-g(X))(g(X)-h(X))] .
\end{aligned}
$$

But,
$E[(Y-g(X))(g(X)-h(X))]=0$ by the projection property. Thus, $E\left[(Y-h(X))^{2}\right] \geq E\left[(Y-g(X))^{2}\right]$.

## 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 $E\left[X_{n}\right]=\mu$ for all $n \geq 1$
Then,

$$
E\left[X_{1}+\cdots+X_{Z}\right]=\mu E[Z] .
$$

## Proof:

$E\left[X_{1}+\cdots+X_{Z} \mid Z=k\right]=\mu k$
Thus, $E\left[X_{1}+\cdots+X_{Z} \mid Z\right]=\mu Z$
Hence, $E\left[X_{1}+\cdots+X_{Z}\right]=E[\mu Z]=\mu E[Z]$.
$E[Y \mid X]$ and $L[Y \mid X]$ as projections

$\hat{Y}=\dot{L}[Y \mid X] \quad\{g(X), g(\cdot): \Re \rightarrow \Re\}-\dot{A}$
$L[Y \mid X]$ is the projection of $Y$ on $\{a+b X, a, b \in \Re\}$ : LLSE $E[Y \mid X]$ is the projection of $Y$ on $\{g(X), g(\cdot): \Re \rightarrow \Re\}$ : MMSE.

Summary

## Conditional Expectation

- Definition: $E[Y \mid X]:=\sum_{y} y \operatorname{Pr}[Y=y \mid X=x]$

Properties: Linearity,
$Y-E[Y \mid X] \perp h(X) ; E[E[Y \mid X]]=E[Y]$

- Some Applications:

Calculating $E[Y \mid X]$
Diluting

- Mixing
- Rumors
- MMSE: $E[Y \mid X]$ minimizes $E\left[(Y-g(X))^{2}\right]$ over all $g(\cdot)$

