

# Machine Learning (VI): Conditional Expectation, Nonparametric and Parametric Estimations

Le Wang

CEF: Motivation and Running Example

Possible Solutions

Solution (1): Kernel Estimation

Solution 2: KKN Estimator

More on Linear Regression

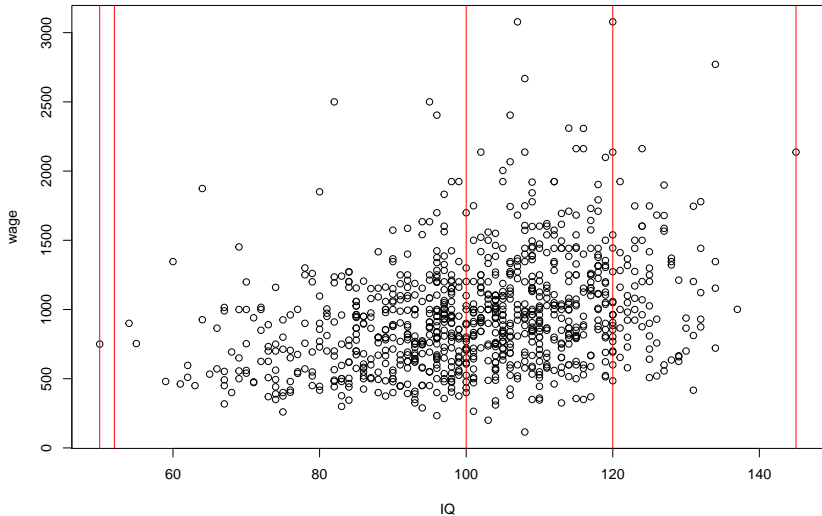
## CEF: Motivation and Running Example

# Motivation

Question: What if the predictor or explanatory variable,  $\mathbf{x}$ , is continuous?

Let's look at one example

**Question:** What is the relationship between IQ and Wages?



You already know: not that many low- or high-IQ individuals! Even if it is theoretically well defined, we cannot estimate it!

How can we obtain

$$\mathbb{E}[\text{wages} \mid \text{IQ}]$$

Of course, we can still calculate the CEF values for those that exist in the data.

```
results<-aggregate(wage,by=list(IQ),FUN=mean)  
as.data.frame(results)
```

##	Group.1	x
## 1	50	750.0000
## 2	54	900.0000
## 3	55	754.0000
## 4	59	480.0000
## 5	60	1346.0000
## 6	61	462.0000
## 7	62	553.0000
## 8	63	450.0000
## 9	64	1400.0000
## 10	65	533.0000
## 11	66	718.0000
## 12	67	636.3333
## 13	68	546.5000
## 14	69	831.6000
## 15	70	810.4000
## 16	71	629.6667

## Possible Solutions



# Possible Solutions

There are many ways to define these solutions (or models):

**Nonparametric** vs. **Parametric**

In **econometrics**: whether or not functional form is assumed

In **machine learning**: does the model have a fixed number of parameters? Or, does the number of parameters grow with the amount of data?

**Parametric models** have the advantage of often being faster to use, but the disadvantage of making stronger (perhaps wrong) assumptions about the nature of the conditional distribution.

**Nonparametric Models** are more flexible, but often computationally intractable for large datasets, let alone big data!

1. Kernel Estimation
2. K-nearest neighbors (KNN)
3. OLS estimation (Linear Regression)

## Solution (1): Kernel Estimation

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We now turn this quantity

$$\mathbb{E}[\text{wages} | \text{IQ} = 60]$$

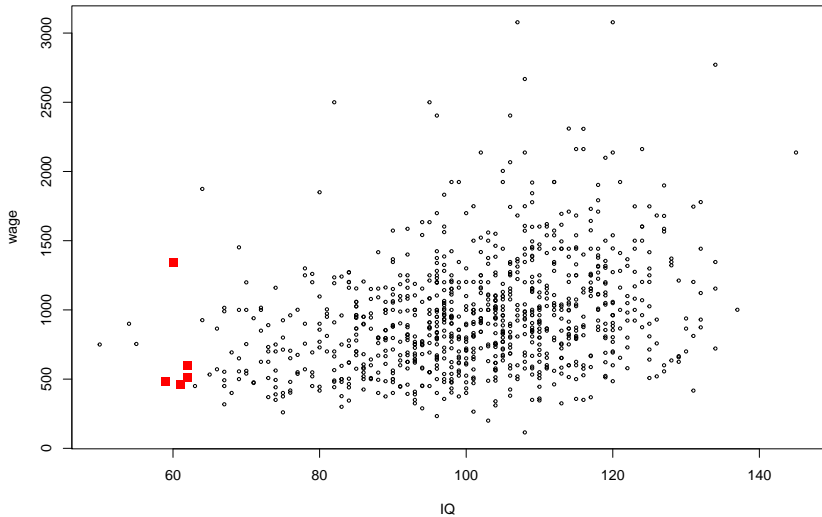
to the wages for those with similar IQ

$$\mathbb{E}[\text{wages} | \text{IQ} \approx 60]$$

**Question:** What do you mean by similar?

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**Similarity:** Perhaps within two-unit differences of one's own IQ? If so, it is pretty straightforward to implement in R.





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  - (b) Calculate the average of the outcome variable (continuous variable) or the conditional distribution of the outcome variable (discrete variable)
  - (c) Report the average (continuous variable) as your prediction, or the most likely outcome (discrete variable) as your prediction.

Let's see how we implement this approach in R

## **Alternative Expression of NP:** Weighted Averages

Another way to express what we just did:

$$\mathbb{E}[\text{wages} \mid \text{IQ} = 50] = \mathbb{E}[\text{wages} \mid \text{IQ} \approx 50]$$

## Alternative Expression of NP: Weighted Averages

Another way to express what we just did:

$$\begin{aligned}\mathbb{E}[\text{wages} \mid \text{IQ} = 50] &= \mathbb{E}[\text{wages} \mid \text{IQ} \approx 50] \\ &= \frac{\sum \mathbb{I}[50 + 2 \geq \text{IQ}_i \geq 50 - 2] \cdot \text{wages}_i}{\sum \mathbb{I}[50 + 2 \geq \text{IQ}_i \geq 50 - 2]}\end{aligned}$$

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$$\text{where } w_i = \frac{\mathbb{I}[50+2 \geq \text{IQ}_i \geq 50-2]}{\sum \mathbb{I}[50+2 \geq \text{IQ}_i \geq 50-2]}$$



## Example

$IQ$	wages	$\mathbb{I}[50 + 2 \geq IQ_i \geq 50 - 2]$
51	100	1
49	50	1
53	110	0
53	115	0
44	45	0

**Approach 1:**  $\frac{100+50}{2} = 75$

## Example

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**Approach 1:**  $\frac{100+50}{2} = 75$

**Approach 2:**

$$\frac{1 \cdot 100 + 1 \cdot 50 + 0 \cdot 110 + 0 \cdot 115 + 0 \cdot 45}{1 + 1 + 0 + 0 + 0}$$

## Example

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**Approach 2:**

$$\frac{1 \cdot 100 + 1 \cdot 50 + 0 \cdot 110 + 0 \cdot 115 + 0 \cdot 45}{1 + 1 + 0 + 0 + 0}$$
$$= \frac{1}{2} \cdot 100 + \frac{1}{2} \cdot 50 + \frac{0}{2} \cdot 110 + \frac{0}{2} \cdot 115 + \frac{0}{2} \cdot 45 = 75$$

## Limitations of Solution 1

Our proposed solution: discretization (as we have seen in one of the previous examples) Shortcoming:

1. Arbitrary bundling of the points.
2. Use of only limited points (sometimes may not be any observations)!

*Question:* What to do?

Solution 1 (Extension): Nonparametric Kernel Estimation:

$$\mathbb{E}[\text{wages} \mid \text{IQ} = 50] = \mathbb{E}[\text{wages} \mid \text{IQ} \approx 50]$$

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$$\begin{aligned}\mathbb{E}[\text{wages} \mid \text{IQ} = 50] &= \mathbb{E}[\text{wages} \mid \text{IQ} \approx 50] \\ &= \frac{\sum \mathbb{K}[50, \text{IQ}_i] \cdot \text{wages}_i}{\sum \mathbb{K}[50, \text{IQ}_i]}\end{aligned}$$

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where  $w_i = \frac{\mathbb{K}[50, \text{IQ}_i]}{\sum \mathbb{K}[50, \text{IQ}_i]}$

Find a kernel function that assigns declining weights with respect to the distance to the data point,  $x$ .

$$\mathbb{K}[50, IQ_i] = \mathbb{K}\left[\frac{IQ_i - 50}{h}\right]$$

where  $h$  is called the **bandwidth** (you can think of it as window)

## Examples of Kernel

### 1. Gaussian or Normal

$$\mathbb{K}(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

### 2. Uniform

$$\mathbb{K}(z) = \frac{1}{2} \mathbb{I}(|u| \leq 1)$$

### 3. Epanechnikov

$$\mathbb{K}(z) = \frac{3}{4} (1 - u^2) \mathbb{I}(|u| \leq 1)$$



Let's look at how to implement it in R

## Solution 2: KKN Estimator

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The book also discusses an alternative approach, which, to some extent, solve the issue where no observations exist for the discretization approach above:

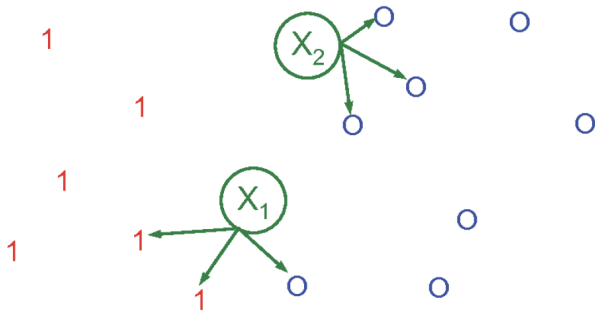
### **K-nearest Neighbors**

As the name suggests, you use only  $K$  nearest neighbors around the value,  $x$ , to calculate the mean and use it to obtain the prediction.

This method is an example of memory-based learning or instance-based learning.

The 3 nearest neighbors of point  $x_{\{1\}}$  have labels 1,1,0, so we

$$\mathbb{E}[y|x = x_1] = \frac{1 + 1 + 0}{3} = \frac{2}{3}$$



## Algorithm

1. Calculate the distance between your value of  $x$  and all  $x$  in your data, sort the data, and pick the first  $k$  observations

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- (a) Report the average as your prediction for these  $k$  observations, or the most likely outcome as your prediction.

## Alternative Expression of KKN: Weighted Averages

Version Another way to express what we just did:

$$\begin{aligned}\mathbb{E}[\text{wages} | \text{IQ} = 50] &= \mathbb{E}[\text{wages} | \text{IQ} \in D] \\ &= \frac{\sum \mathbb{I}[\text{IQ} \in D] \cdot \text{wages}_i}{\sum \mathbb{I}[\text{IQ} \in D]} \\ &= \sum w_i \cdot \text{wages}_i\end{aligned}$$

My prediction from the previous model

$$\text{wage} = 116.992 + 8.303 \cdot \text{IQ}$$

One time for all values!

$$\text{IQ} = 50 \implies \mathbb{E}[\text{wage} | \text{IQ} = 50] = 116.992 + 8.303 \cdot 50$$

$$\text{IQ} = 60 \implies \mathbb{E}[\text{wage} | \text{IQ} = 60] = 116.992 + 8.303 \cdot 60$$

## Alternative Expression of OLS: Weighted Averages

Remember that it is an estimator of the underlying conditional mean. We are somehow weighting some of the observations to obtain an estimate of the conditional mean. But what does this weighting function look like?

$$\mathbb{E}[\text{wage} | \text{IQ} = 50] = \beta_0 + \beta_1 \cdot 50$$

$$\beta_0 = \bar{y} - \beta_1 \cdot \bar{x}$$

$$\beta_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$$



## Alternative Expression of OLS: Weighted Averages

Let me show you one results before proceeding

$$\begin{aligned}\beta_1 &= \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2} = \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} - \frac{\sum(x_i - \bar{x})\bar{y}}{\sum(x_i - \bar{x})^2} \\&= \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} - \frac{\bar{y} \cdot \sum(x_i - \bar{x})}{\sum(x_i - \bar{x})^2} \\&= \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} - \frac{\bar{y} \cdot N \cdot \frac{1}{N} \sum(x_i - \bar{x})}{\sum(x_i - \bar{x})^2} \\&= \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} - \frac{\bar{y} \cdot N \cdot \left[ \frac{1}{N} \sum x_i - \frac{1}{N} \sum \bar{x} \right]}{\sum(x_i - \bar{x})^2} \\&= \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} - \frac{\bar{y} \cdot N \cdot \left[ \bar{x} - \frac{1}{N} \cdot N \cdot \bar{x} \right]}{\sum(x_i - \bar{x})^2} \\&= \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2}\end{aligned}$$

$$\begin{aligned}
\beta_0 + \beta_1 \cdot 50 &= (\bar{y} - \beta_1 \cdot \bar{x}) + \beta_1 \cdot 50 \\
&= \bar{y} + \beta_1(50 - \bar{x}) \\
&= \bar{y} + \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2} \cdot (50 - \bar{x}) \\
&= \frac{1}{N} \sum y_i + \frac{\sum(x_i - \bar{x})y_i}{\sum(x_i - \bar{x})^2} \cdot (50 - \bar{x}) \\
&= \sum \frac{1}{N} \cdot y_i + \sum \frac{(50 - \bar{x}) \cdot (x_i - \bar{x})}{\sum(x_i - \bar{x})^2} y_i \\
&= \sum \left[ \frac{1}{N} + \frac{(50 - \bar{x}) \cdot (x_i - \bar{x})}{\sum(x_i - \bar{x})^2} \right] y_i \\
&= \sum w_i \cdot y_i
\end{aligned}$$

## More on Linear Regression

## Linear Regression: Prediction

Now, we know the underlying mechanism behind how we calculate the conditional mean. We turn to a more convenient way to calculate our conditional mean function and the prediction.

Suppose that the model that you run is given by

$$y = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \cdots + \beta_k \cdot x_k + \epsilon$$

The implied conditional mean is given by

$$\mathbb{E}[y|x] = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \cdots + \beta_k \cdot x_k$$

You can just substitute in your  $x$  values to this equation.

```
results<-lm(wage~married+IQ+black,data=wagedata)
results
```

```
##
```

```
## Call:
```

```
## lm(formula = wage ~ married + IQ + black, data = wagedata)
```

```
##
```

```
## Coefficients:
```

## (Intercept)	married	IQ	black
## 71.734	177.020	7.339	-118.031

$$\begin{aligned}\mathbb{E}[\text{wage}|\text{married},\text{black},\text{IQ}] &= 71.734355 + 177.020344 \cdot \text{married} \\ &\quad + 7.338611 \cdot \text{IQ} - 118.030901 \cdot \text{black}\end{aligned}$$

**Example:** What is our prediction for non-married, black workers with an IQ of 120?

$$\begin{aligned}\mathbb{E}[\text{wage} \mid \text{married}, \text{black}, \text{IQ}] \\ &= 71.734355 + 177.020344 \cdot 0 + 7.338611 \cdot 120 - 118.030901 \cdot 1 \\ &= 834.3367\end{aligned}$$

## Linear Regression: Partial Effects

Remember that the second use of our conditional mean function is to figure out what the partial effects of a variable is

$$\mathbb{E}[\text{wage}|\text{IQ} = x_1] - \mathbb{E}[\text{wage}|\text{IQ} = x_0]$$

**Examples:**

$$\begin{aligned}\mathbb{E}[\text{wage}|\text{IQ} = 51] - \mathbb{E}[\text{wage}|\text{IQ} = 50] \\&= (\beta_0 + \beta_1 \cdot 51) - (\beta_0 + \beta_1 \cdot 50) \\&= \beta_1\end{aligned}$$

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$$\begin{aligned}\mathbb{E}[\text{wage}|\text{IQ} = 52] - \mathbb{E}[\text{wage}|\text{IQ} = 51] \\&= (\beta_0 + \beta_1 \cdot 52) - (\beta_0 + \beta_1 \cdot 51) \\&= \beta_1\end{aligned}$$



## Partial Effects: More General Form

$$\mathbb{E}[y|x_1, x_2, x_3 \dots, x_k] = m(x) = m(x_1, x_2, \dots, x_k)$$

## Partial Effects:

$$\frac{\partial}{\partial x_1} \mathbb{E}[y|x_1, x_2, x_3 \dots, x_k] = \frac{\partial}{\partial x_1} m(x)$$

## Interpretation:

When  $x_1$  increases by one unit, by how much will  $y$  (or the averages of  $y$ ) will increase?

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#### 1. Linear Models

$$\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \dots + \beta_k \cdot x_k$$

### Partial Effects:

$$\frac{\partial}{\partial x_k} [\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \dots + \beta_k \cdot x_k] = \beta_k$$

## Example

$$\mathbb{E}[\text{wage}|\text{married},\text{black},\text{IQ}]$$

$$= 71.734355 + 177.020344 \cdot \text{married} + 7.338611 \cdot \text{IQ} - 118.030901 \cdot \text{black}$$

1. One-unit increase in IQ will lead to

## Example

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$$\begin{aligned} \frac{\partial}{\partial \text{IQ}} [71.734355 + 177.020344 \cdot \text{married} + 7.338611 \cdot \text{IQ} - 118.030901 \cdot \text{black}] \\ = 7.338611 \end{aligned}$$

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2. One unit increase in marital status (change from 0 to 1): (it is not really derivative, but for consistency)

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$$\begin{aligned}\frac{\partial}{\partial \text{married}} [71.734355 + 177.020344 \cdot 1 + 7.338611 \cdot \text{IQ} - 118.030901 \cdot \text{black}] \\ = 177.020344\end{aligned}$$

Again, it does not depend on any other things such as  $x$ . It is a constant!

# Why do we still use OLS?

We know that the linear regression or the OLS approach gives us

1. A weird form of weighted averages
2. A constant partial effect

**Question:** Why is it still useful?!

**Answer:** It is the best linear approximation!

$$\min \mathbb{E} \left[ (m(x) - x'\beta)^2 \right] \implies \beta = \mathbb{E}[xx']^{-1} \mathbb{E}[x'y]$$



## Improvements of OLS

The fact that it is the best linear approximation does NOT mean that we can further improve the approximation using the linear form of nonlinear equations

### 1. Interaction Terms

- (a) Interaction terms between the same variables: Polynomial terms (partial effects depend on itself)
- (b) Interaction terms between two different variables: Partial effects depend on the other variable

## 1. Quadratic Models:

$$\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_1^2 + \cdots + \beta_k \cdot x_k$$

Partial Effects:

$$\frac{\partial}{\partial x_1} [\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_1^2 + \cdots + \beta_k \cdot x_k] = \beta_1 + 2 \cdot \beta_2 \cdot x_1$$

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## 2. Interaction Models

$$\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \beta_3 \cdot x_1 \cdot x_2 + \dots$$

Partial Effects:

$$\frac{\partial}{\partial x_1} [\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \beta_3 \cdot x_1 \cdot x_2 + \dots] = \beta_1 + \beta_3 \cdot x_2$$

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Partial Effects:

$$\frac{\partial}{\partial x_1} [\beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \beta_3 \cdot x_1 \cdot x_2 + \dots] = \beta_1 + \beta_3 \cdot x_2$$

## 3. Infinite number of possible models

## Model Selection

Two questions naturally follow:

1. Can I test the model specification?
2. Which model is preferred? Model selection criteria.

Symbol	Usage
~	Separates response variables on the left from the explanatory variables on the right. For example, a prediction of $y$ from $x$ , $z$ , and $w$ would be coded $y \sim x + z + w$ .
+	Separates predictor variables.
:	Denotes an interaction between predictor variables. A prediction of $y$ from $x$ , $z$ , and the interaction between $x$ and $z$ would be coded $y \sim x + z + x:z$ .
*	A shortcut for denoting all possible interactions. The code $y \sim x * z * w$ expands to $y \sim x + z + w + x:z + x:w + z:w + x:z:w$ .
^	Denotes interactions up to a specified degree. The code $y \sim (x + z + w)^2$ expands to $y \sim x + z + w + x:z + x:w + z:w$ .
.	A placeholder for all other variables in the data frame except the dependent variable. For example, if a data frame contained the variables $x$ , $y$ , $z$ , and $w$ , then the code $y \sim .$ would expand to $y \sim x + z + w$ .
-	A minus sign removes a variable from the equation. For example, $y \sim (x + z + w)^2 - x:w$ expands to $y \sim x + z + w + x:z + z:w$ .
-1	Suppresses the intercept. For example, the formula $y \sim x - 1$ fits a regression of $y$ on $x$ , and forces the line through the origin at $x=0$ .