# Regression

CISC 7026: Introduction to Deep Learning

University of Macau

#### ML

Many problems in ML can be reduced to **regression** or **classification** 

**Regression** asks how many

**Regression** asks how many

• How much money will I make?

**Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?

**Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

**Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

**Classification** asks which one

#### **Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

#### **Classification** asks which one

• Is this a dog or muffin?

#### **Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

#### **Classification** asks which one

- Is this a dog or muffin?
- Will it rain tomorrow? Yes or no?

#### **Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

#### Classification asks which one

- Is this a dog or muffin?
- Will it rain tomorrow? Yes or no?
- What color is this object?

#### **Regression** asks how many

- How much money will I make?
- How much rain will there be tomorrow?
- How far away is this object?

#### Classification asks which one

- Is this a dog or muffin?
- Will it rain tomorrow? Yes or no?
- What color is this object?

Let us start with regression

1. Define an example problem

- 1. Define an example problem
- 2. Define our machine learning model f

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

**Task:** Given your education, predict your life expectancy

**Task:** Given your education, predict your life expectancy

X: Years in school

**Task:** Given your education, predict your life expectancy

X: Years in school

Y: Age of death

**Task:** Given your education, predict your life expectancy

X : Years in school

Y: Age of death

**Approach:** Learn the parameters  $\theta$  such that

$$f(x,\theta) = y$$

**Task:** Given your education, predict your life expectancy

X: Years in school

Y: Age of death

**Approach:** Learn the parameters  $\theta$  such that

$$f(x,\theta) = y$$

**Goal:** Given someone's education, you can predict how long they will live

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

Soon, f will be a deep neural network

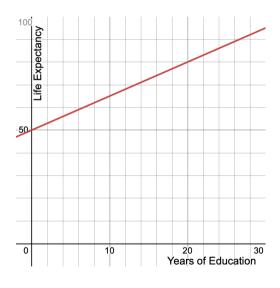
Soon, f will be a deep neural network

For now, it is easier if we make f a **linear function** 

Soon, f will be a deep neural network

For now, it is easier if we make f a **linear function** 

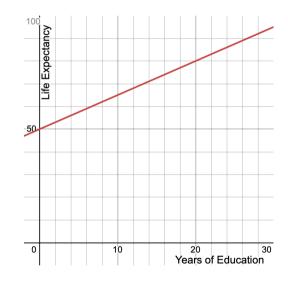
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



Soon, f will be a deep neural network

For now, it is easier if we make f a **linear function** 

$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



Now, we need to find the parameters  $m{\theta} = \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}$  that makes  $f(x, m{\theta}) = y$ 

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

Now, we need to find the parameters 
$$\pmb{\theta} = \begin{bmatrix} \theta_2 \\ \theta_1 \end{bmatrix}$$
 that make  $f(x,\pmb{\theta}) = y$ 

Now, we need to find the parameters  $\pmb{\theta} = \begin{vmatrix} \theta_2 \\ \theta_1 \end{vmatrix}$  that make  $f(x, \pmb{\theta}) = y$ 

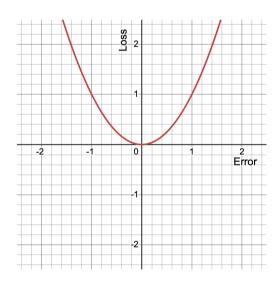
**Question:** How do we find  $\theta$ ? (Hint: We want  $f(x, \theta) = y$ )

Now, we need to find the parameters  $\pmb{\theta} = \begin{bmatrix} \theta_2 \\ \theta_1 \end{bmatrix}$  that make  $f(x,\pmb{\theta}) = y$ 

**Question:** How do we find  $\theta$ ? (Hint: We want  $f(x, \theta) = y$ )

**Answer:** We will minimize the **loss** (error) between  $f(x, \theta)$  and y

E.g., 
$$\min_{\pmb{\theta}} \left( f(x, \pmb{\theta}) - y \right)^2 = 0$$



We compute the loss using the **loss function**  $\mathcal{L}$ 

We compute the loss using the **loss function**  $\mathcal{L}$ 

$$\mathcal{L}(x, y, \boldsymbol{\theta})$$

We compute the loss using the **loss function**  $\mathcal{L}$ 

$$\mathcal{L}(x, y, \boldsymbol{\theta})$$

The loss function tells us how close f(x) is to y

We compute the loss using the **loss function**  $\mathcal{L}$ 

$$\mathcal{L}(x, y, \boldsymbol{\theta})$$

The loss function tells us how close f(x) is to y

By **minimizing** the loss function, we make f(x) = y

We compute the loss using the **loss function**  $\mathcal{L}$ 

$$\mathcal{L}(x, y, \boldsymbol{\theta})$$

The loss function tells us how close f(x) is to y

By **minimizing** the loss function, we make f(x) = y

There are many possible loss functions, but for now we will use the **mean-square error** 

We compute the loss using the **loss function**  $\mathcal{L}$ 

$$\mathcal{L}(x, y, \boldsymbol{\theta})$$

The loss function tells us how close f(x) is to y

By **minimizing** the loss function, we make f(x) = y

There are many possible loss functions, but for now we will use the **mean-square error** 

$$\operatorname{error}(y, \hat{y}) = (y - \hat{y})^2$$

Let's derive the error function

Let's derive the error function

$$f(x, \boldsymbol{\theta}) = y$$

f(x) should predict y

Let's derive the error function

$$f(x, \boldsymbol{\theta}) = y$$

$$f(x, \boldsymbol{\theta}) - y = 0$$

f(x) should predict y

Move y to LHS

Let's derive the error function

$$f(x, \boldsymbol{\theta}) = y$$

$$f(x, \boldsymbol{\theta}) - y = 0$$

$$(f(x, \boldsymbol{\theta}) - y)^2 = 0$$

f(x) should predict y

Move y to LHS

Square for minimization

Let's derive the error function

$$f(x, \boldsymbol{\theta}) = y$$

$$f(x, \boldsymbol{\theta}) - y = 0$$

$$\left(f(x,\boldsymbol{\theta}) - y\right)^2 = 0$$

$$\operatorname{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

f(x) should predict y

Move y to LHS

Square for minimization

Let's derive the error function

$$f(x, \boldsymbol{\theta}) = y$$

$$f(x, \boldsymbol{\theta}) - y = 0$$

$$\left(f(x,\boldsymbol{\theta}) - y\right)^2 = 0$$

$$\operatorname{error}(f(x, \boldsymbol{\theta}), y) = (f(x, \boldsymbol{\theta}) - y)^2$$

f(x) should predict y

Move y to LHS

Square for minimization

We can write the loss function for a single datapoint  $x_i, y_i$  as

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

We can write the loss function for a single datapoint  $x_i, y_i$  as

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

By minimizing  $\mathcal{L}$ , we can find the parameters  $\boldsymbol{\theta}$ 

We can write the loss function for a single datapoint  $x_i, y_i$  as

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

By minimizing  $\mathcal{L}$ , we can find the parameters  $\theta$ 

$$\min_{\pmb{\theta}} \mathcal{L}(x_i, y_i, \pmb{\theta}) = \min_{\pmb{\theta}} \operatorname{error}(f(x_i, \pmb{\theta}), y_i) = \min_{\pmb{\theta}} \left(f(x_i, \pmb{\theta}) - y_i\right)^2$$

We can write the loss function for a single datapoint  $x_i, y_i$  as

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

By minimizing  $\mathcal{L}$ , we can find the parameters  $\theta$ 

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

**Question:** Any issues with  $\mathcal{L}$ ?

We can write the loss function for a single datapoint  $x_i, y_i$  as

$$\mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

By minimizing  $\mathcal{L}$ , we can find the parameters  $\boldsymbol{\theta}$ 

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

**Question:** Any issues with  $\mathcal{L}$ ?

**Answer:** We only consider a single datapoint! We want to learn  $\boldsymbol{\theta}$  for the entire dataset

For a single  $x_i, y_i$ :

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

For a single  $x_i, y_i$ :

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

For the entire dataset:

$$\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x}_i, \boldsymbol{y}_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \operatorname{error}(f(\boldsymbol{x}_i, \boldsymbol{\theta}), \boldsymbol{y}_i) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \left(f(\boldsymbol{x}_i, \boldsymbol{\theta}) - \boldsymbol{y}_i\right)^2$$

For a single  $x_i, y_i$ :

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

For the entire dataset:

$$\min_{\pmb{\theta}} \mathcal{L}(x_i, y_i, \pmb{\theta}) = \min_{\pmb{\theta}} \sum_{i=1}^n \operatorname{error}(f(x_i, \pmb{\theta}), y_i) = \min_{\pmb{\theta}} \sum_{i=1}^n \left(f(x_i, \pmb{\theta}) - y_i\right)^2$$

Minimizing this loss function will give us the optimal parameters!

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

Lecture 1: Introduction

**Question:** How do we minimize:

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

**Question:** How do we minimize:

$$\min_{\boldsymbol{\theta}} \mathcal{L}(x_i, y_i, \boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \operatorname{error}(f(x_i, \boldsymbol{\theta}), y_i) = \min_{\boldsymbol{\theta}} \sum_{i=1}^n \left(f(x_i, \boldsymbol{\theta}) - y_i\right)^2$$

**Answer:** For now, magic! We need more knowledge before we can derive this.

First, construct a **design matrix**X containing input data x and a constant 1 for the bias. Also construct a y vector!

And remember the parameters heta

$$oldsymbol{X} = egin{bmatrix} x_1 & 1 \ x_2 & 1 \ dots & dots \ x_n & 1 \end{bmatrix}, oldsymbol{y} = egin{bmatrix} y_1 \ y_2 \ dots \ y_n \end{bmatrix}$$

$$oldsymbol{ heta} = egin{bmatrix} heta_1 \ heta_0 \end{bmatrix},$$

$$oldsymbol{ heta} = \left( oldsymbol{X}^ op oldsymbol{X} 
ight)^{-1} oldsymbol{X}^ op oldsymbol{y}$$

The solution to linear regression

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

Lecture 1: Introduction

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

Back to the example...

Back to the example...

**Task:** Given your education, predict your life expectancy

Back to the example...

**Task:** Given your education, predict your life expectancy

X: Years in school

Back to the example...

Task: Given your education, predict your life expectancy

X : Years in school

Y: Age of death

Back to the example...

**Task:** Given your education, predict your life expectancy

X : Years in school

Y: Age of death

**Goal:** Learn the parameters  $\theta$  such that

$$f(x, \boldsymbol{\theta}) = y$$

Back to the example...

**Task:** Given your education, predict your life expectancy

X: Years in school

Y: Age of death

**Goal:** Learn the parameters  $\theta$  such that

$$f(x, \boldsymbol{\theta}) = y$$

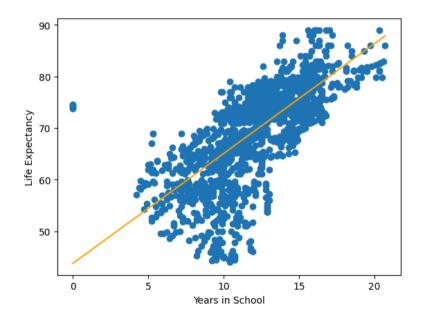
You will be doing this in your first assignment!

Back to the example...

**Task:** Given your education, predict your life expectancy

Back to the example...

**Task:** Given your education, predict your life expectancy



Tips for assignment 1

```
Tips for assignment 1

def f(theta, design):
    # Linear function
    return theta @ design
```

Lecture 1: Introduction

# Tips for assignment 1 def f(theta, design): # Linear function return theta @ design

Not all matrices can be inverted! Ensure the matrices are square and the condition number is low

```
A.shape
cond = jax.numpy.linalg.cond(A)
```

1. Define an example problem

- 1. Define an example problem
- 2. Define our machine learning model f

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f

- 1. Define an example problem
- 2. Define our machine learning model f
- 3. Define a loss function  $\mathcal{L}$
- 4. Use  $\mathcal{L}$  to learn the parameters  $\theta$  of f
- 5. Investigate the results

# Relax

• Outliers

- Outliers
- Can we go beyond linear?

- Outliers
- Can we go beyond linear?
- Overfitting

- Outliers
- Can we go beyond linear?
- Overfitting
- Test and train splits

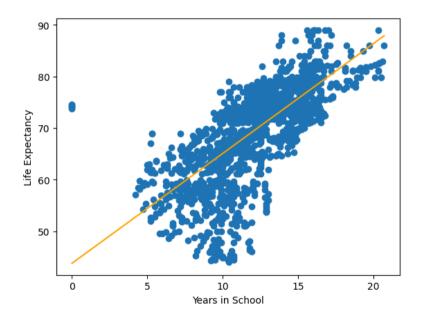
- Outliers
- Can we go beyond linear?
- Overfitting
- Test and train splits

Back to the example...

**Task:** Given your education, predict your life expectancy

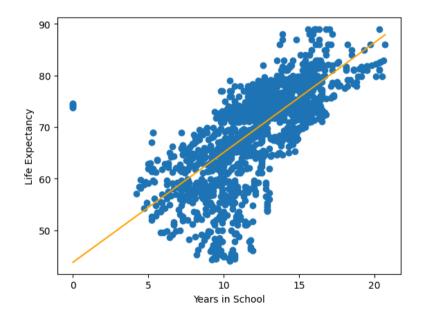
Back to the example...

**Task:** Given your education, predict your life expectancy



Back to the example...

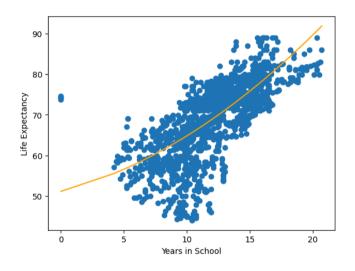
**Task:** Given your education, predict your life expectancy



Could we do better than a linear function f?

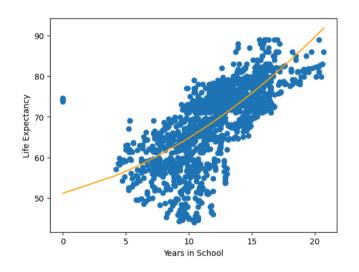
Could we do better than a linear function f?

#### Could we do better than a linear function f?



What if we used a polynomial instead?

#### Could we do better than a linear function f?



What if we used a polynomial instead?

$$f(x) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 + x^1 + \theta_0$$

$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 + x^1 + \theta_0$$

$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix}\right) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 + x^1 + \theta_0$$

$$f(x, \pmb{\theta}) = [\theta_n \;\; \theta_{n-1} \;\; \dots \;\; \theta_1 \;\; b] \begin{bmatrix} x^n \\ x^{n-1} \\ \vdots \\ x^1 \\ 1 \end{bmatrix}$$

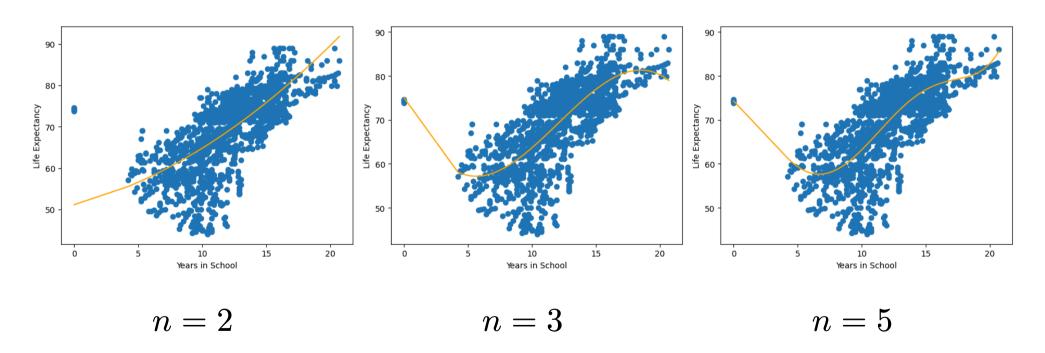
$$f(x, \theta) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 x^1 + \theta_0$$

$$f(x, \theta) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 x^1 + \theta_0$$

How do we choose n? Let us try different n

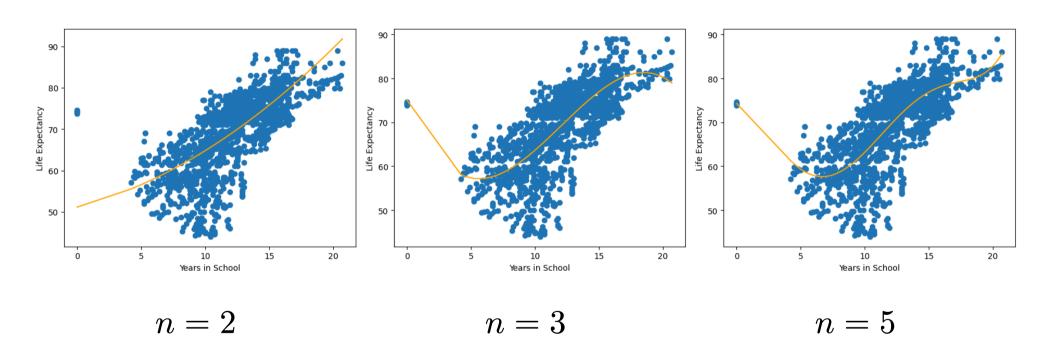
$$f(x, \theta) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 x^1 + \theta_0$$

How do we choose n? Let us try different n



$$f(x, \theta) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 + x^1 + \theta_0$$

$$f(x, \theta) = \theta_n x^n + \theta_{n-1} x^{n-1}, ..., \theta_1 + x^1 + \theta_0$$



**Question:** Which *n* should we pick? Why?

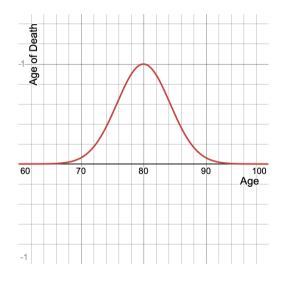
Data is inherently noisy

Data is inherently noisy

The world is governed by random processes

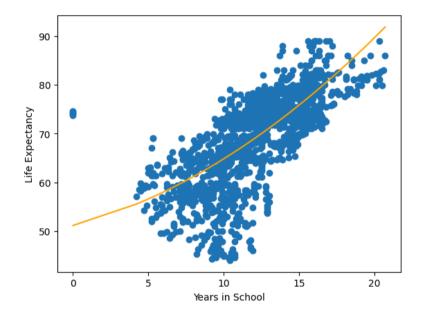
Data is inherently noisy

The world is governed by random processes

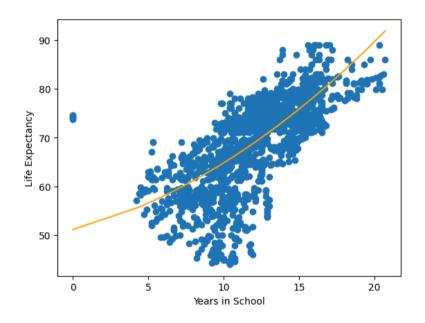


,

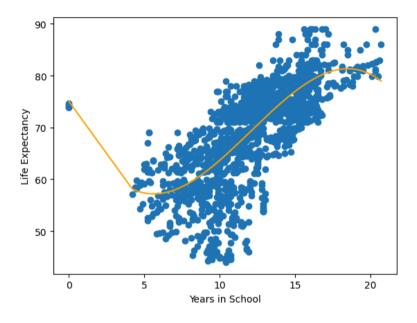
#### This is just an estimate

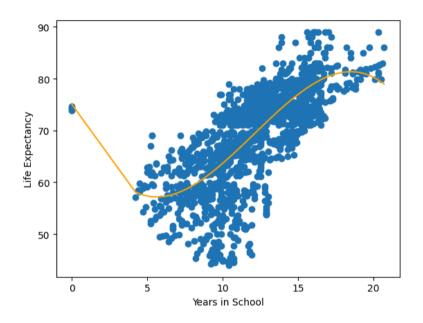


This is just an estimate

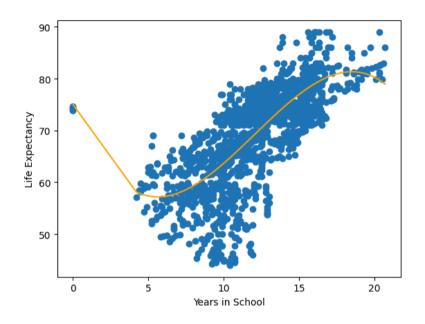


Going to school for 20 years will not save you from a hungry bear





When we fit to noise instead of the trend, we call it **overfitting** 



When we fit to noise instead of the trend, we call it **overfitting** Overfitting is bad because our predictions will be inaccurate

How can we measure overfitting?

How can we measure overfitting?

Learn our parameters from one subset of data: training dataset

How can we measure overfitting?

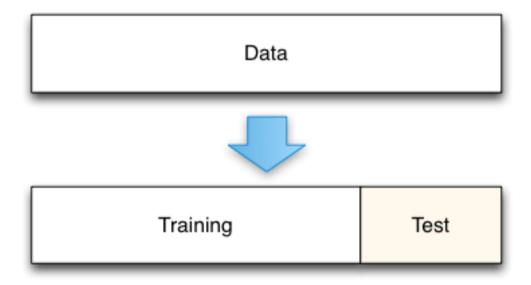
Learn our parameters from one subset of data: training dataset

Test our model on a different subset of data: **testing dataset** 

How can we measure overfitting?

Learn our parameters from one subset of data: training dataset

Test our model on a different subset of data: **testing dataset** 



**Question:** How do we choose the training and testing datasets?

**Question:** How do we choose the training and testing datasets?

$$\mathcal{D}_{\text{train}} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\mathcal{D}_{ ext{test}} = egin{bmatrix} x_4 \\ x_5 \end{bmatrix}$$

$$\mathcal{D}_{ ext{train}} = egin{bmatrix} x_4 \ x_1 \ x_3 \end{bmatrix}$$

$$\mathcal{D}_{ ext{test}} = egin{bmatrix} x_2 \ x_5 \end{bmatrix}$$

**Answer:** Always shuffle the data

**Question:** How do we choose the training and testing datasets?

$$egin{align} \mathcal{D}_{ ext{train}} &= egin{bmatrix} x_1 \ x_2 \ x_3 \end{bmatrix} & \mathcal{D}_{ ext{train}} &= egin{bmatrix} x_4 \ x_1 \ x_3 \end{bmatrix} \ \mathcal{D}_{ ext{test}} &= egin{bmatrix} x_2 \ x_3 \end{bmatrix} & \mathcal{D}_{ ext{test}} &= egin{bmatrix} x_2 \ x_3 \end{bmatrix} \end{aligned}$$

**Answer:** Always shuffle the data

ML relies on the **Independent and Identically Distributed (IID)** assumption

- Overfitting
- Outliers
- Regularization
- Etc