Regression

CISC 7026: Introduction to Deep Learning

University of Macau

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Probably the oldest method for machine learning (Gauss and Legendre)

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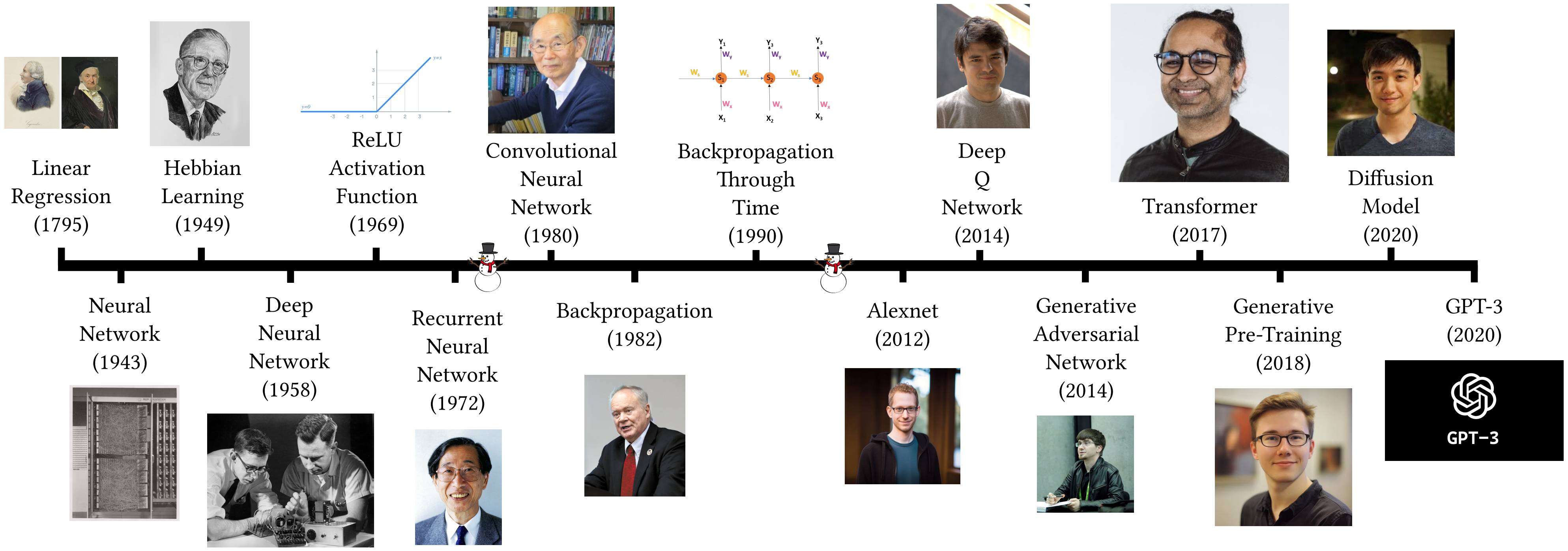

Linear Regression (1795)

Neural Network (1943)

Hebbian Learning (1949)

Deep Neural Network (1958)

ReLU Activation Function (1969)

Recurrent Neural Network (1972)

Convolutional Neural Network (1980)

Backpropagation (1982)

Backpropagation Through Time (1990)

Alexnet (2012)

Deep Q Network (2014)

Generative Adversarial Network (2014)

Transformer (2017)

Generative Pre-Training (2018)

Diffusion Model (2020)

GPT-3 (2020)

ML

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

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Let us start with regression

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Linear Regression

The World Health Organization (WHO) has collected data on life expectancy

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World Health Organization
ions
World Health Organization
Health Topics
Countries
Newsroom
THE GLOBAL HEALTH OBSERVATORY
Explore a world of health data
GHO Home
Indicators
Countries
Data API
M
Data / GHO / Themes / Global Health Estimates: Life expectancy and lead
GHE: Life expectancy and healthy life expectancy

Available for free at https://www.who.int/data/gho/data/themes/mortality-and-global-health-estimates/ghe-life-expectancy-and-healthy-life-expectancy

Linear Regression

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For each person, they recorded:

Linear Regression

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For each person, they recorded:

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We can use this data to make future predictions

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Linear Regression

Since everyone here is very educated, we will focus on how education affects life expectancy

There are studies showing a causal effect on education on health

- *The causal effects of education on health outcomes in the UK Biobank.* Davies et al. *Nature Human Behaviour.*
- By staying in school, you are likely to live longer

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Task: Given your education, predict your life expectancy

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Approach: Learn the parameters θ such that

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

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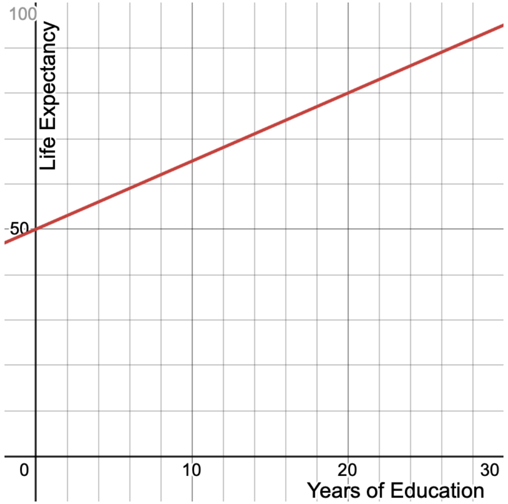
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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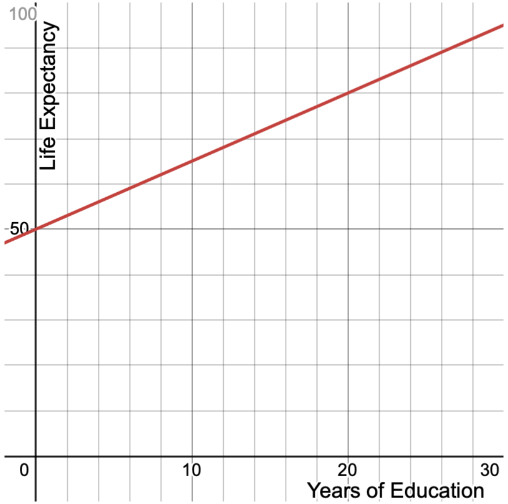

Now, we need to find the parameters $\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}$ that makes $f(x, \boldsymbol{\theta}) = y$

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

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

$$x \in X, y \in Y$$

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We compute the loss using the **loss function** $\mathcal{L} : X \times Y \times \Theta \mapsto \mathbb{R}$

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

Linear Regression

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Square for minimization

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

Linear Regression

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

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

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For the entire dataset:

$$\boldsymbol{x} = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}^\top, \boldsymbol{y} = \begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix}^\top$$

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Minimizing this loss function will give us the optimal parameters!

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Question: How do we minimize:

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

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$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}$$

Linear Regression

We add the column of ones so that we can multiply $\boldsymbol{X}_D^\top$ with $\boldsymbol{\theta}$ to get a linear function $\theta_1 x + \theta_0$ evaluated at each data point

$$\boldsymbol{X}_D \boldsymbol{\theta} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix} = \begin{bmatrix} \theta_1 x_1 + \theta_0 \\ \theta_1 x_2 + \theta_0 \\ \vdots \\ \theta_1 x_n + \theta_0 \end{bmatrix}$$

Linear Regression

With our design matrix $\boldsymbol{X}_D$ and desired output $\boldsymbol{y}$,

$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}, \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

and our parameters $\boldsymbol{\theta}$,

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix},$$

$$\boldsymbol{\theta} = \left(\boldsymbol{X}_D^\top \boldsymbol{X}_D\right)^{-1} \boldsymbol{X}_D^\top \boldsymbol{y}$$

We can find the parameters that minimize $\mathcal{L}$

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Example

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$X \in \mathbb{R}_+$: Years in school

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You will be doing this in your first assignment!

Tips for assignment 1

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```
def f(theta, design):
  # Linear function
  return design @ theta
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Not all matrices can be inverted! Ensure the matrices are square and the condition number is low

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cond = jax.numpy.linalg.cond(A)
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Everything you need is in the lecture notes

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Relax

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Plot the datapoints $(x_1, y_1), (x_2, y_2), \ldots$

Plot the curve $f(x, \boldsymbol{\theta}) = \theta_1 x + \theta_0; \quad x \in [0, 25]$

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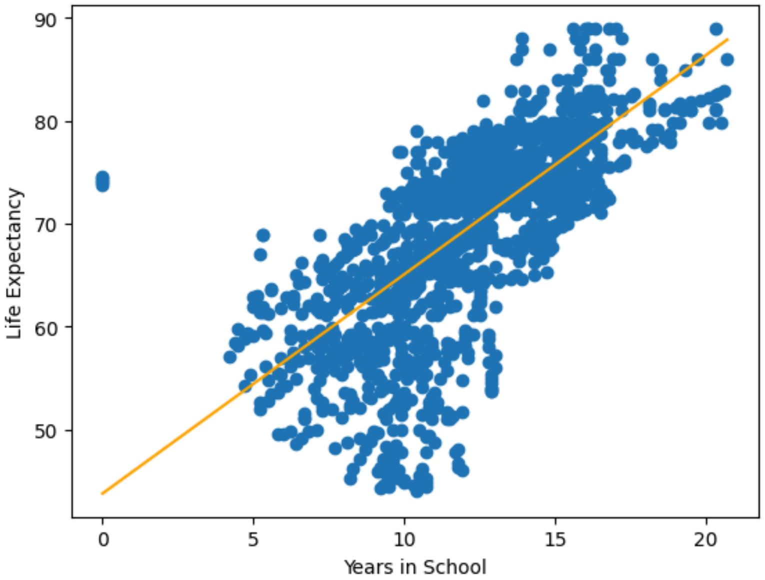

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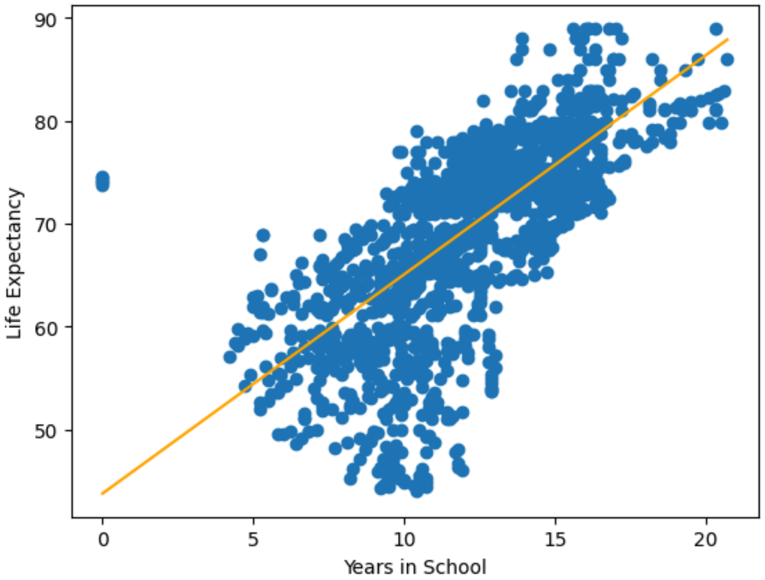
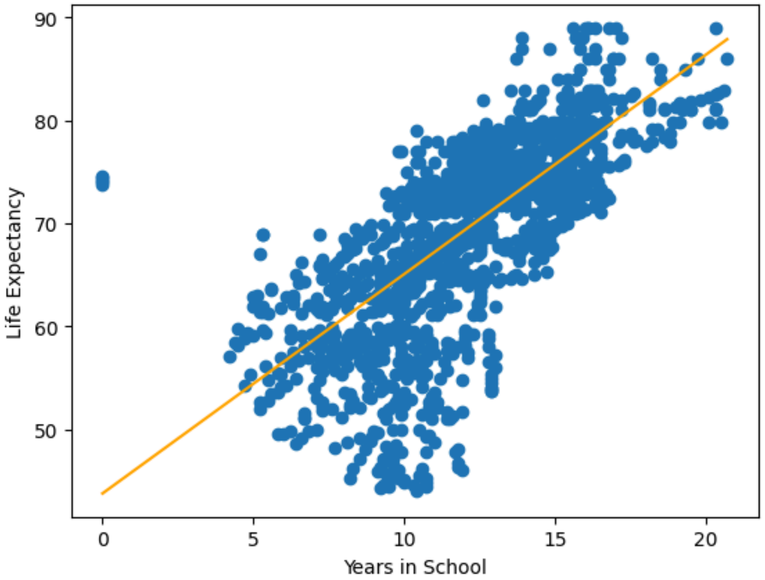
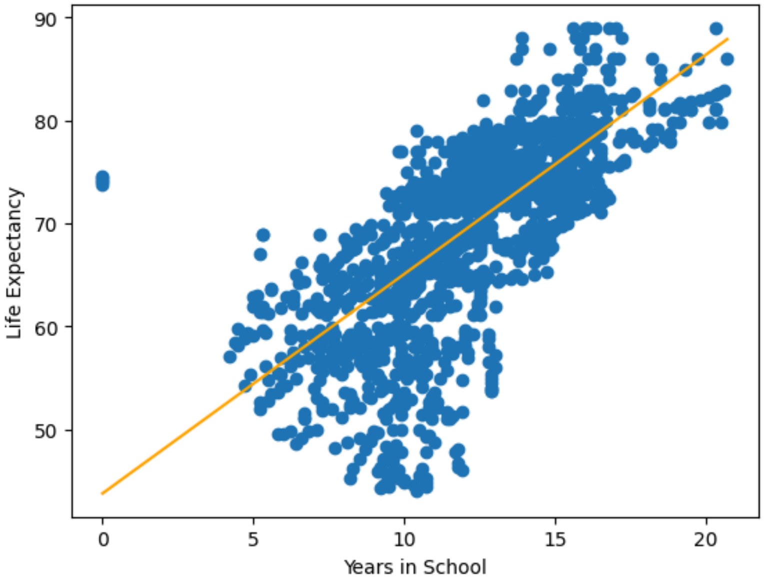




We figured out linear regression!



We figured out linear regression!

But can we do better?

1. Beyond linear functions

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2. Overfitting

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Does the data look linear?

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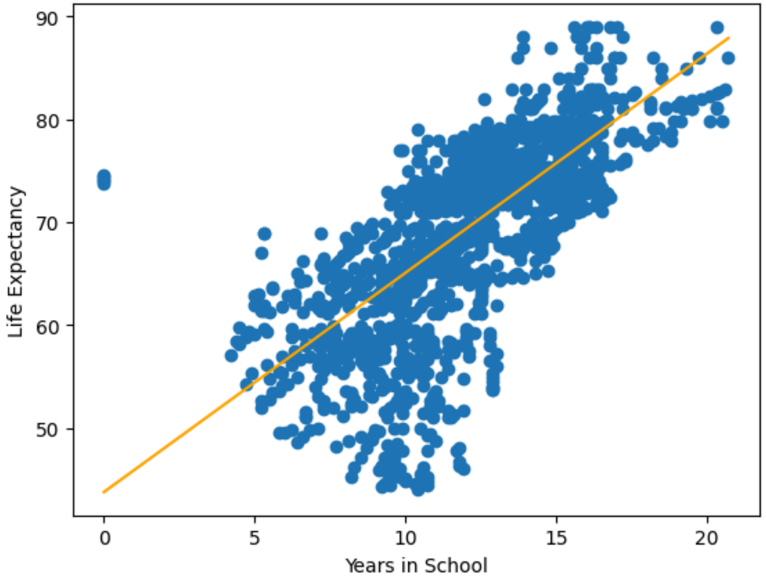

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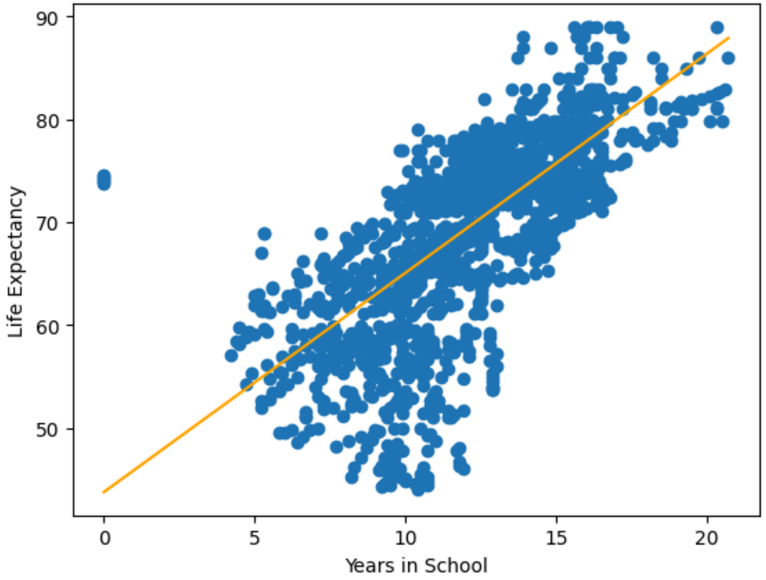

Or maybe more logarithmic?

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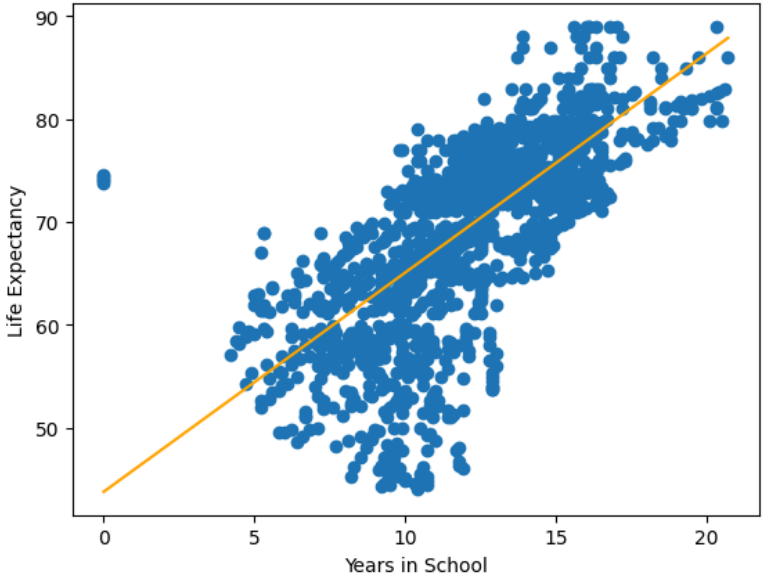

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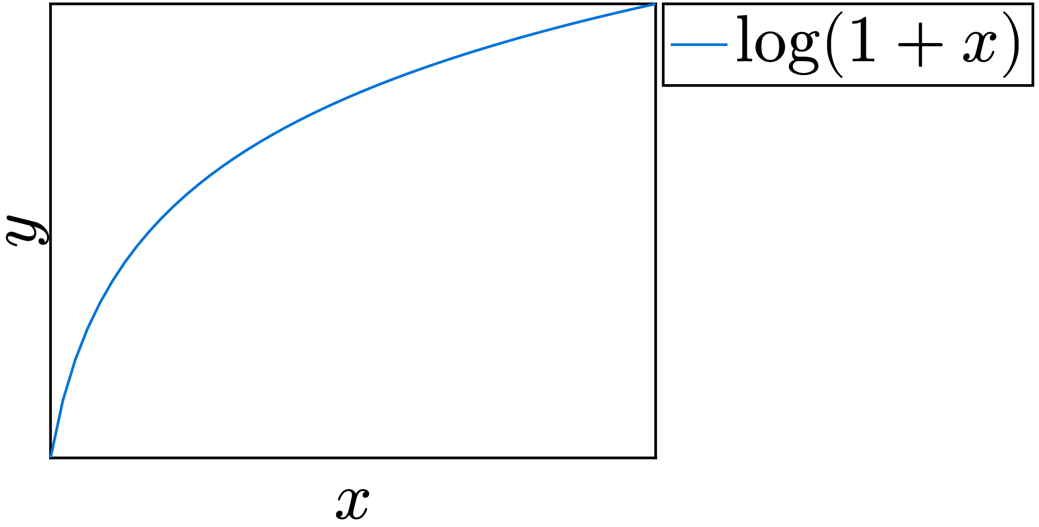

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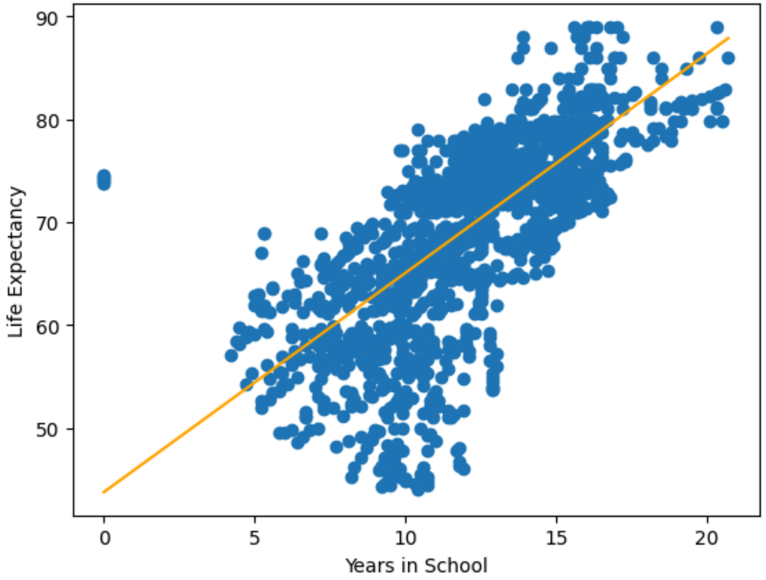

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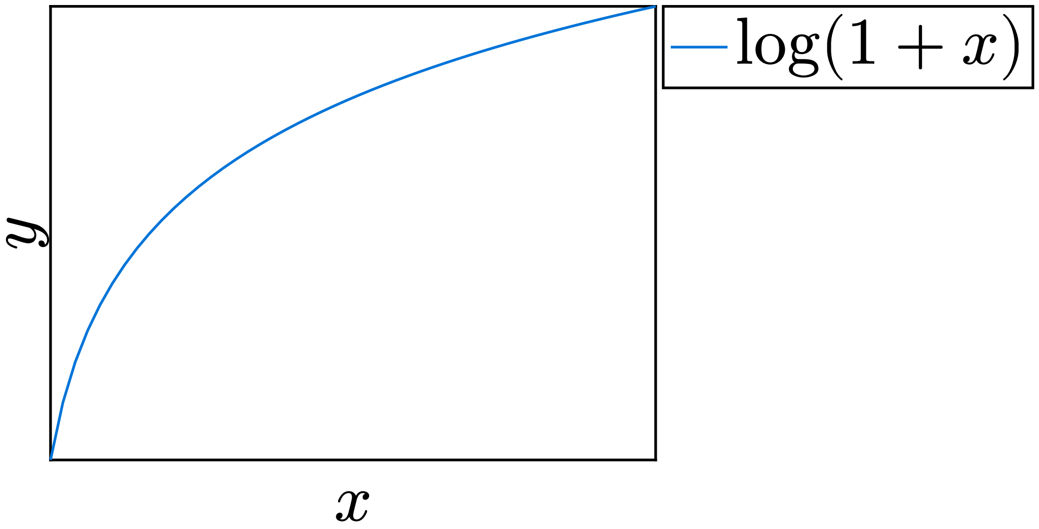

However, linear regression must be linear!

Question: What does it mean when we say linear regression is linear?

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Answer: The function $f(x, \theta)$ is a linear function of x

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$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} \log(1 + x_1) & 1 \\ \log(1 + x_2) & 1 \\ \vdots & \vdots \\ \log(1 + x_n) & 1 \end{bmatrix}$$

Now, f is a linear function of $\log(1 + x)$ – a nonlinear function of x!

New design matrix...

$$\boldsymbol{X}_D = \begin{bmatrix} \log(1 + x_1) & 1 \\ \log(1 + x_2) & 1 \\ \vdots & \vdots \\ \log(1 + x_n) & 1 \end{bmatrix}$$

New function...

$$f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 \log(1 + x) + \theta_0$$

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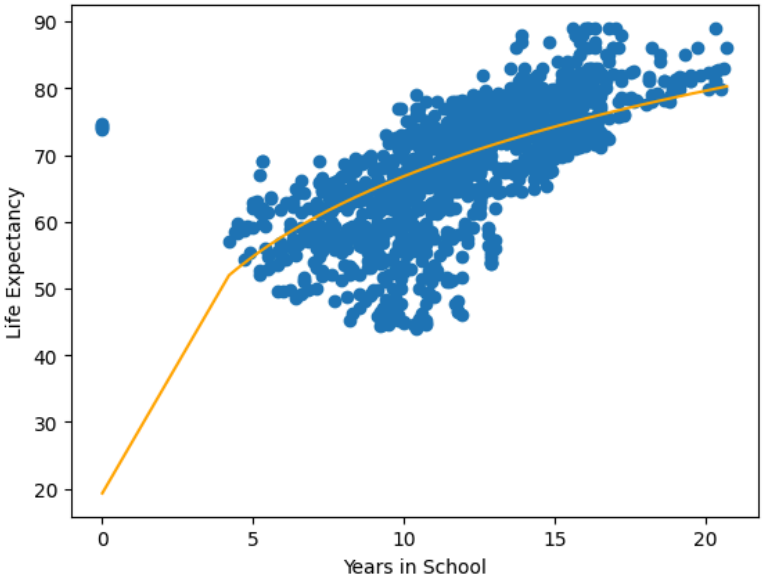
Same solution...

$$\boldsymbol{\theta} = \left(\boldsymbol{X}_D^\top \boldsymbol{X}_D\right)^{-1} \boldsymbol{X}_D^\top \boldsymbol{y}$$


90
80
70
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50
40
30
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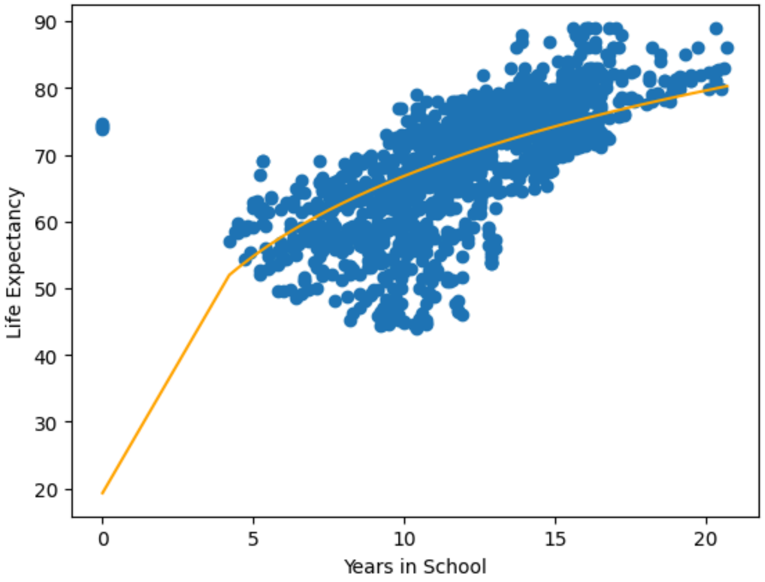
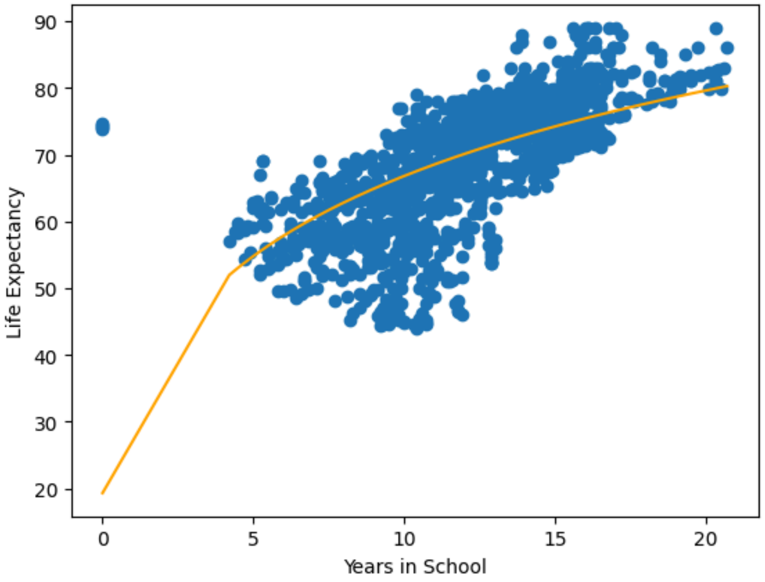
Life Expectancy
0
5
10
15
20
Years in School



Better, but still not perfect



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Can we do even better?

What about polynomials?

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Can we extend linear regression to polynomials?

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And add some new parameters...

$$\boldsymbol{\theta} = [\theta_1 \ \ \theta_0]^\top \Rightarrow \boldsymbol{\theta} = [\theta_n \ \ \theta_{n-1} \ \ \ldots \ \ \theta_1 \ \ \theta_0]^\top$$

$$\boldsymbol{X}_D \boldsymbol{\theta} = \begin{bmatrix} x_1^n & x_1^{n-1} & \dots & x_1 & 1 \\ x_2^n & x_2^{n-1} & \dots & x_2 & 1 \\ \vdots & \vdots & \ddots & & \\ x_n & x_n^{n-1} & \dots & x_n & 1 \end{bmatrix} \begin{bmatrix} \theta_n \\ \theta_{n-1} \\ \vdots \\ \theta_0 \end{bmatrix} = \begin{bmatrix} \theta_n x_1^n + \theta_{n-1} x_1^{n-1} + \dots + \theta_0 \\ \theta_n x_2 + \theta_{n-1} x_2^{n-1} + \dots + \theta_0 \\ \vdots \\ \theta_n x_n^n + \theta_{n-1} x_n^{n-1} + \dots + \theta_0 \end{bmatrix}$$

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Summary: By changing the input space, we can fit a polynomial to the data using a linear fit!

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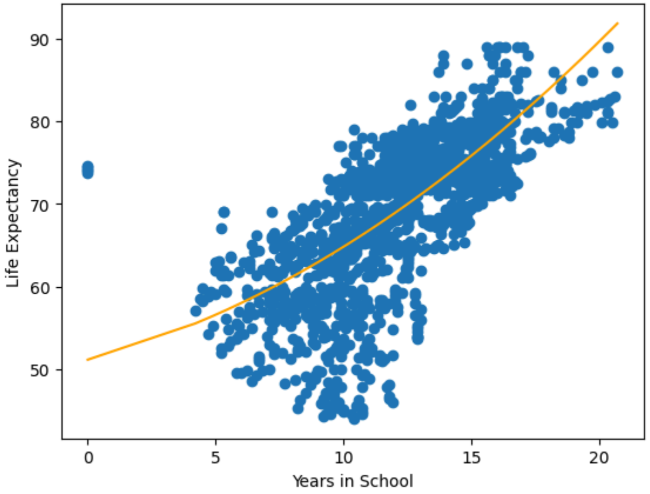
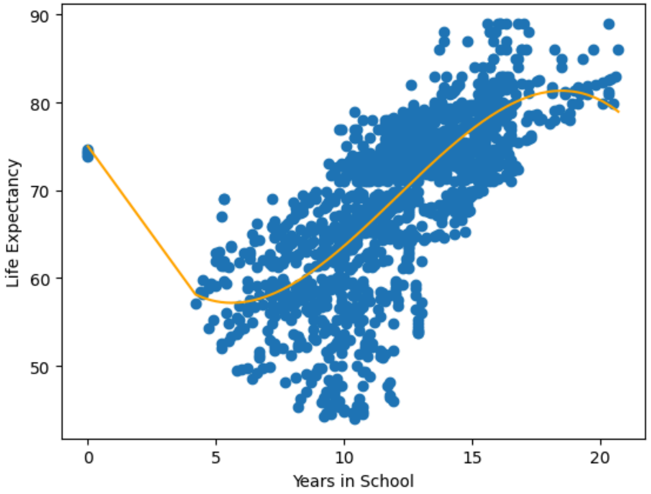


$n = 2$



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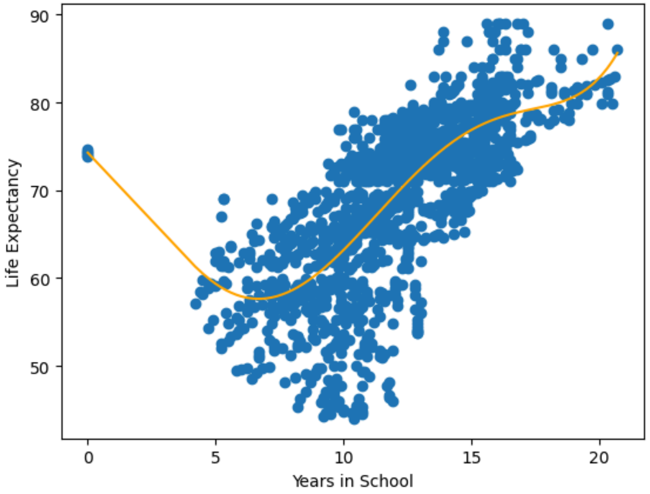

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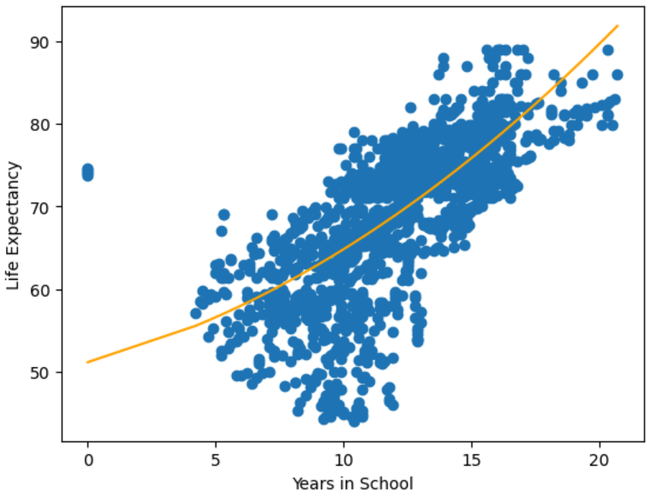

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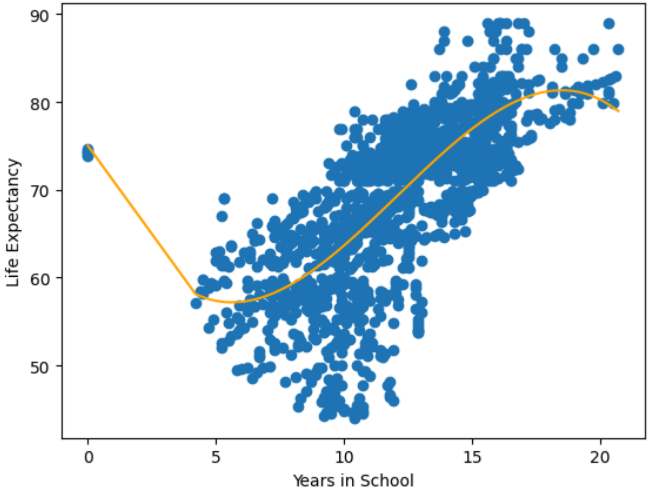

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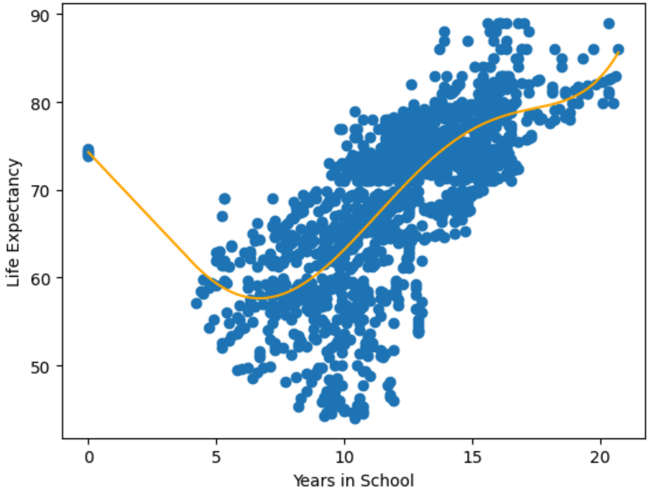
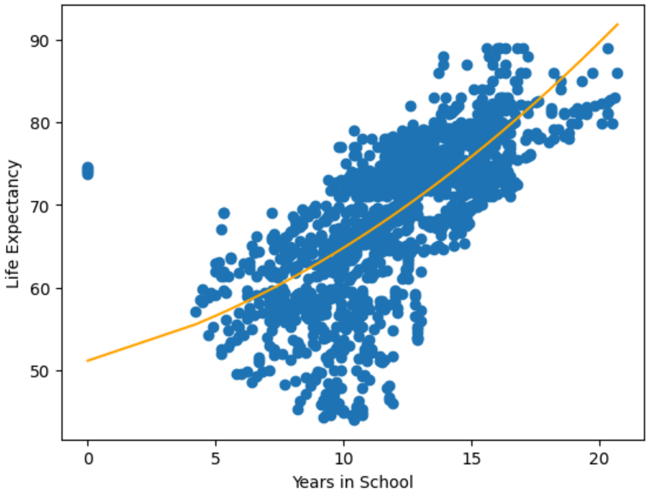


$$n = 5$$

Pick the n with the smallest loss

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



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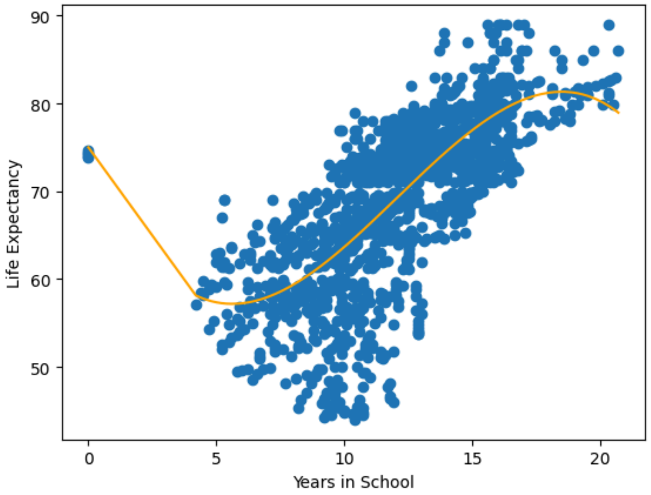

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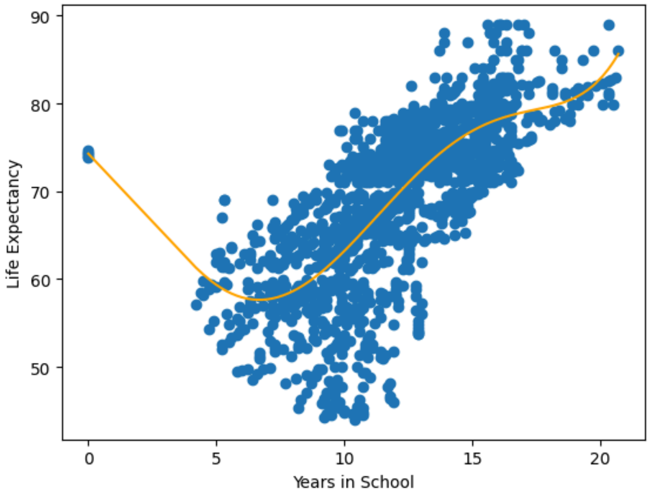

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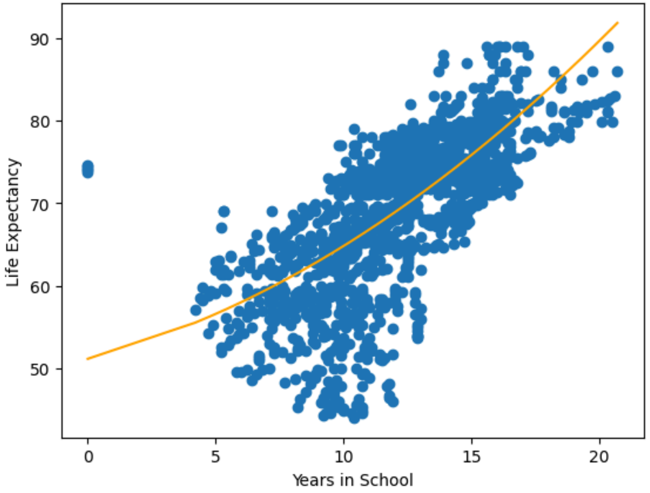
Question: Which n do you think has the smallest loss?



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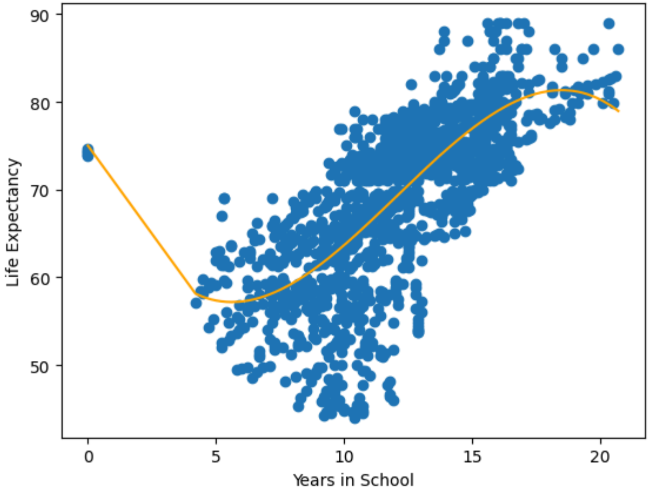

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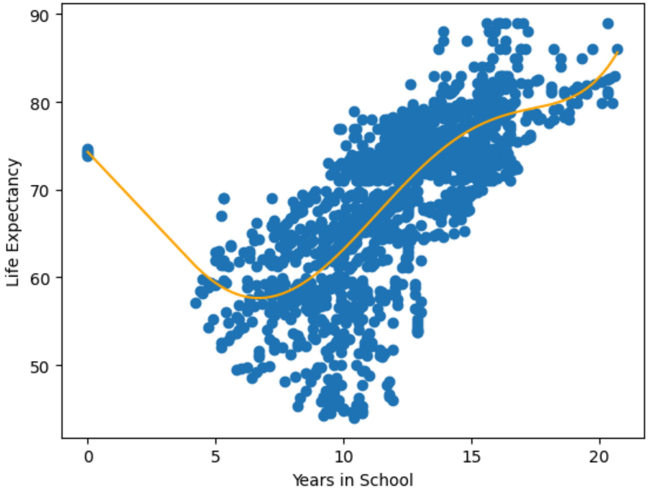

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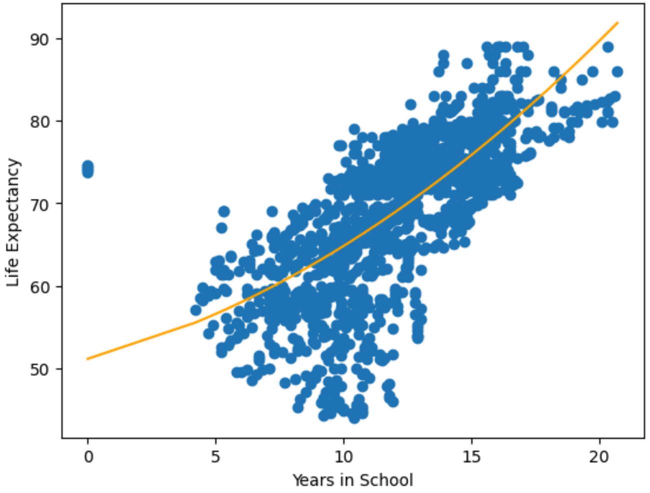
Question: Which n do you think has the smallest loss?

Answer: $n = 5$, but intuitively, $n = 5$ does not seem very good...



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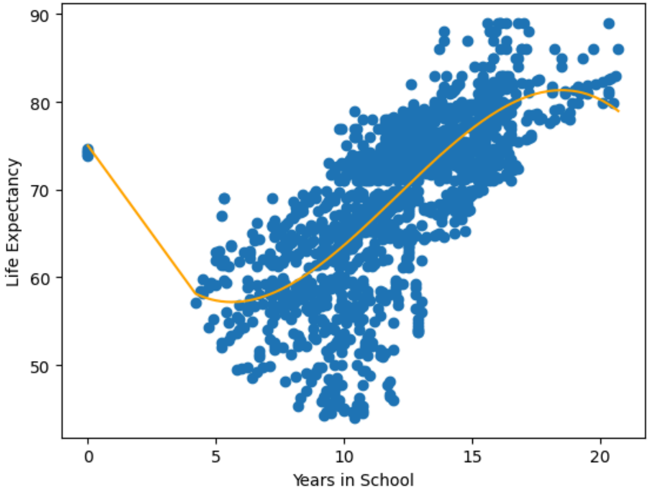

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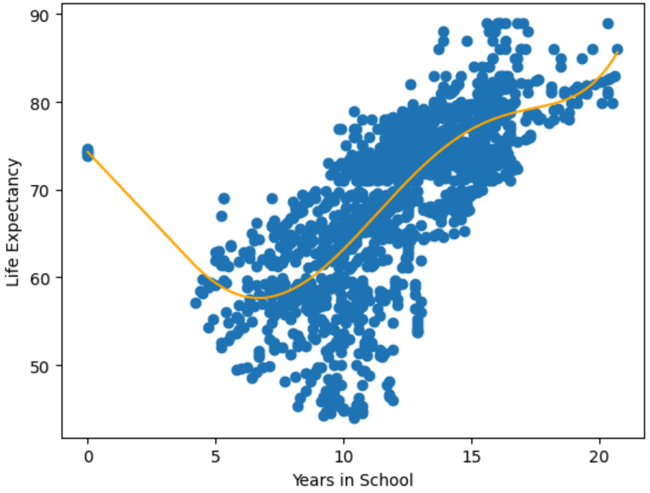
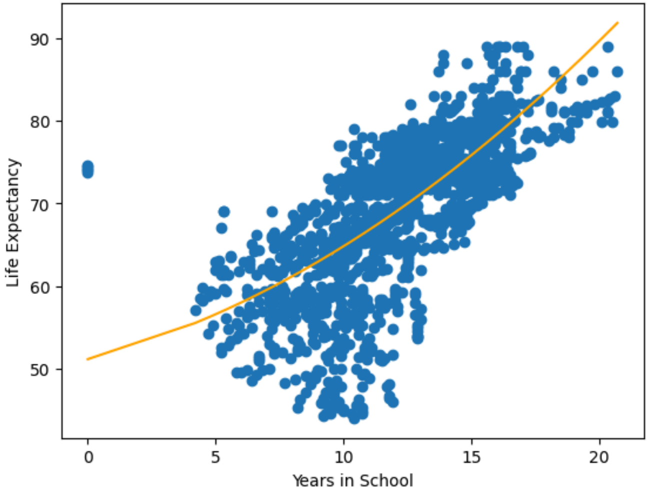


$n = 5$

More specifically, $n = 5$ will not generalize to new data



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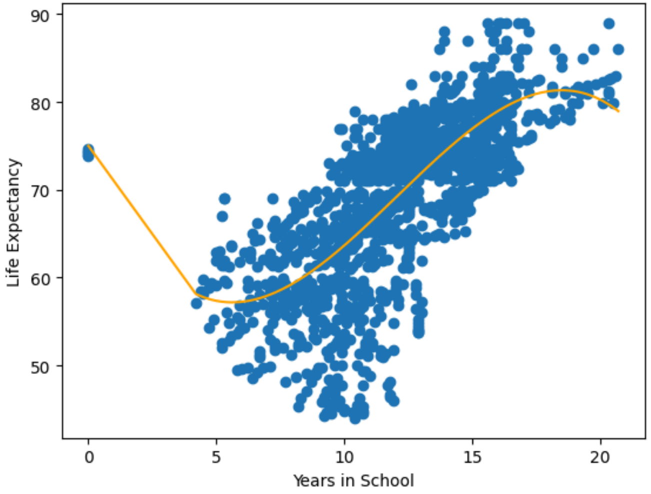

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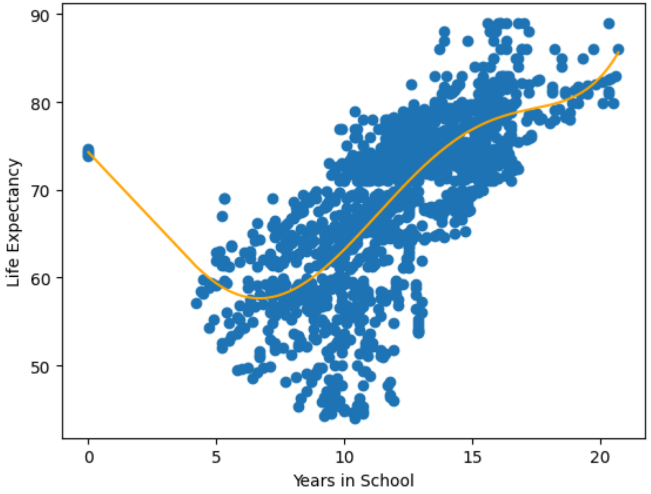

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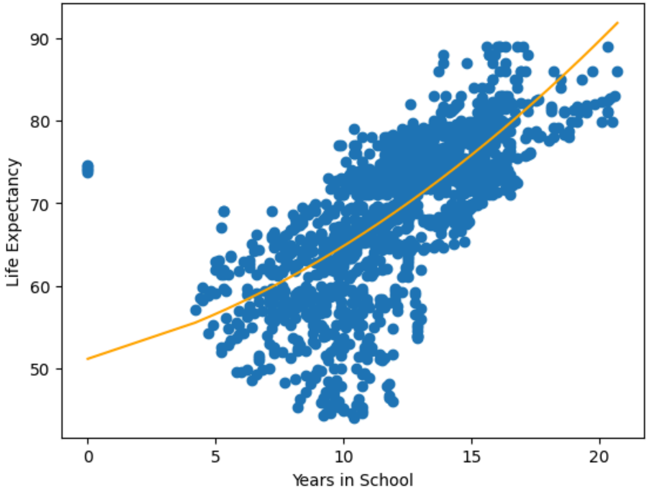

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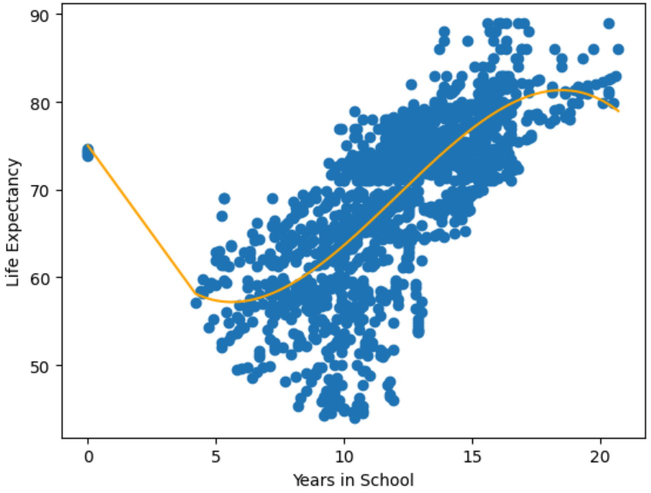

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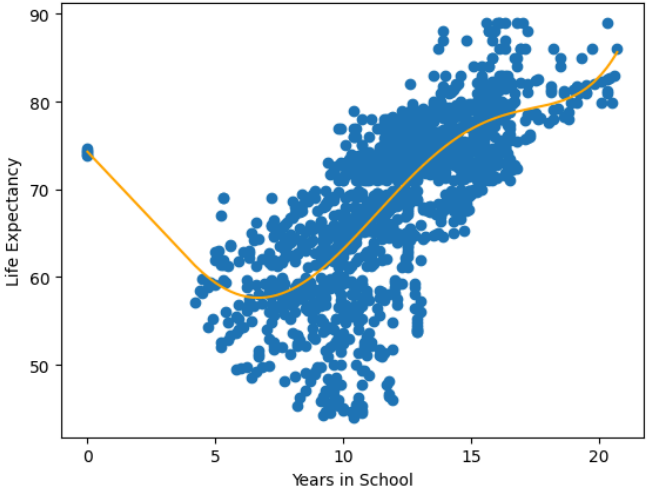

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Answer: Compute the loss on unseen data!

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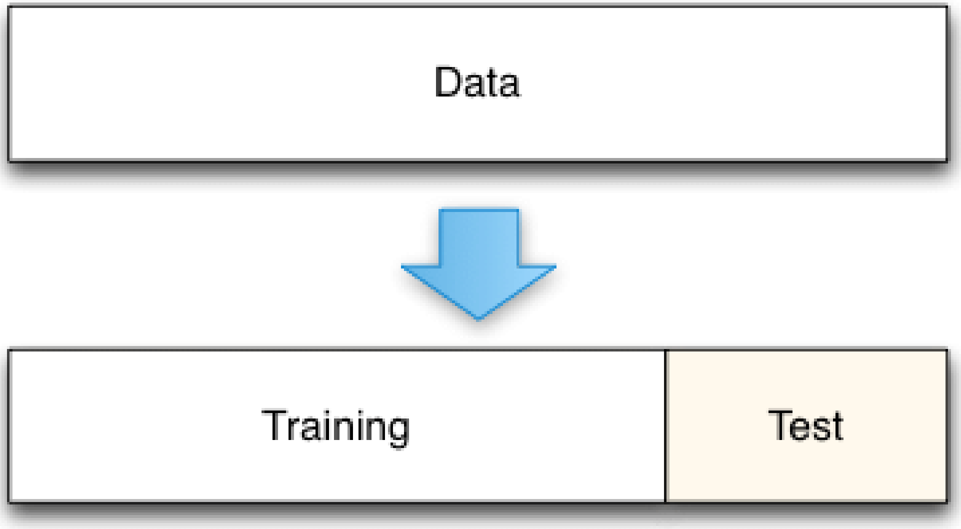

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Note: The model must never see the testing dataset during training. This is very important!

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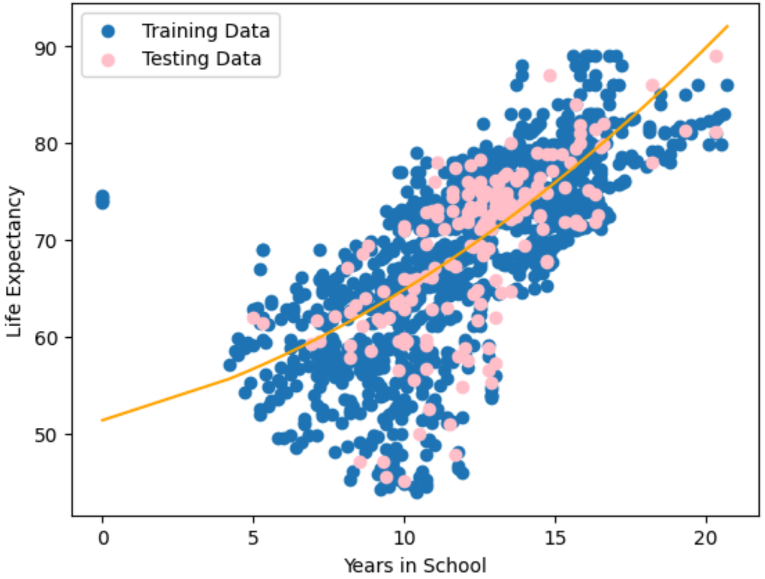

Learn parameters from the train dataset, evaluate on the test dataset

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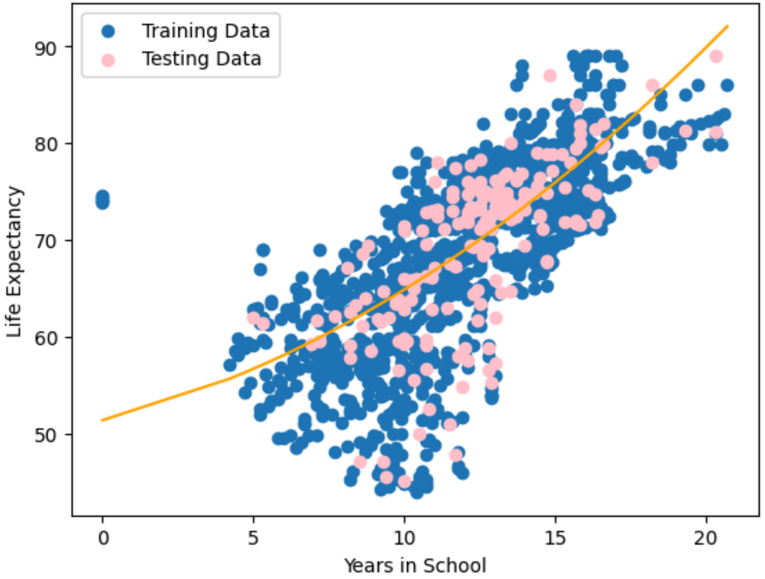

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$$\mathcal{L}(\boldsymbol{X}_{\text{train}}, \boldsymbol{y}_{\text{train}}, \boldsymbol{\theta}) \qquad \mathcal{L}(\boldsymbol{X}_{\text{test}}, \boldsymbol{y}_{\text{test}}, \boldsymbol{\theta})$$

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