

Regression

CISC 7026: Introduction to Deep Learning

University of Macau

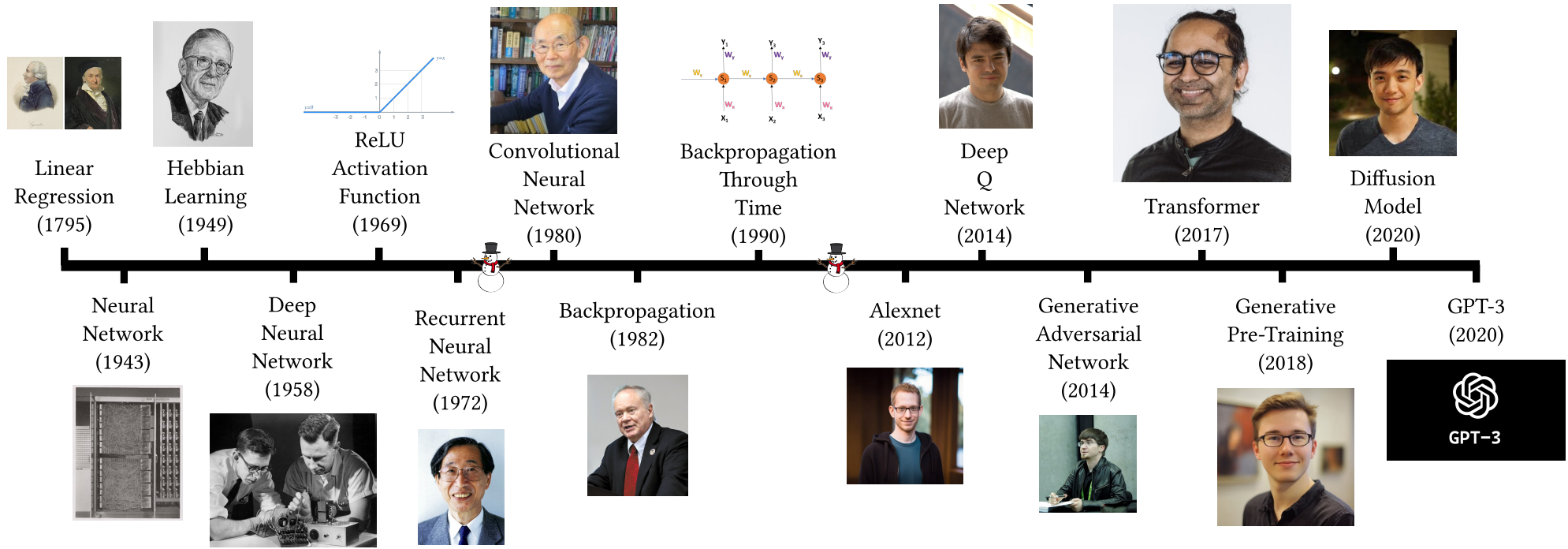
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Let us start with regression

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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:

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We can use this data to make future predictions

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- *The causal effects of education on health outcomes in the UK Biobank.*
Davies et al. *Nature Human Behaviour*.

Linear Regression

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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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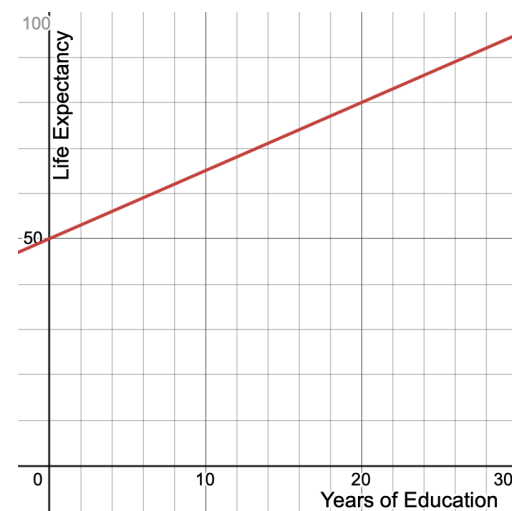
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Linear Regression

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

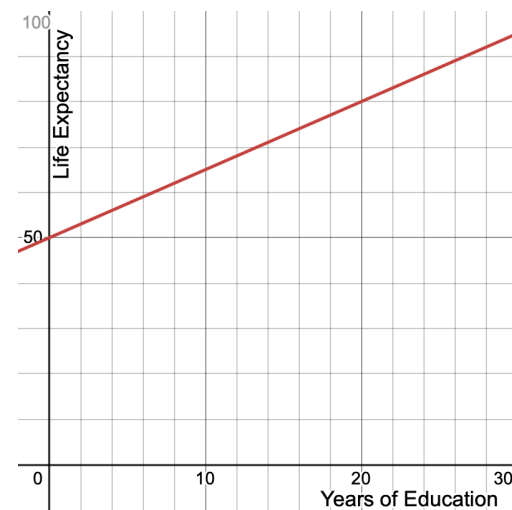


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Question: How do we find θ ? (Hint: We want $f(x, \theta) = y$)

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

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

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

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Move y to LHS

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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 θ for the entire dataset

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For the entire dataset:

$$\boldsymbol{x} = [x_1 \ x_2 \ \dots \ x_n]^\top, \boldsymbol{y} = [y_1 \ y_2 \ \dots \ y_n]^\top$$

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Minimizing this loss function will give us the optimal parameters!

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

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

Linear Regression

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

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

Linear Regression

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

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

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

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

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

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

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You will be doing this in your first assignment!

Tips for assignment 1

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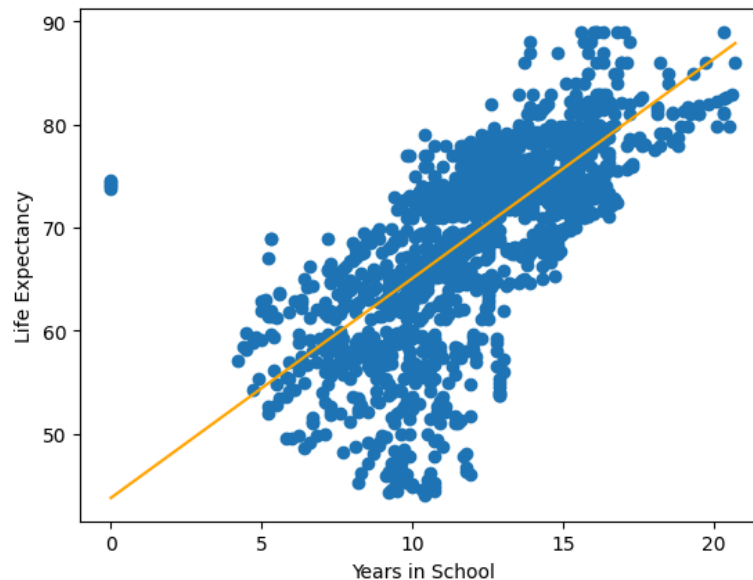
Plot the curve $f(x, \boldsymbol{\theta}) = \theta_1 x + \theta_0; \quad x \in [0, 25]$

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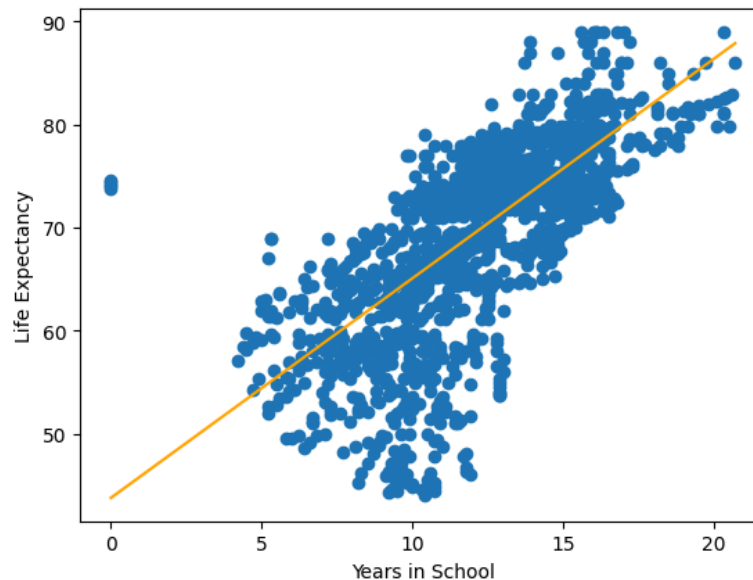


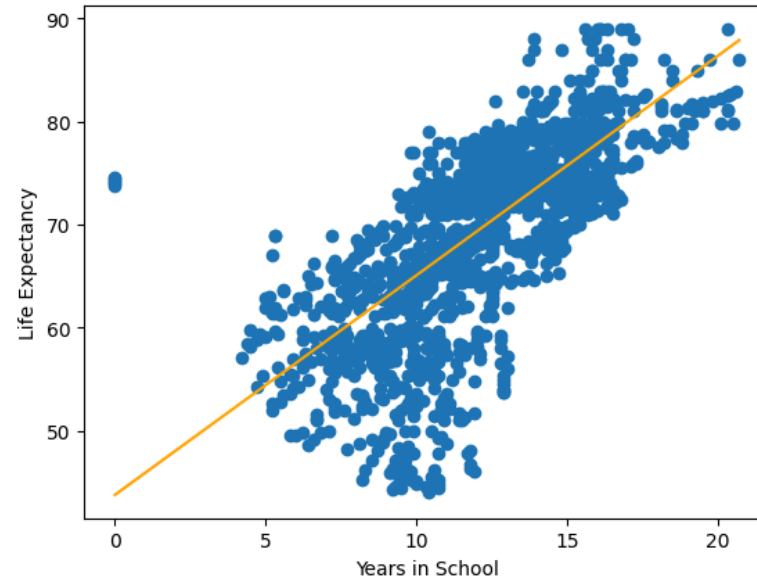
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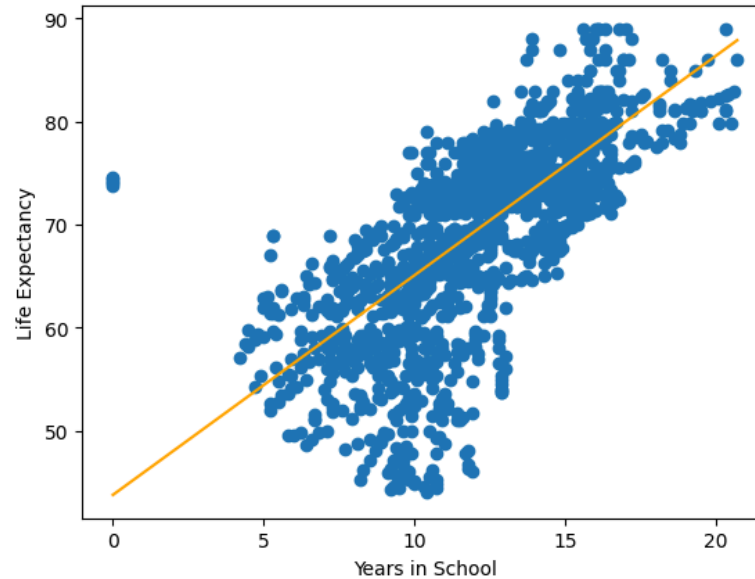
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We figured out linear regression!



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But can we do better?

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2. Overfitting

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3. Outliers

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3. Outliers
4. Regularization

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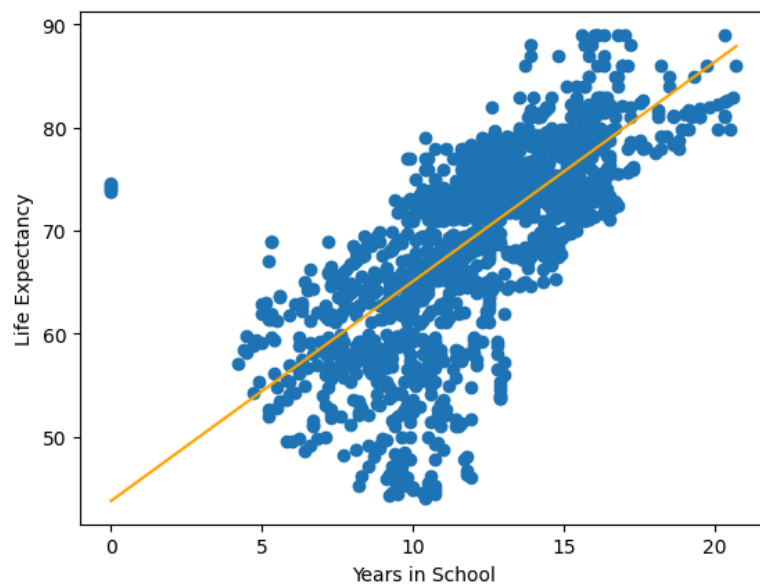
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Does the data look linear?

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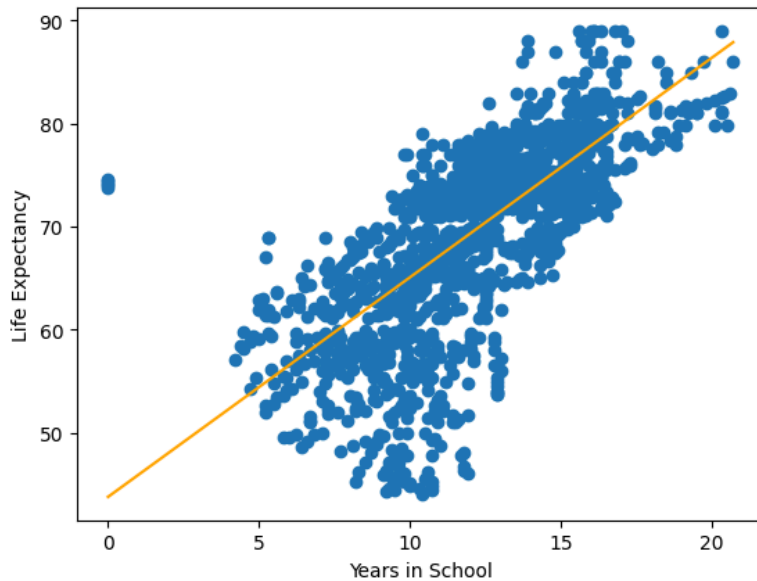
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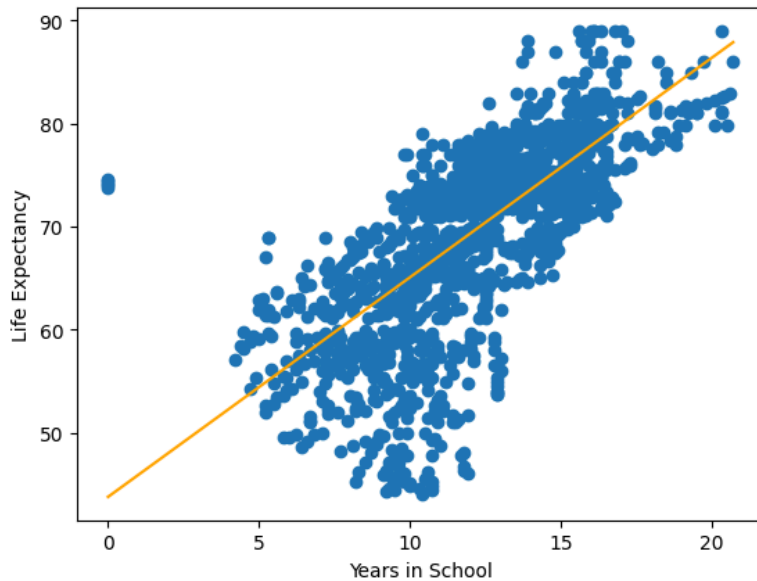
Does the data look linear?

Or maybe more logarithmic?

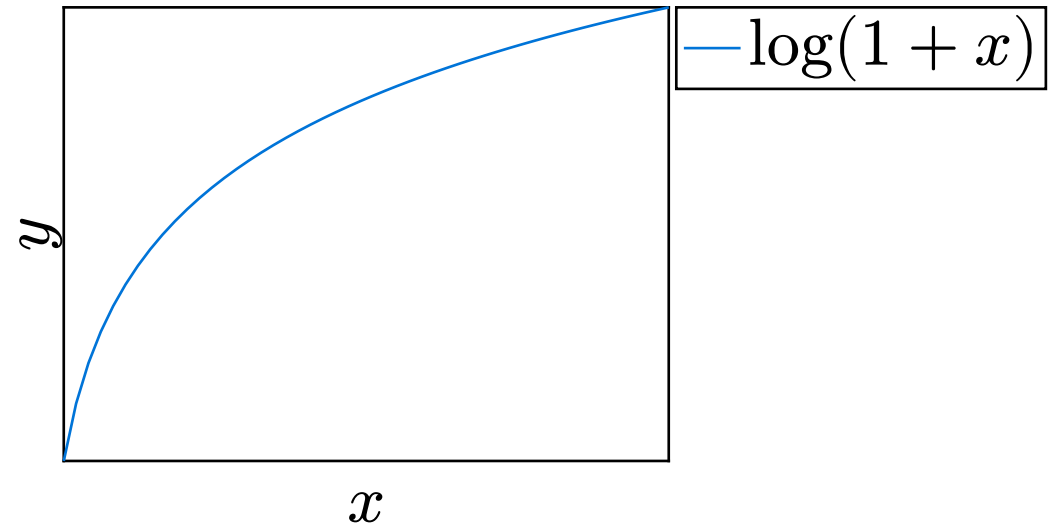


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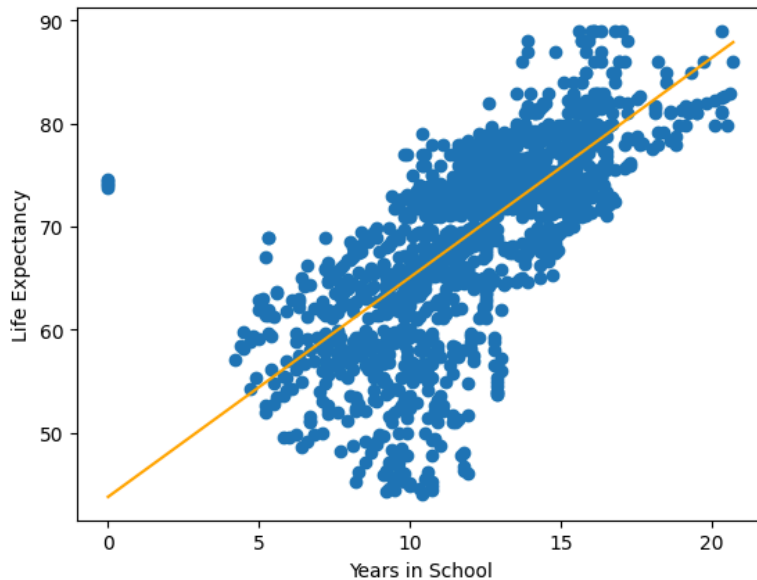


Or maybe more logarithmic?

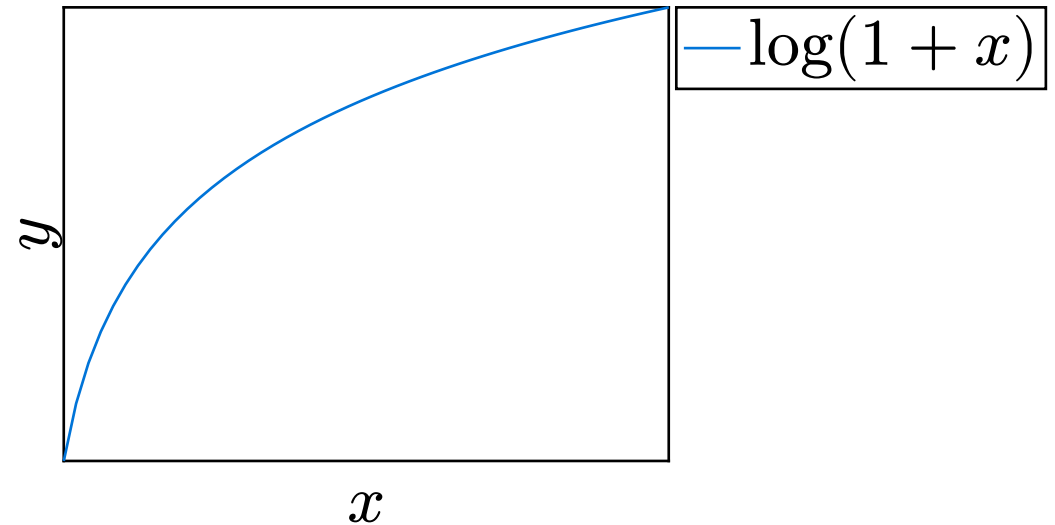


Question:

Does the data look linear?



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However, linear regression must be linear!

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Trick: Change of variables to make f nonlinear: $x_{\text{new}} = \log(1 + x_{\text{data}})$

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

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

New design matrix...

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

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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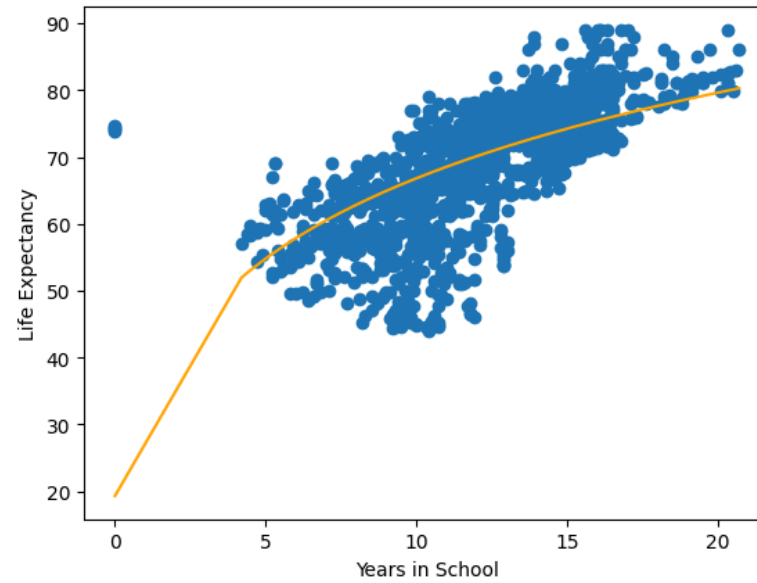
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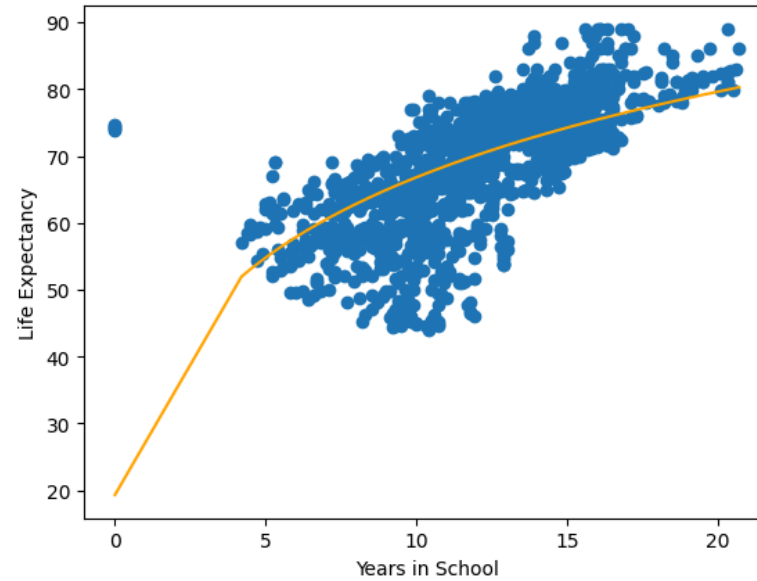
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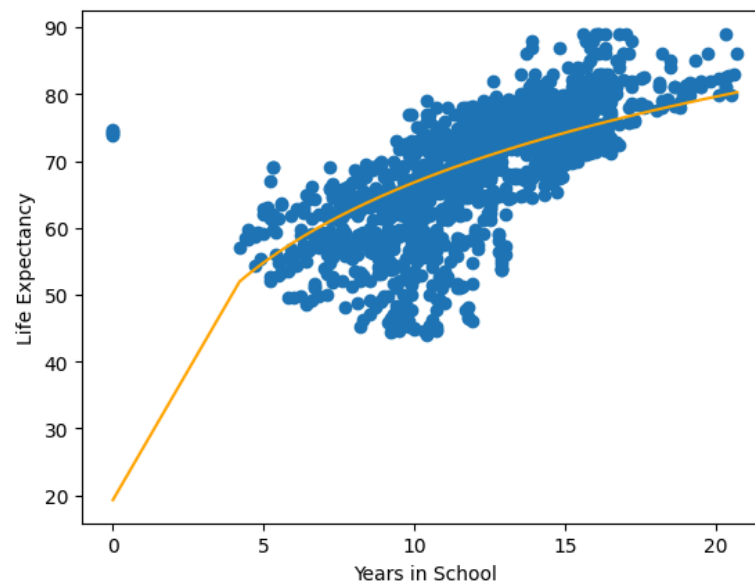
Same solution...

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





Better, but still not perfect



Better, but still not perfect

Can we do even better?

What about polynomials?

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$$f(x) = ax^n + bx^{n-1} + \dots + cx + d$$

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Can we extend linear regression to polynomials?

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And add some new parameters...

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

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

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New function...

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

1. **Beyond linear functions**
2. Overfitting
3. Outliers
4. Regularization

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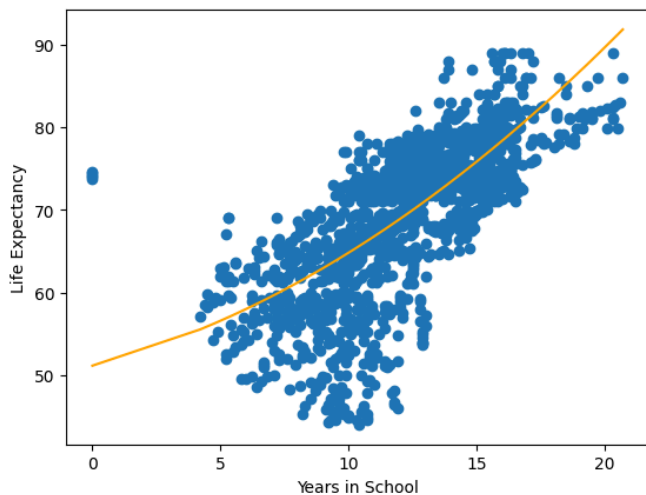
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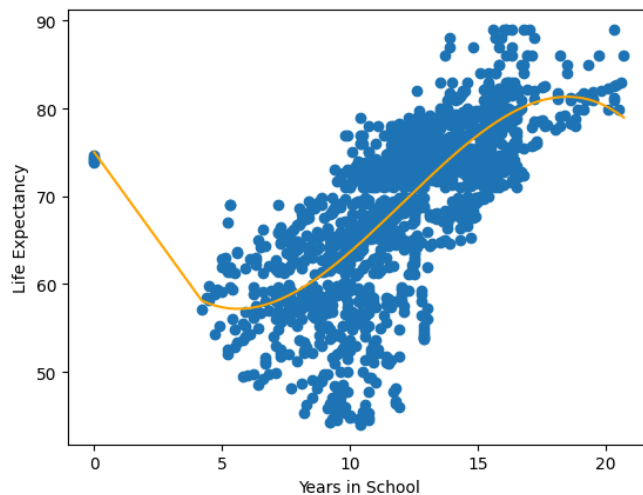
How do we choose n (polynomial order) that provides the best fit?

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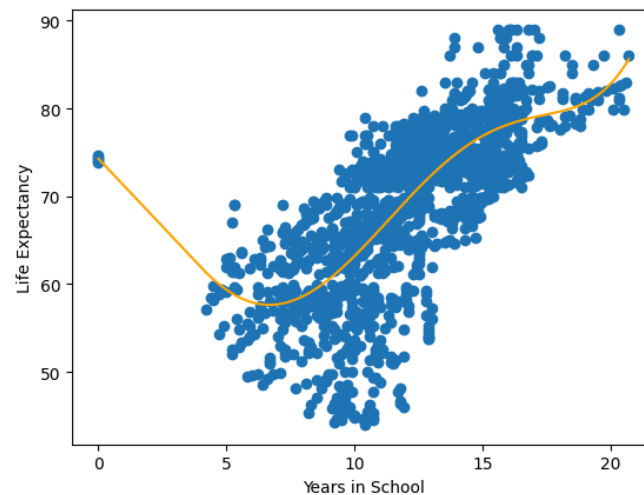
How do we choose n (polynomial order) that provides the best fit?



$n = 2$

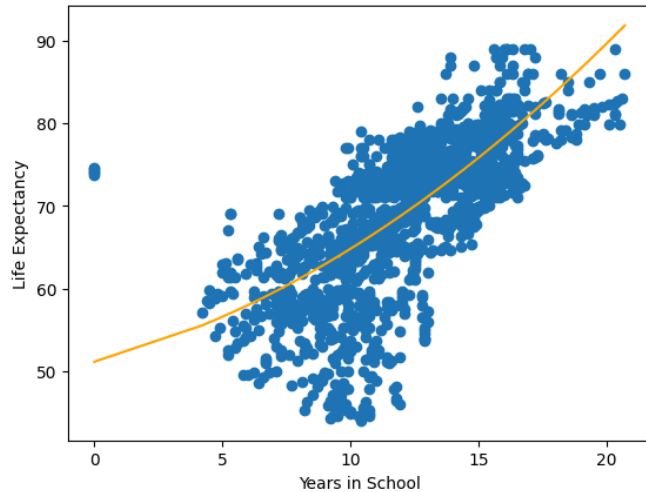


$n = 3$

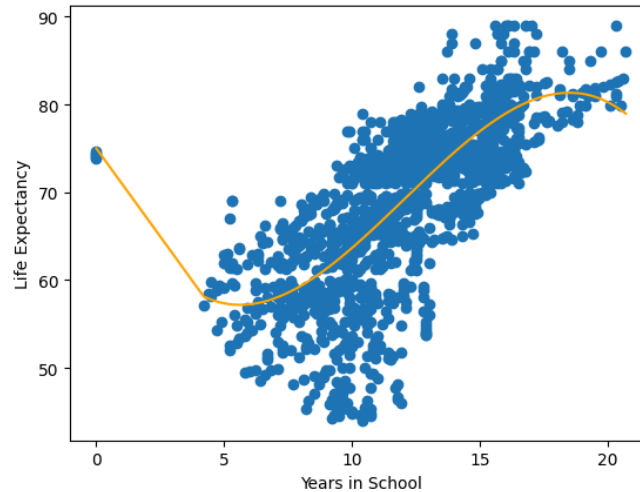


$n = 5$

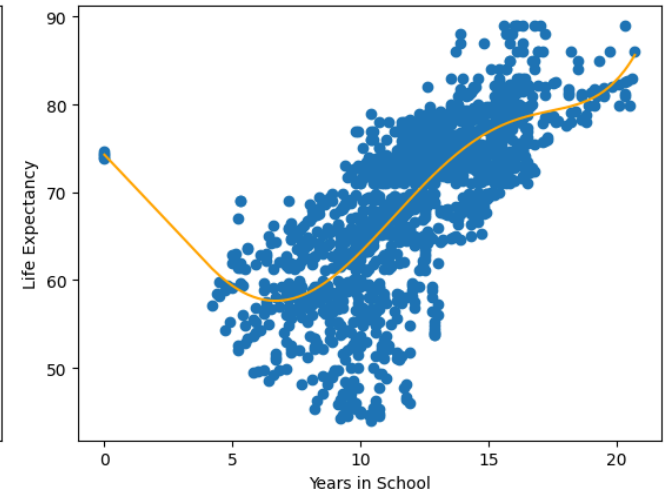
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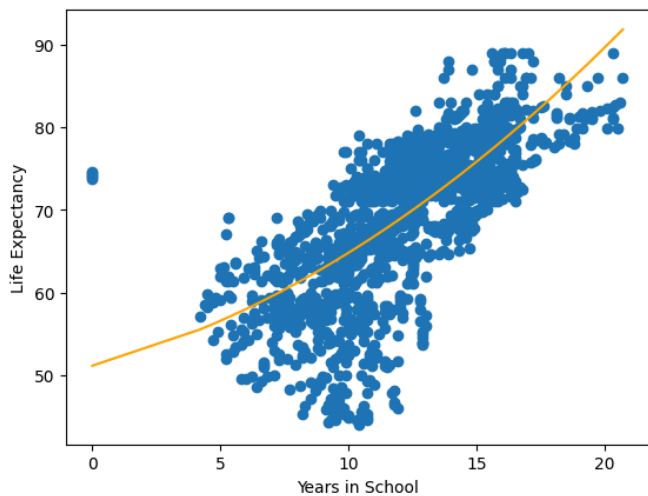
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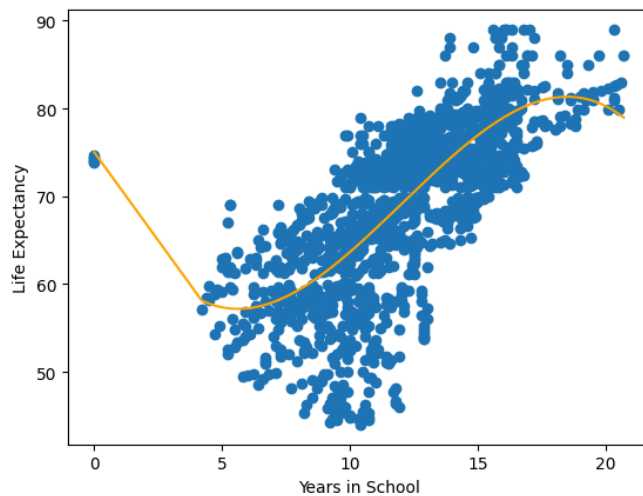
$$n = 5$$

Pick the n with the smallest loss

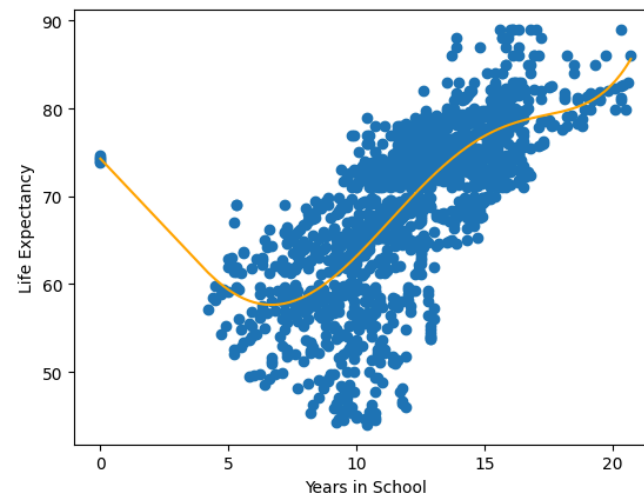
$$\arg \min_{\theta, n} \mathcal{L}(x, y, (\theta, n))$$



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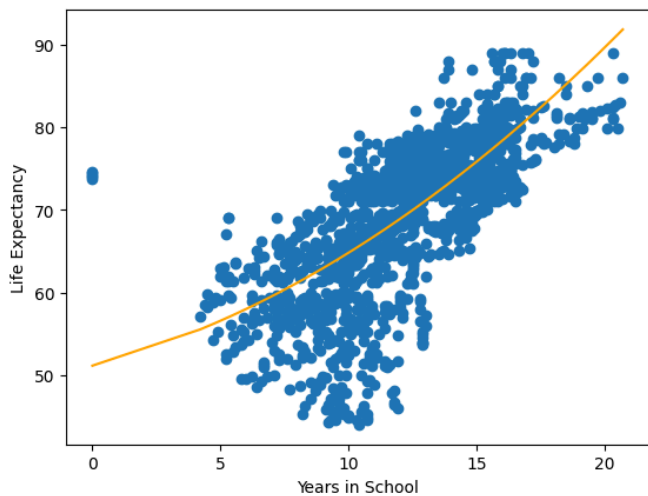


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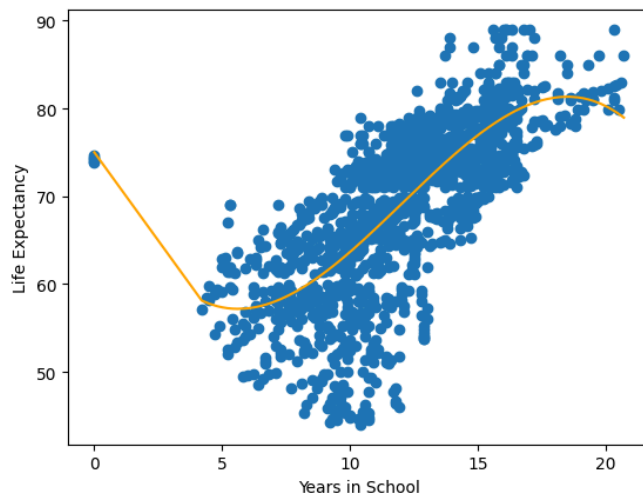


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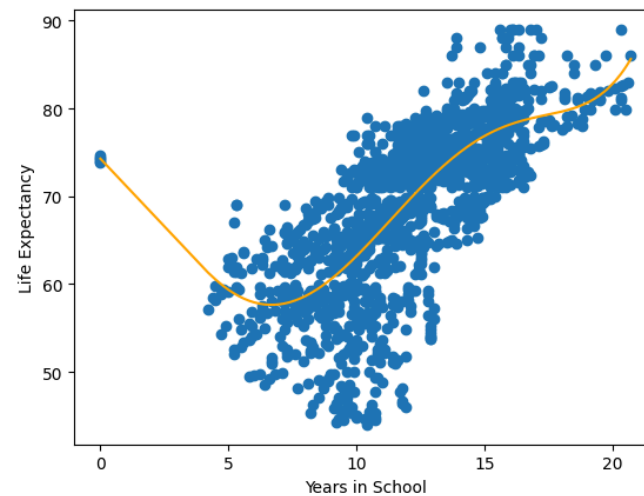
Question: Which n do you think has the smallest loss?



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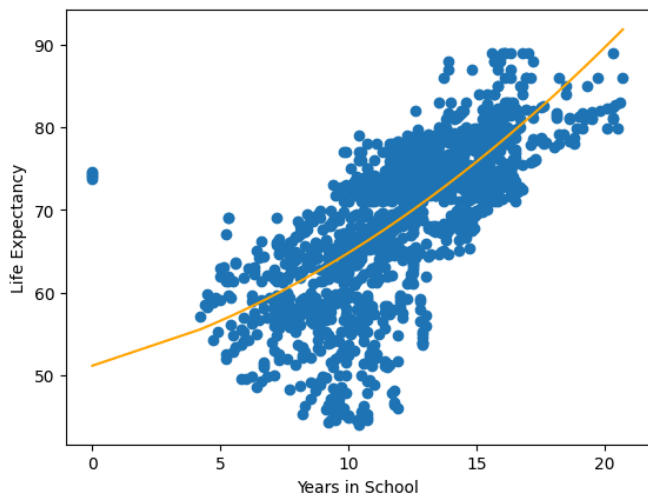
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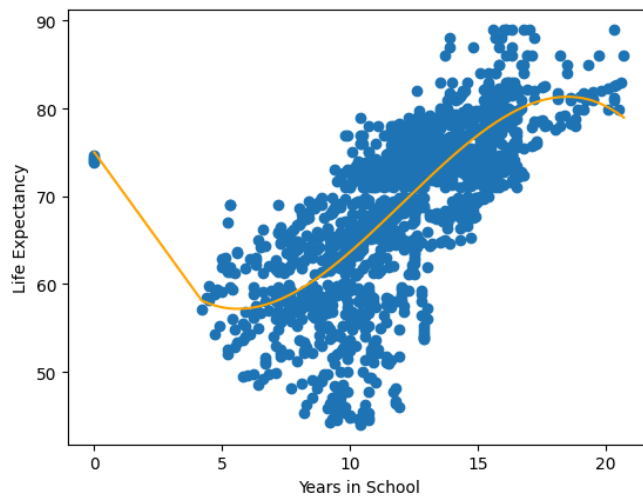
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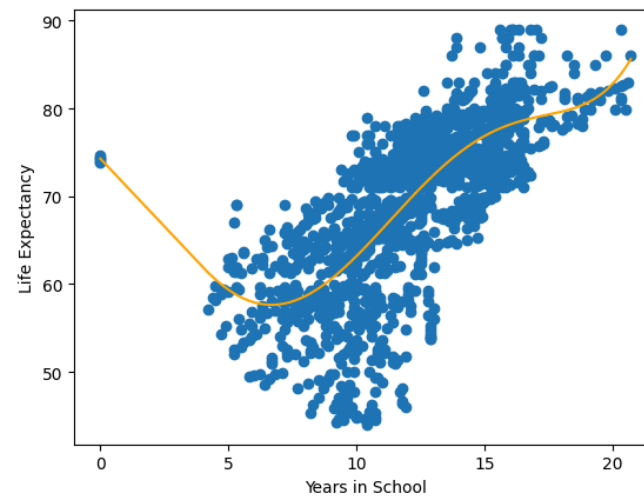
Answer: $n = 5$, but intuitively, $n = 5$ does not seem very good...



$$n = 2$$

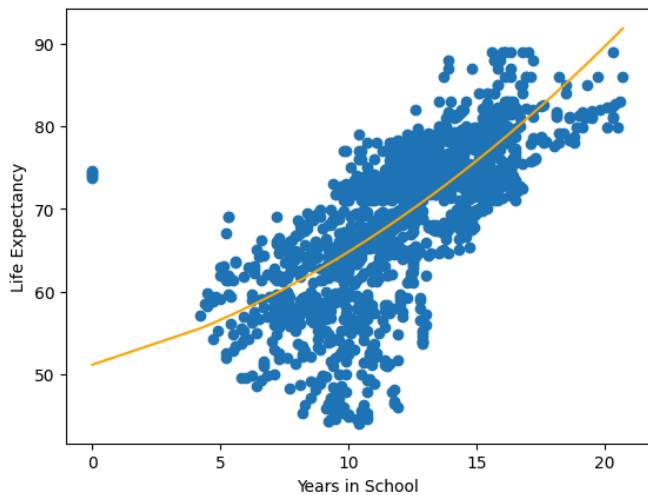


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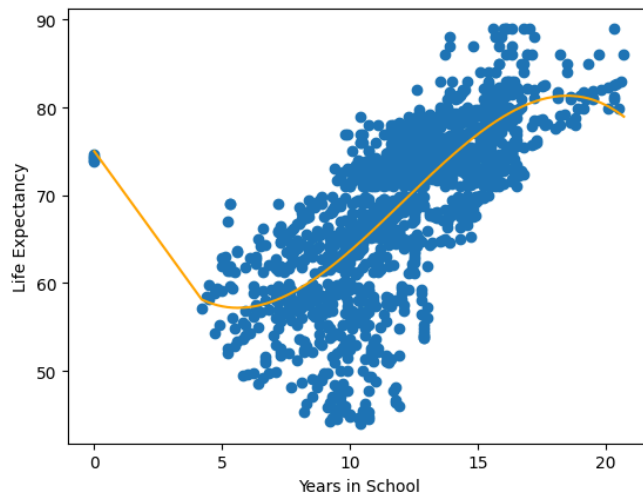


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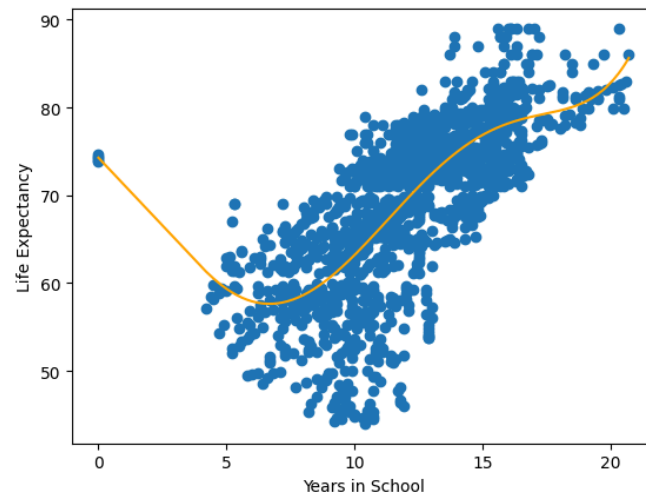
More specifically, $n = 5$ will not generalize to new data



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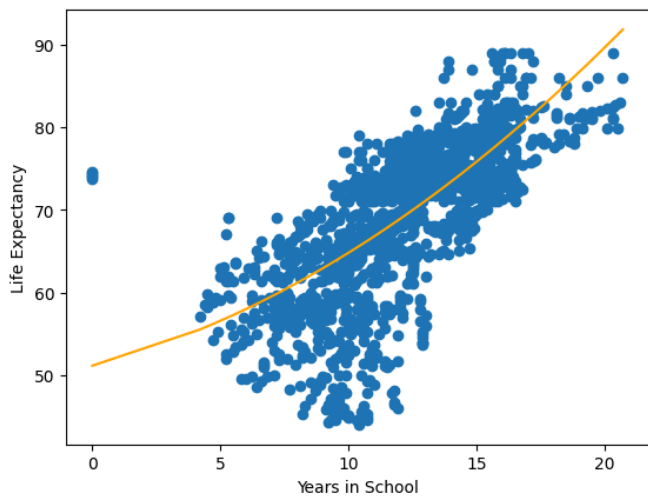
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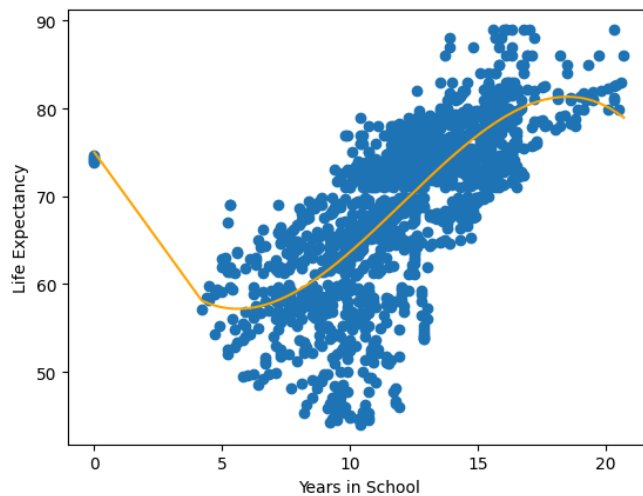
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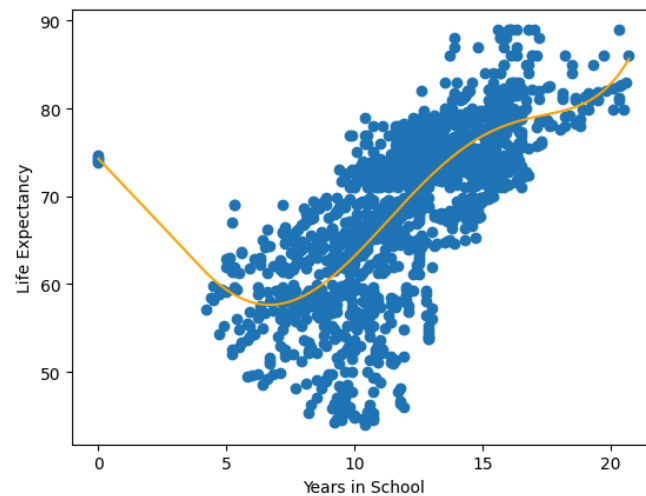
We will only use our model for new data (we already have the y for a known x)!



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Answer: Compute the loss on unseen data!

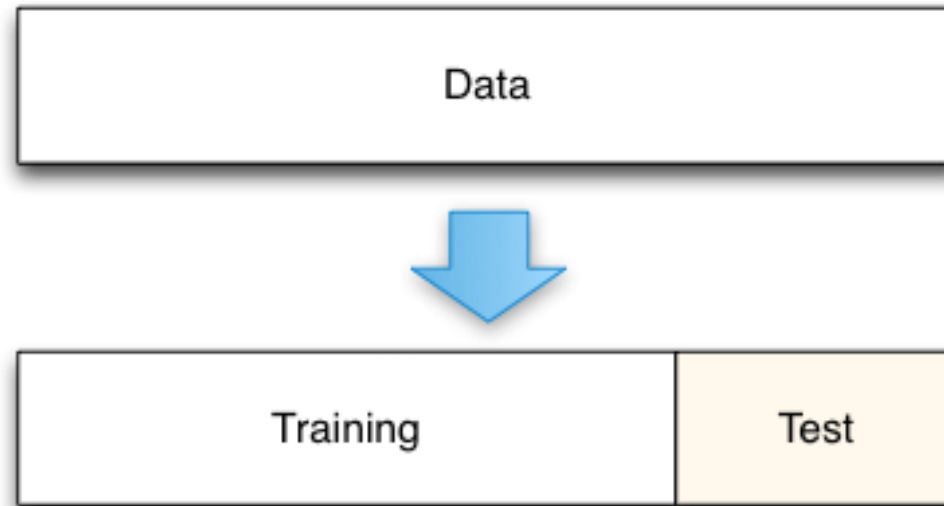
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Note: The model must never see the testing dataset during training. This is very important!

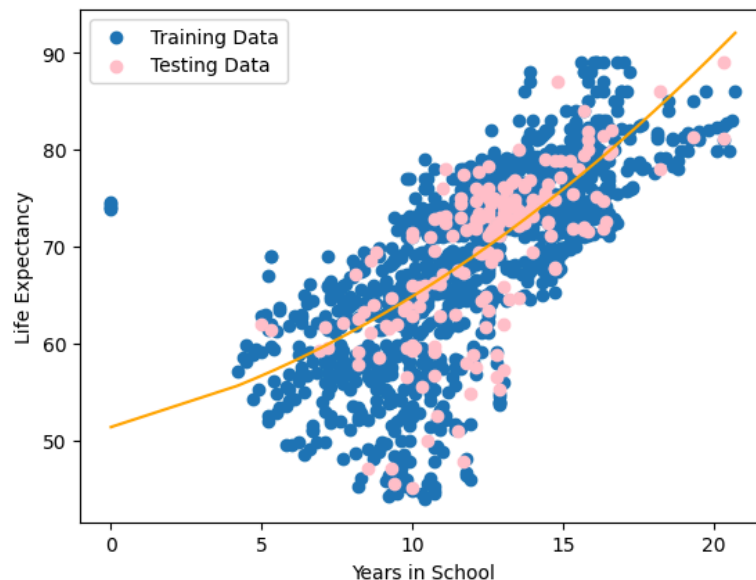
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$$\mathcal{L}(\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}, \boldsymbol{\theta})$$

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

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