Regression

CISC 7026: Introduction to Deep Learning

University of Macau

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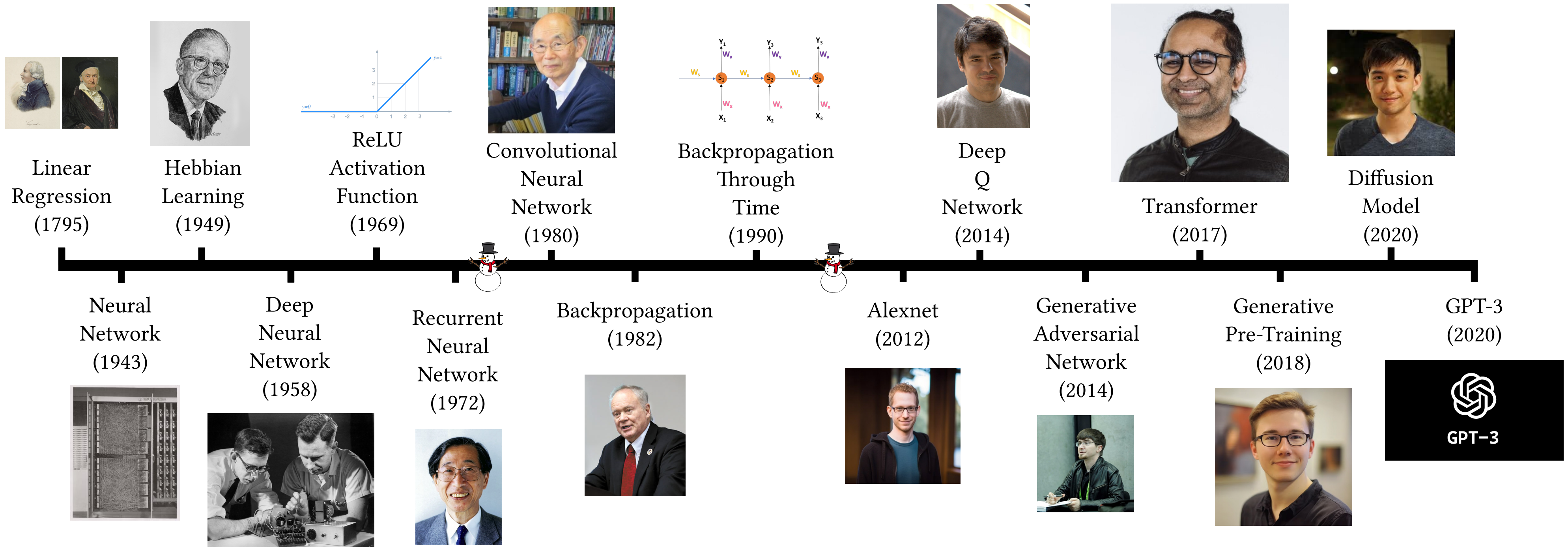

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Let us start with regression

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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

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We can use this data to make future predictions

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- By staying in school, you are likely to live longer

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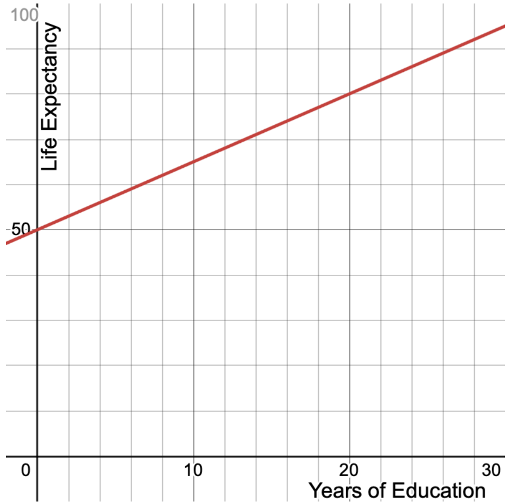

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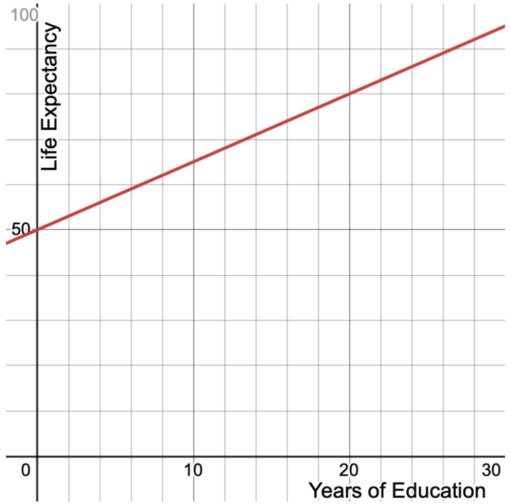

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Question: How do we find $\boldsymbol{\theta}$? (Hint: We want $f(x, \boldsymbol{\theta}) = y$)

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

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Move y to LHS

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

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:

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

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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You will be doing this in your first assignment!

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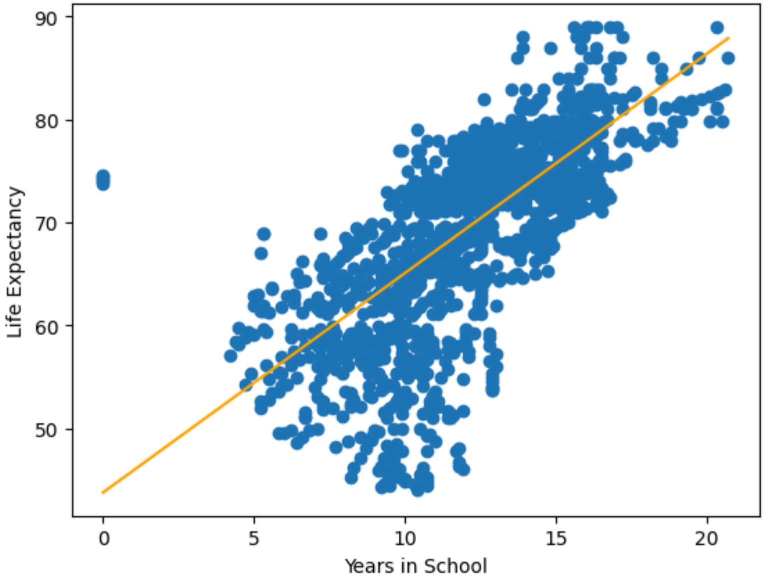

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Everything you need is in the lecture notes

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Relax

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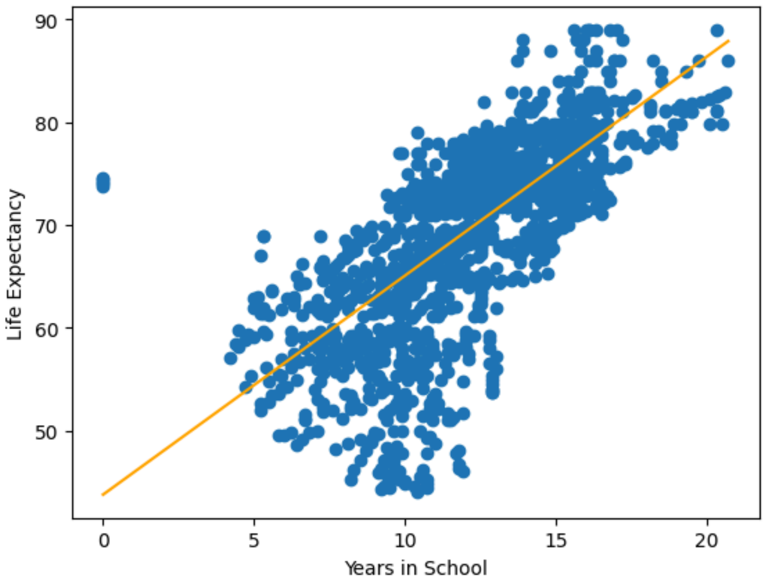

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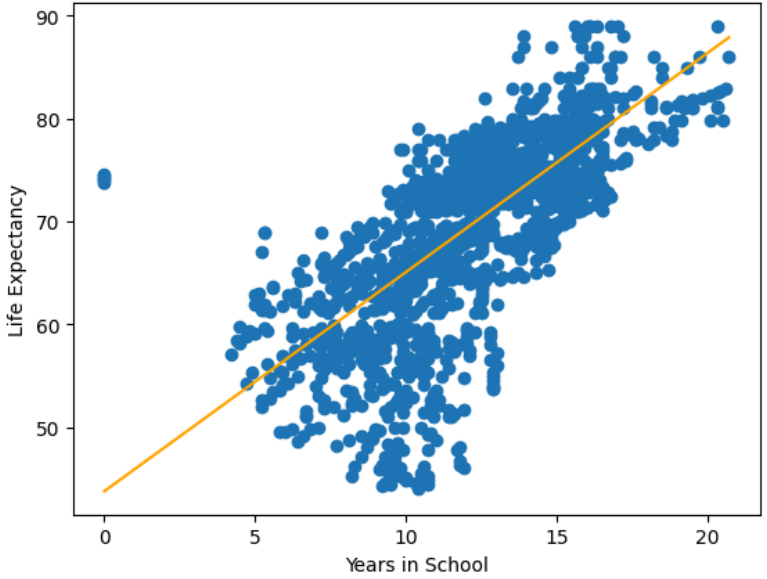

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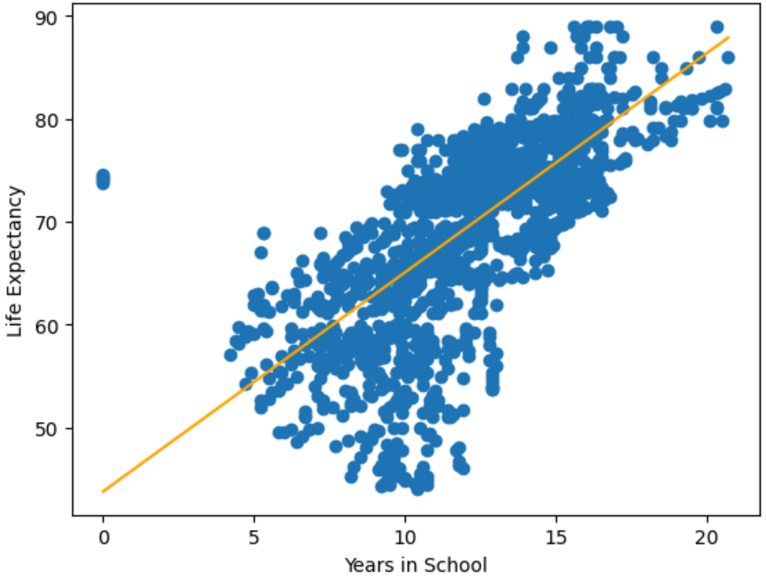

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But can we do better?

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2. Overfitting

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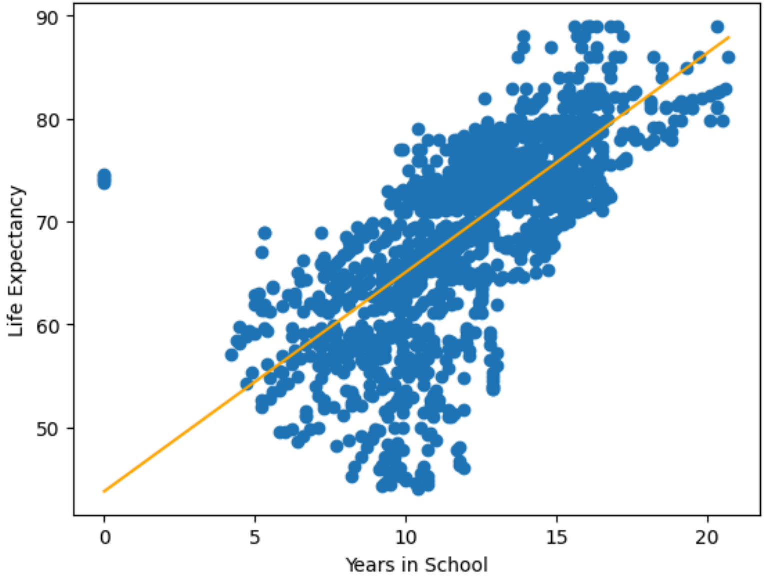

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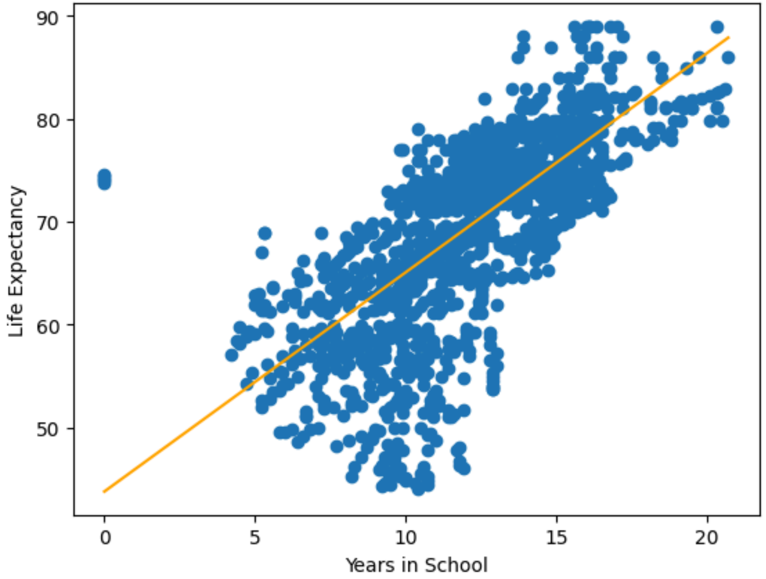

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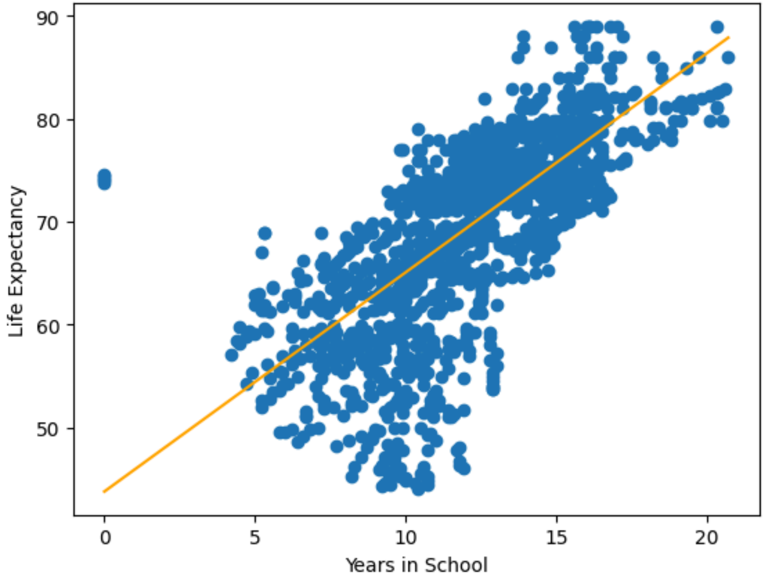

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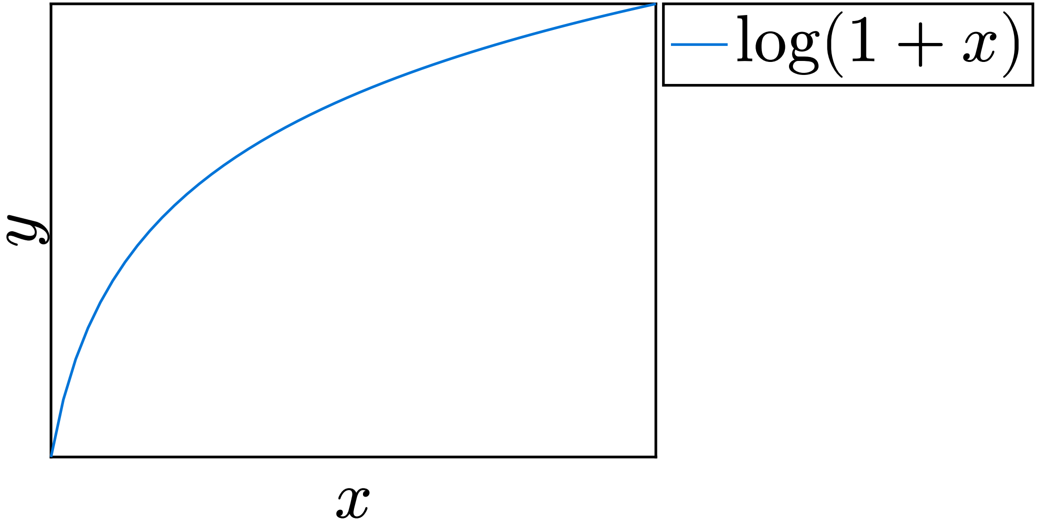
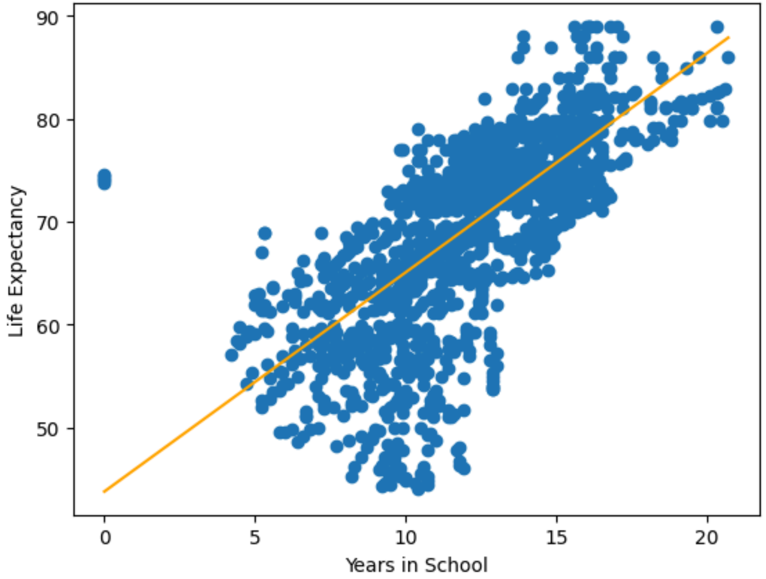


Does the data look linear?



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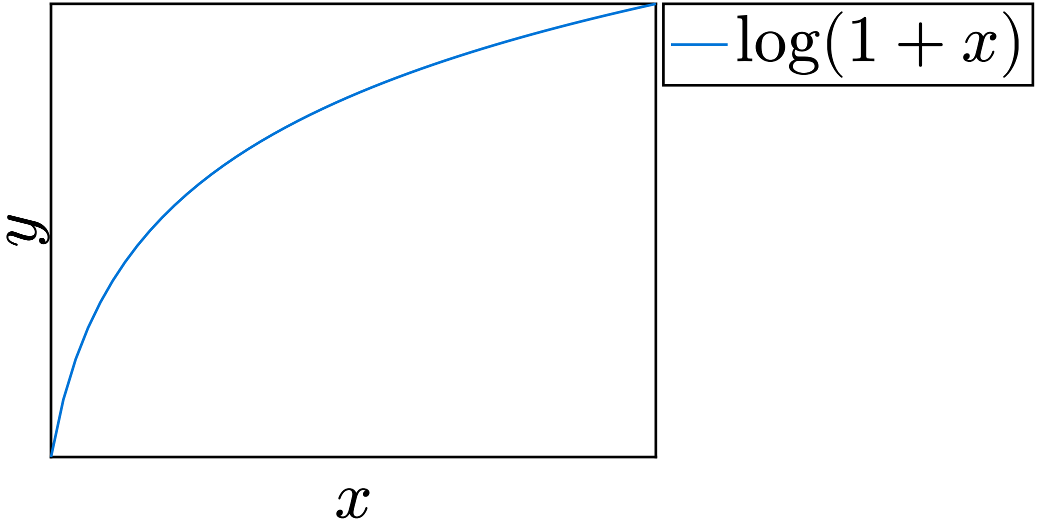

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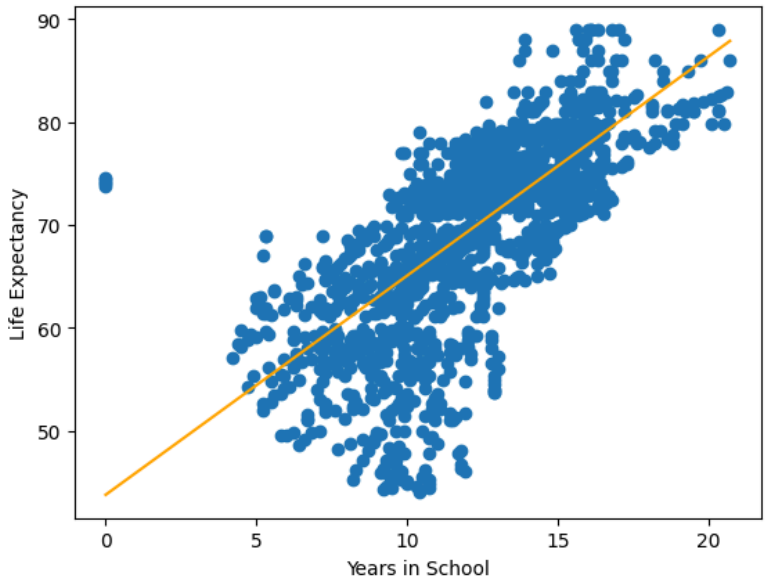

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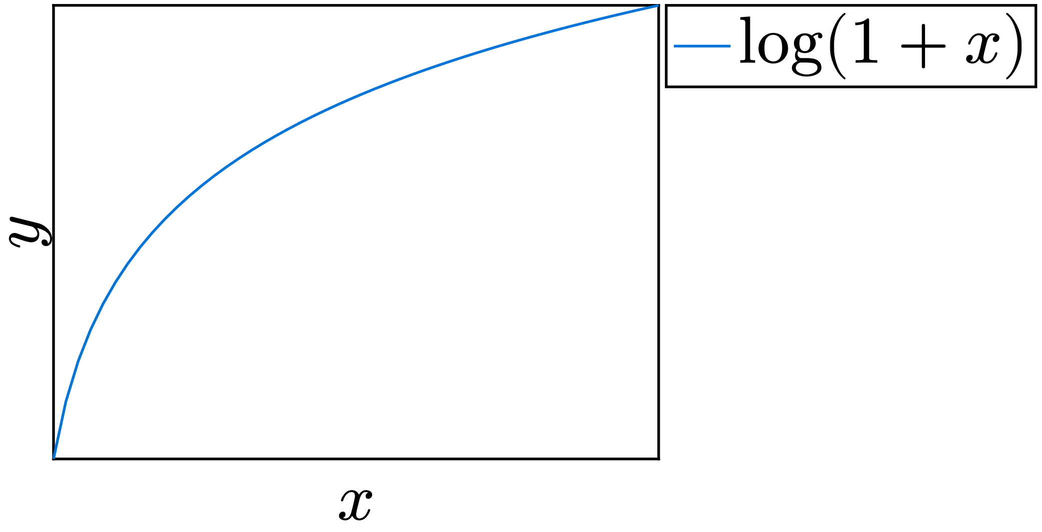

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$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} \log(1 + x_1) & 1 \\ \log(1 + x_2) & 1 \\ \vdots & \vdots \\ \log(1 + x_n) & 1 \end{bmatrix}$$

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

New design matrix…

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

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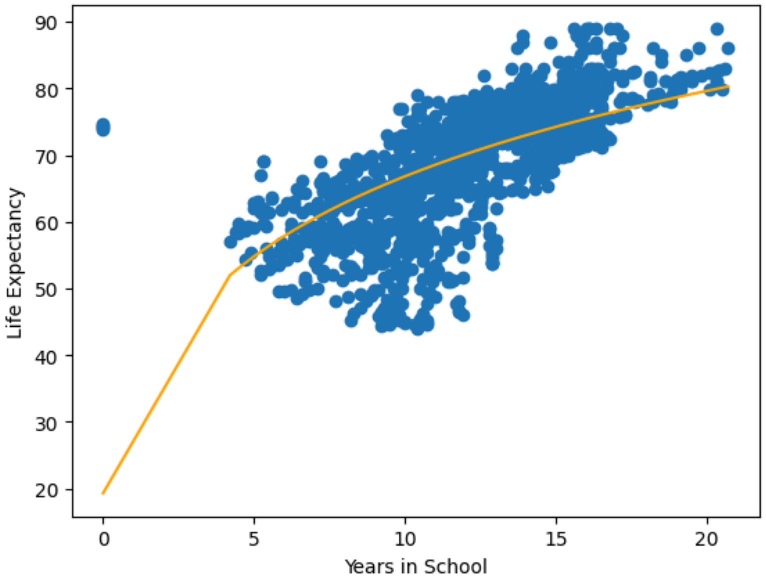
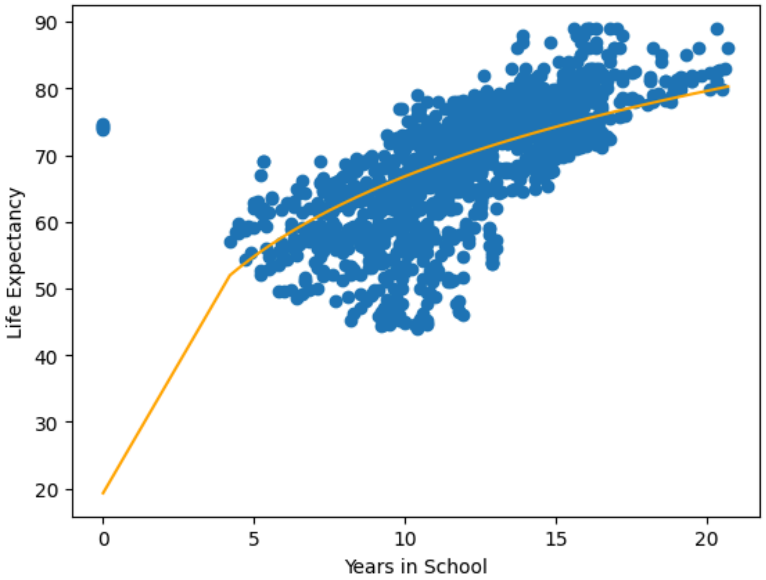
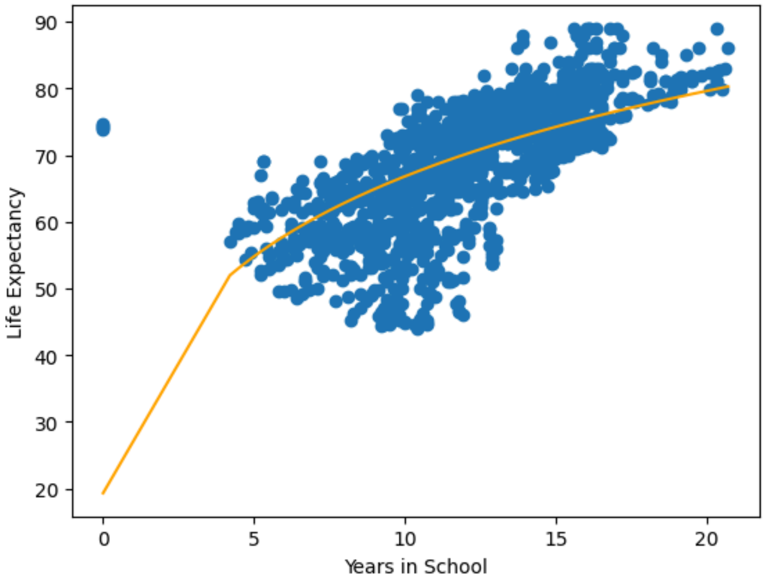
Same solution...

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


90
80
70
60
50
40
30
20
Life Expectancy
0
5
10
15
20
Years in School



Better, but still not perfect



Better, but still not perfect

Can we do even better?

What about polynomials?

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

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And add some new parameters…

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

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

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$$

New function...

$$
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$$

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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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2. Overfitting
3. Outliers
4. Regularization

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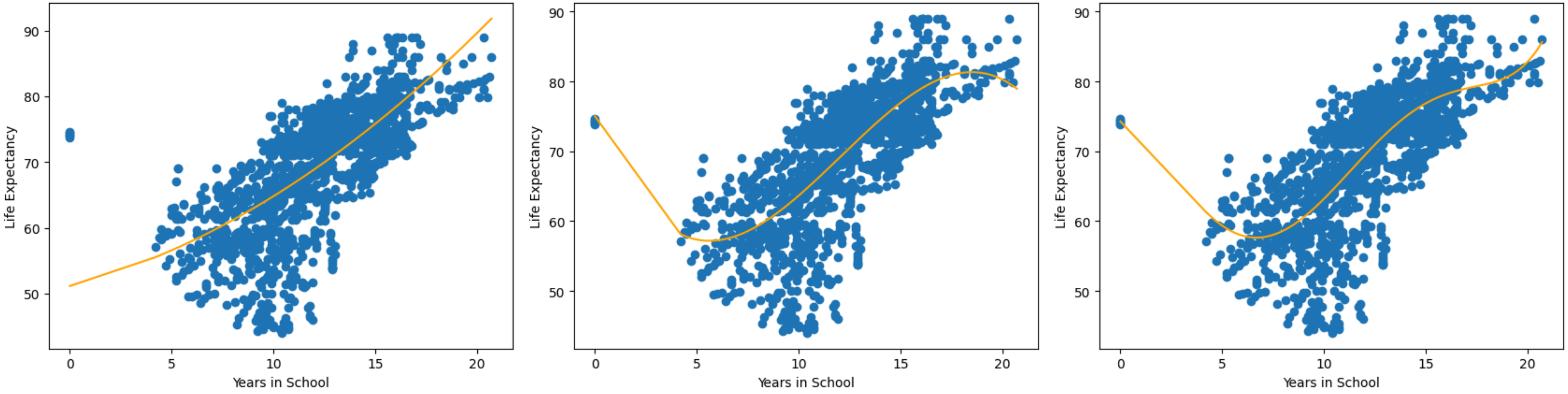

$n = 2$ $n = 3$ $n = 5$

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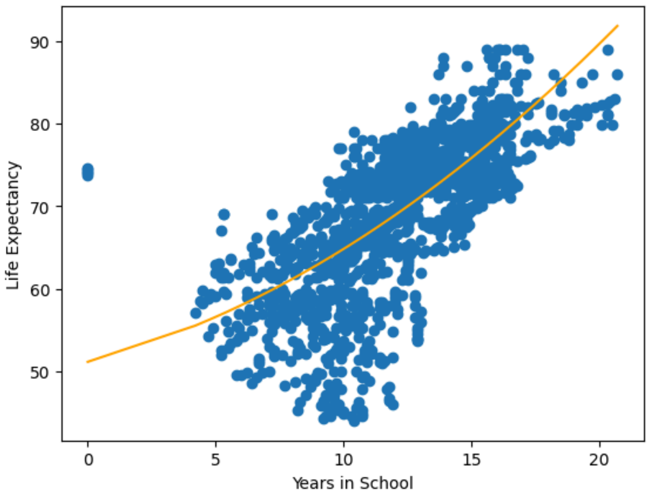

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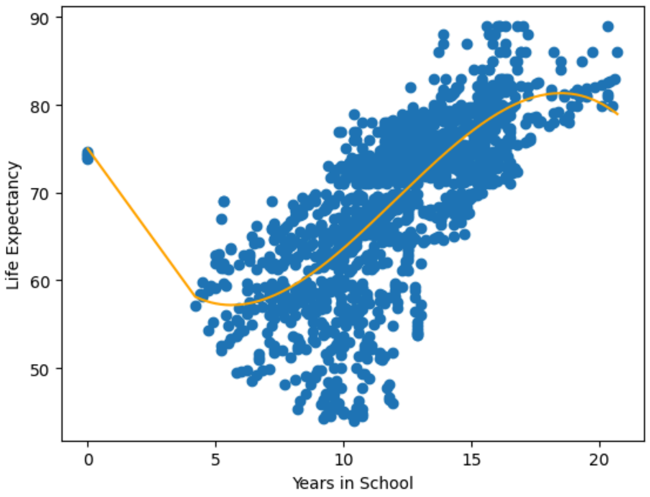

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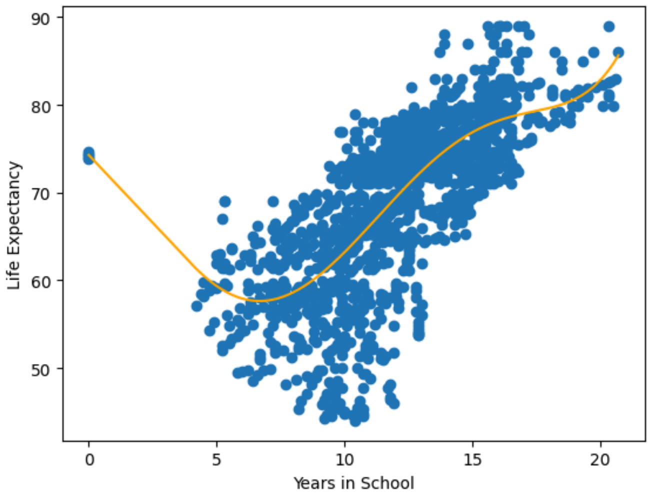
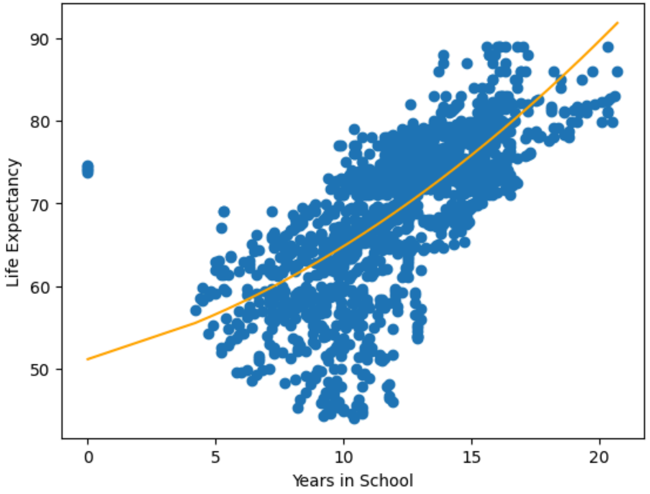


$n = 5$

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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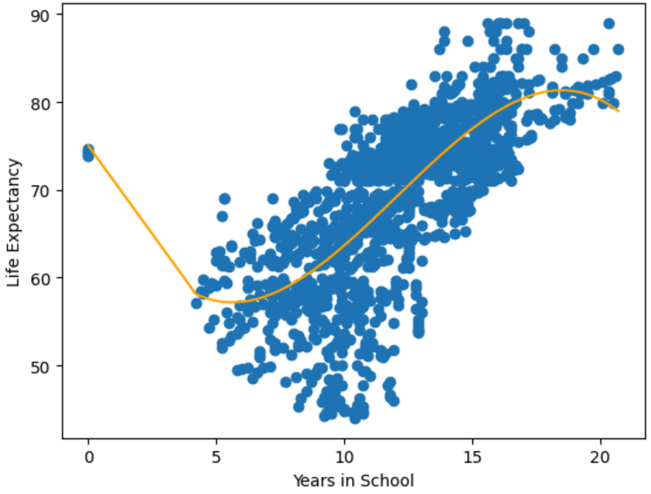

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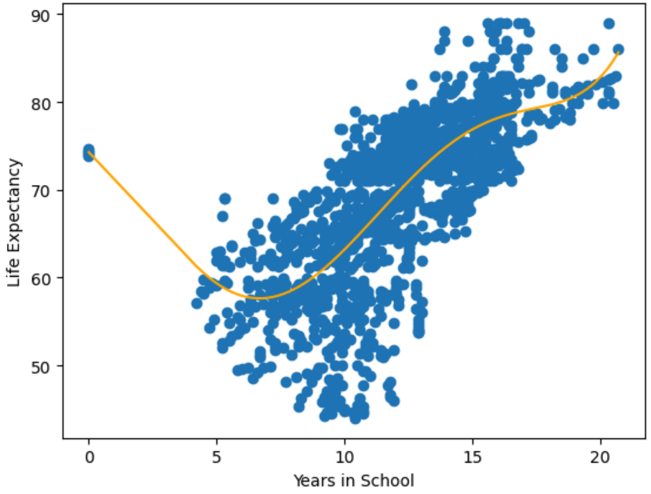

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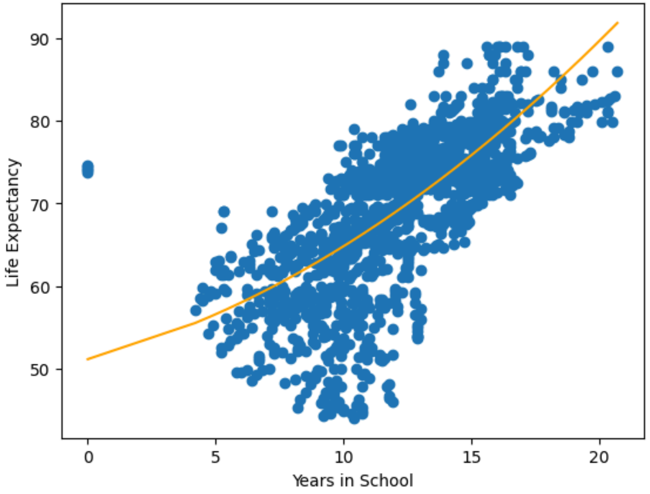
Question: Which n do you think has the smallest loss?



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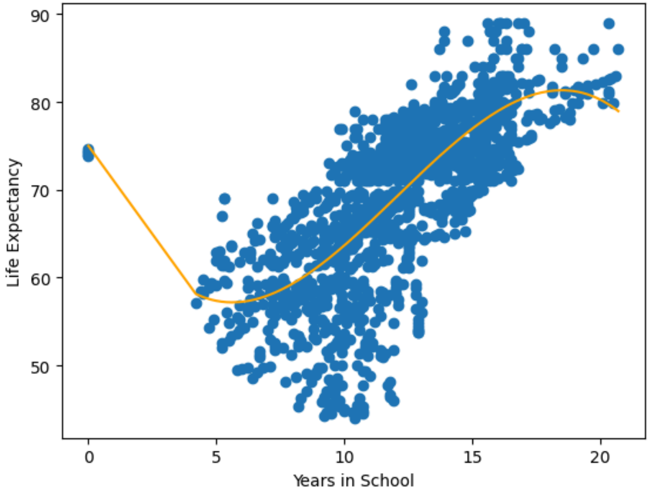

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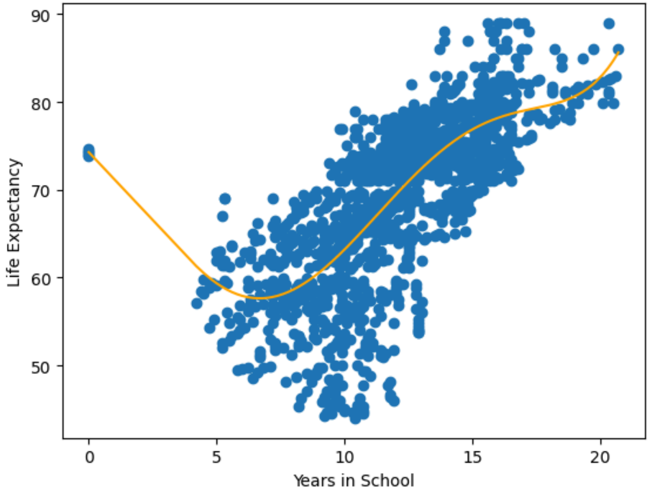

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Answer: $n = 5$ – but intuitively, $n = 5$ does not seem very good...

Example

Back to the example...

Task: Given your education, predict your life expectancy

Example

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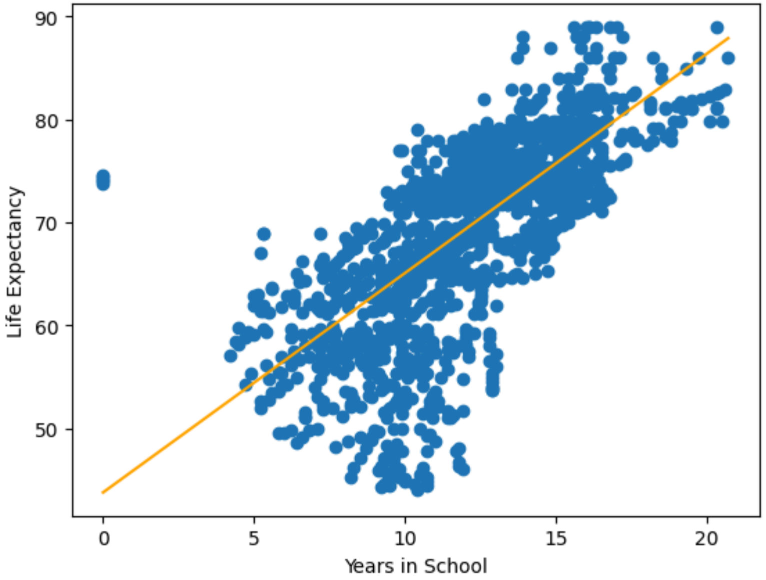

Example

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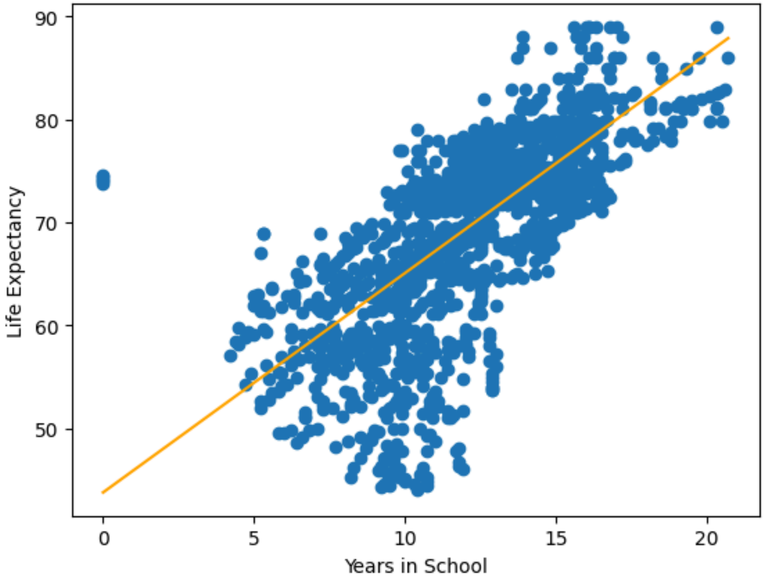

Could we do better than a linear function f?

Example

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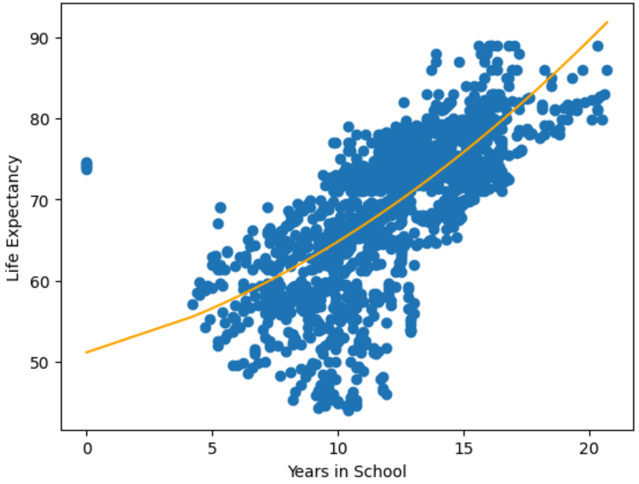

What if we used a polynomial instead?

Example

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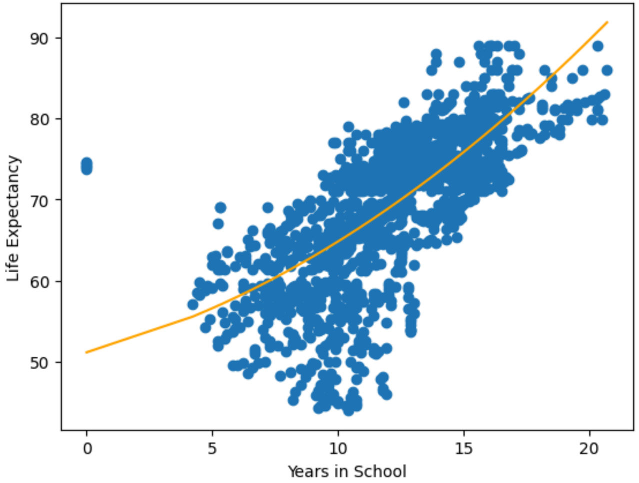

What if we used a polynomial instead?

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

Example

But we said we were using a linear model, how can we come up with a nonlinear polynomial?

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

Example

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Example

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How do we choose n? Let us try different n

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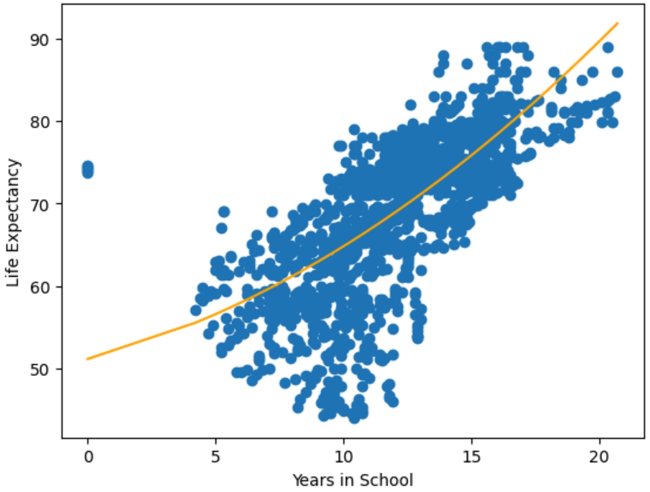
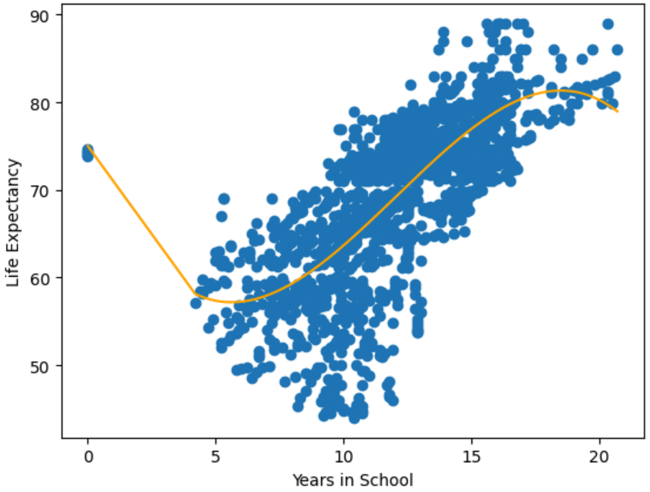


$n = 2$



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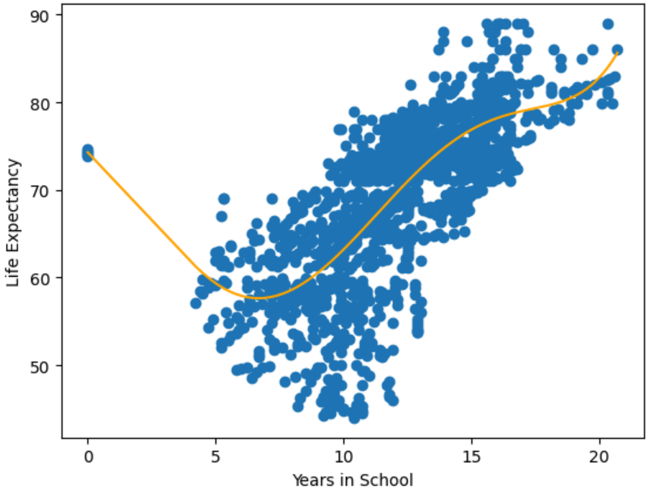

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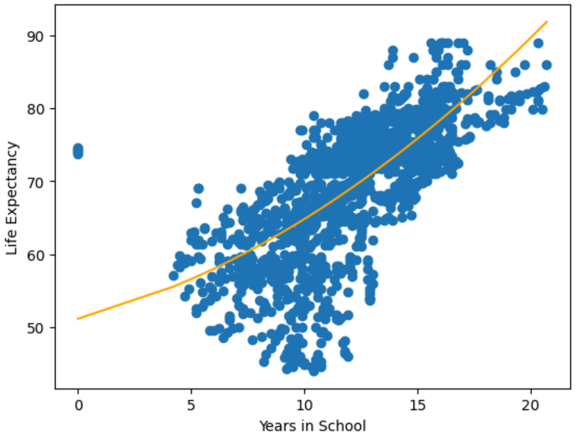

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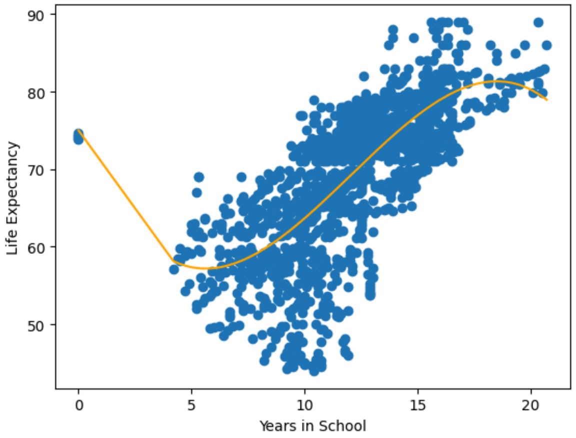

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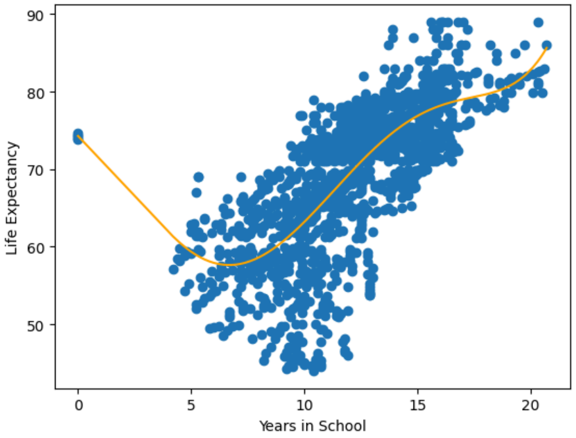

$n = 5$

Question: Which n should we pick?

Example

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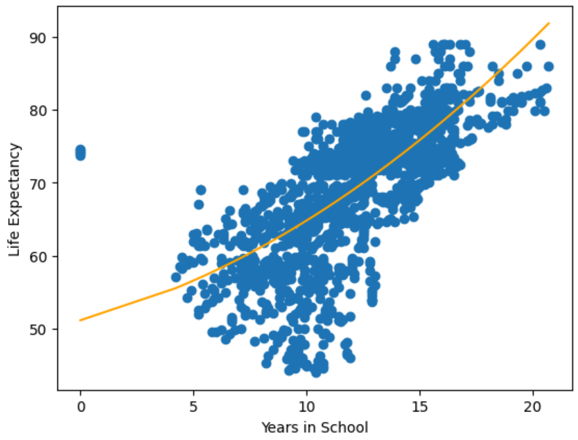
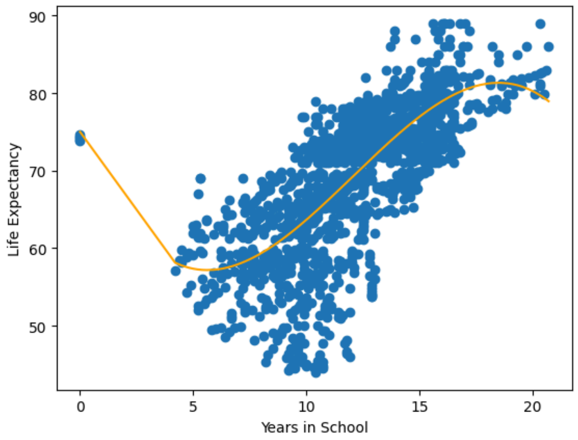
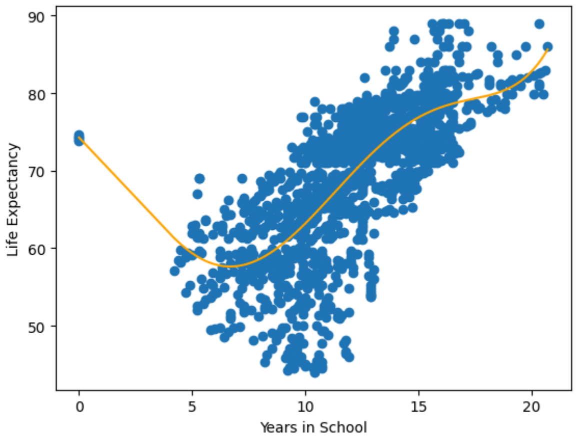




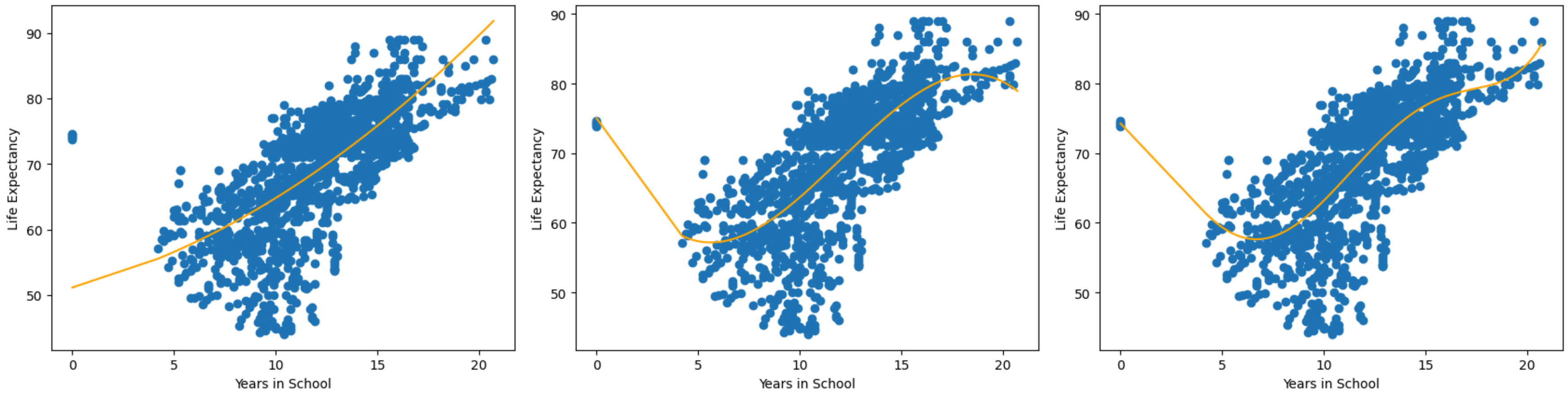


$n = 2$ $n = 3$ $n = 5$

Question: Which n should we pick?

Answer: $n = 2$ feels right, but why?

Example



$n = 2$ $\qquad$ $n = 3$ $\qquad$ $n = 5$

Data can be noisy and we want to fit the trend, not the noise

Example

The world is governed by random processes

Example

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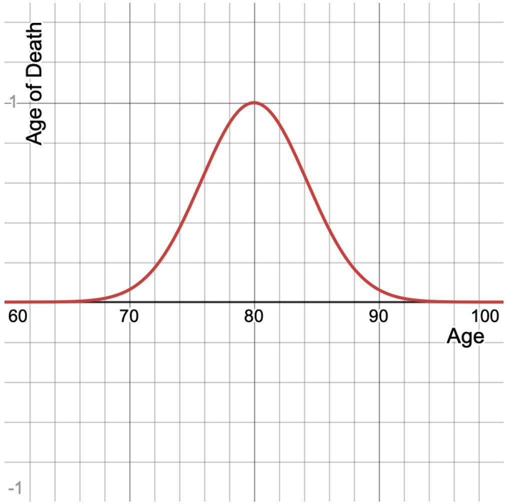

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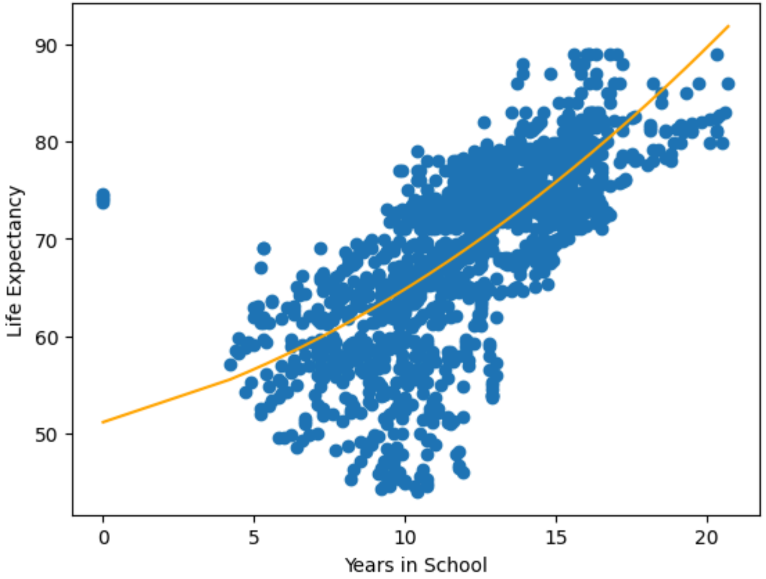
Example

This is just an estimate



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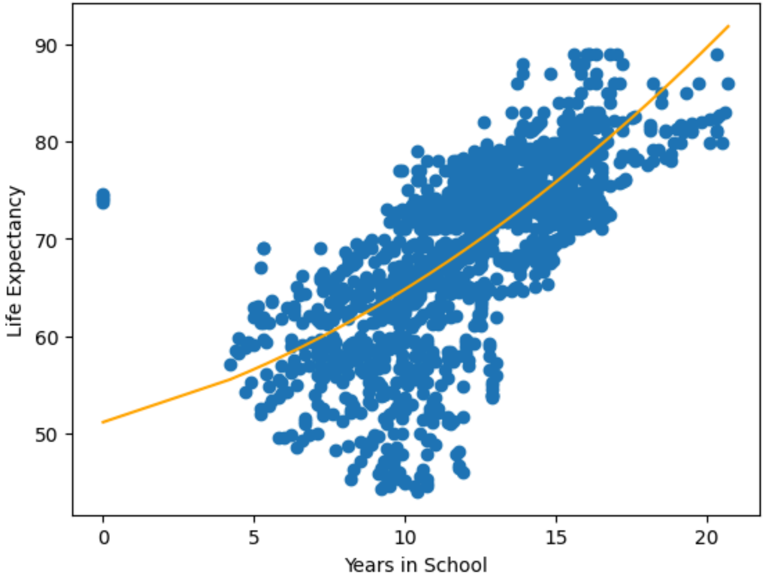
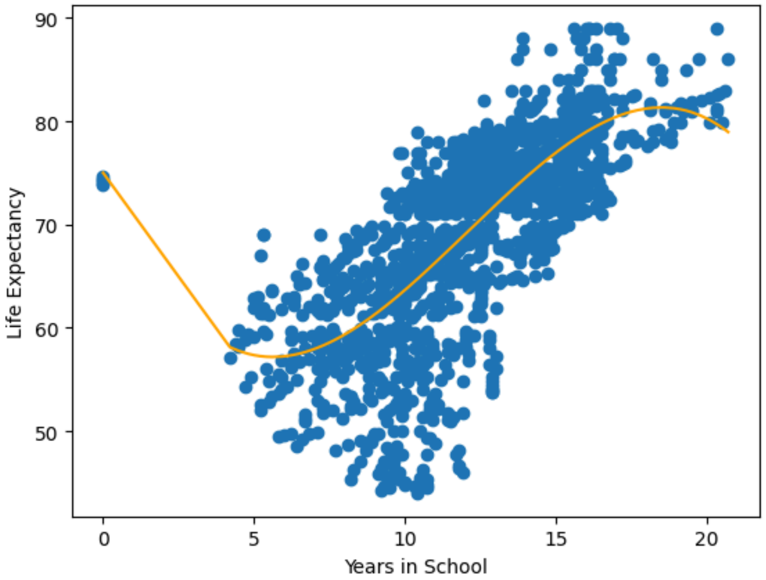
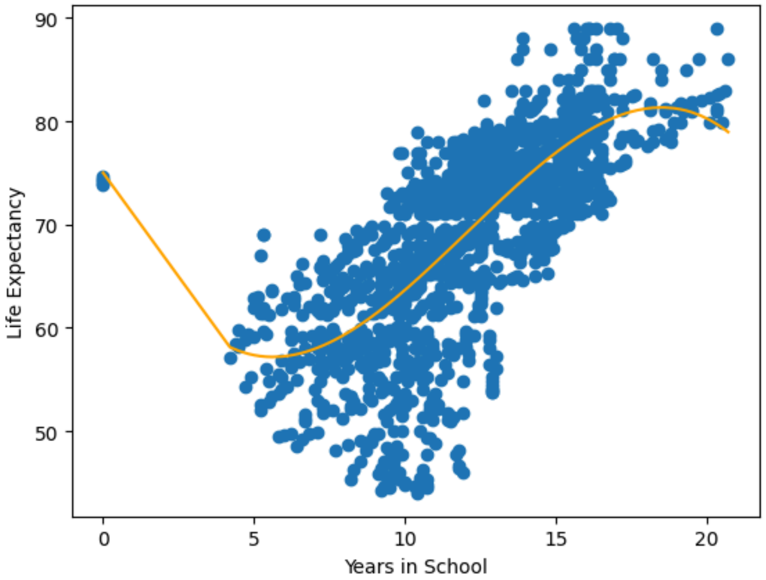


Going to school for 20 years will not save you from a hungry bear

Example

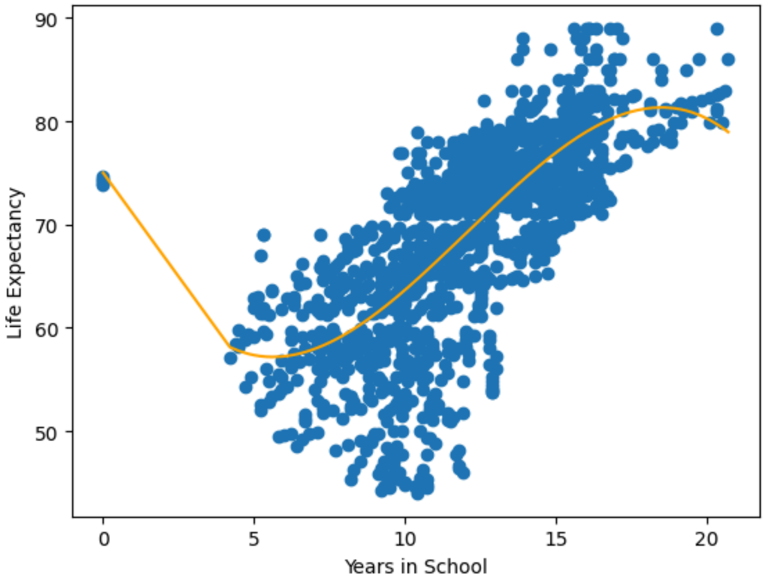


Example



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

Example



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

Overfitting is bad because new predictions will be inaccurate

Example

How can we measure overfitting?

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Learn our parameters from one subset of data: **training dataset**

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

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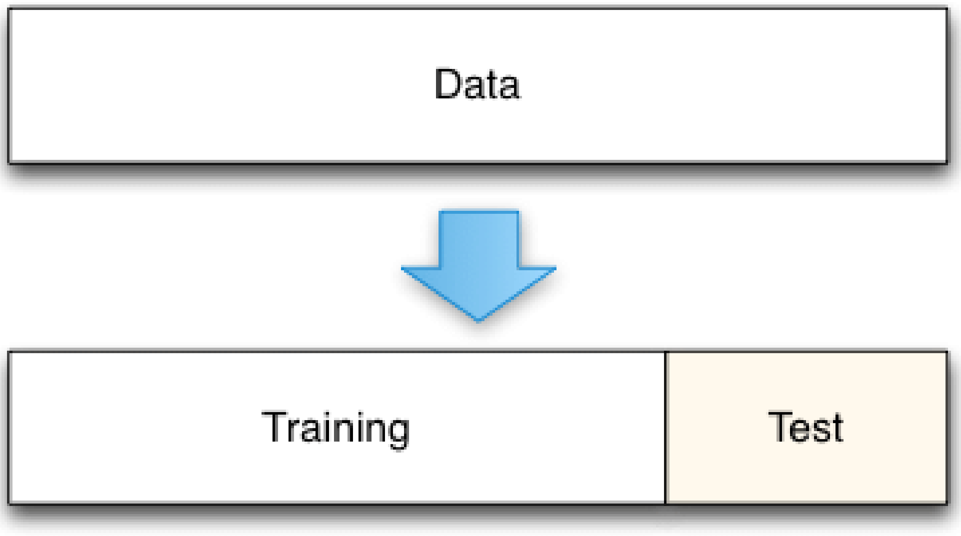

Example

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

Example

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

$$\mathcal{D}_{\text{train}} = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} \qquad \mathcal{D}_{\text{train}} = \begin{bmatrix} x_4 & y_4 \\ x_1 & y_1 \\ x_3 & y_3 \end{bmatrix}$$

$$\mathcal{D}_{\text{test}} = \begin{bmatrix} x_4 & y_4 \\ x_5 & y_5 \end{bmatrix} \qquad \mathcal{D}_{\text{test}} = \begin{bmatrix} x_2 & y_2 \\ x_5 & y_5 \end{bmatrix}$$

Answer: Always shuffle the data

Example

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Answer: Always shuffle the data

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

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- Proposed a linear model
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- Used a trick to extend linear regression to nonlinear functions
- Discussed overfitting and test/train splits