Regression

CISC 7026: Introduction to Deep Learning

University of Macau

Participation

Everyone take out paper and a pen

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Fold the paper into thirds, and write your full name in English and your student ID

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Participate more than once: perfect participation grade

Agenda

1. Review

Agenda

1. Review
2. Quiz

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3. Linear Regression

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Review

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We want to know if the picture is [dog | muffin] $y \in Y$

We learn a function or mapping from X to Y

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$$f\left(你好吗, \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \end{bmatrix} \right) = \text{You good?}$$

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$$x = 你好吗, \quad X = \text{Chinese sentences}$$

$$y = \text{You good?}, \quad Y = \text{English sentences}$$

Review

Create vectors, matrices, or tensors in `jax`

```
import jax.numpy as jnp
a = jnp.array(1) # Scalar
b = jnp.array([1, 2]) # Vector
C = jnp.array([[1,2], [3,4]]) # 2x2 Matrix
D = jnp.ones((3,3,3)) # 3x3x3 Tensor
```

You can determine the dimensions of a variable using `shape`

```
b.shape # Prints (2,)
C.shape # Prints (2,2)
D.shape # prints (3,3,3)
```

Review

Create vectors, matrices, or tensors in `pytorch`

```
import torch
a = torch.tensor(1) # Scalar
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Review

```python
import jax.numpy as jnp

s = 5 * jnp.array([1, 2])
print(s) # jnp.array(5, 10)
x = jnp.array([1, 2]) + jnp.array([3, 4])
print(x) # jnp.array([4, 6])
y = jnp.array([1, 2]) * jnp.array([3, 4]) # Careful!
print(y) # jnp.array([3, 8])
z = jnp.array([[1], [2]]) @ jnp.array([[3, 4]])
print(z) # A^t B (dot product), jnp.array([[11]])
```

Review

`pytorch` is very similar to `jax`

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Review

You can also call various methods on arrays/tensors

```
import jax.numpy as jnp

x = jnp.array([[1, 2], [3, 4]]).sum(axis=0)
print(x) # Sum across leading axis, array([4, 6])
y = jnp.array([[1, 2], [3, 4]]).mean()
print(y) # Mean across all axes, array(2.5)
z = jnp.array([[1, 2], [3, 4]]).reshape((4,))
print(z) # jnp.array([1, 2, 3, 4])
```

Review

Same thing for `pytorch`

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Quiz

Q1: What is the function signature for machine learning?

$$\_\_ : \_\_\_\_\_ \mapsto \_\_$$

Q2: What does the following code print?

```
jnp.array([1, 2]) * jnp.array([2, 1]) + jnp.array([5, 6])
```

Q3: What does the following code print?

```
jnp.array([[1, 2], [3, 4]]).sum(axis=1)
```

Q4: What does the following code print?

```
torch.arange(4)
```

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[1 * 2 + 5, 2 * 1 + 6]
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A2: `Array([7, 8], dtype=int32)`, $\qquad$ `[7, 8]` also ok

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A3: `Array([3, 7], dtype=int32)`, `[3, 7]` also ok

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```

```
[1 + 2, 3 + 4]
```

A3: `Array([3, 7], dtype=int32)`, `[3, 7]` also ok

Q4: What does the following code print?

```
jnp.arange(4)
```

A4: `Array([0, 1, 2, 3], dtype=int32)`, `[0, 1, 2, 3]` also ok

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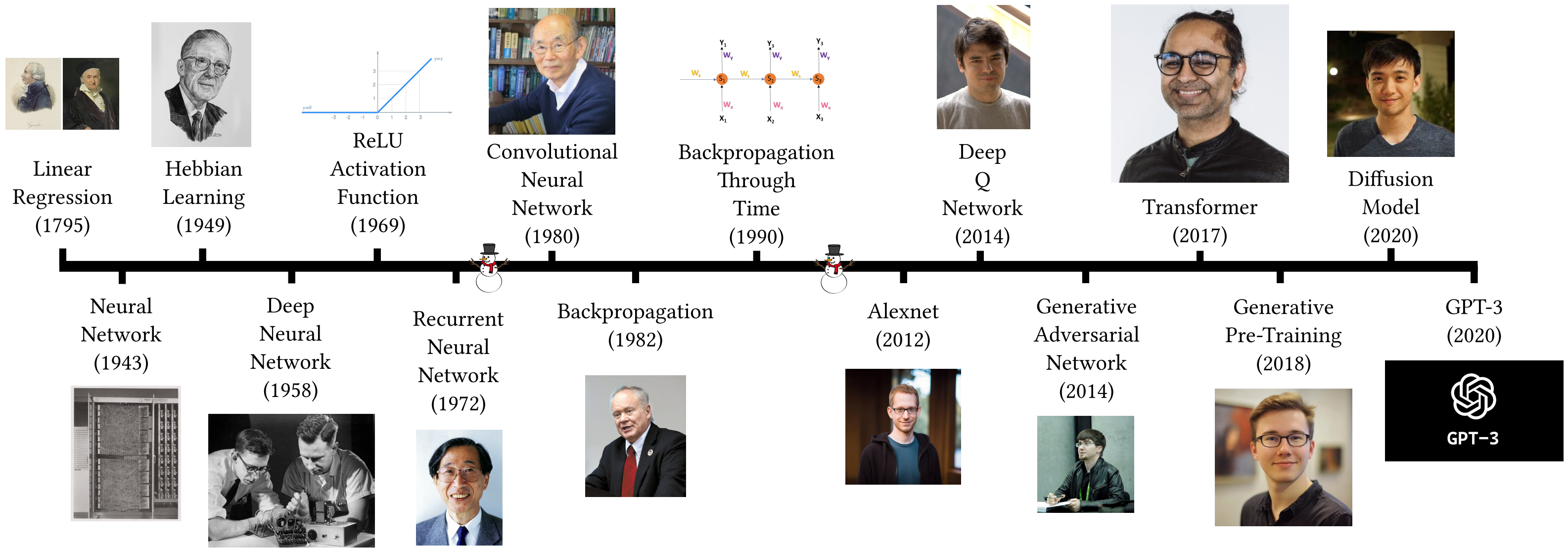

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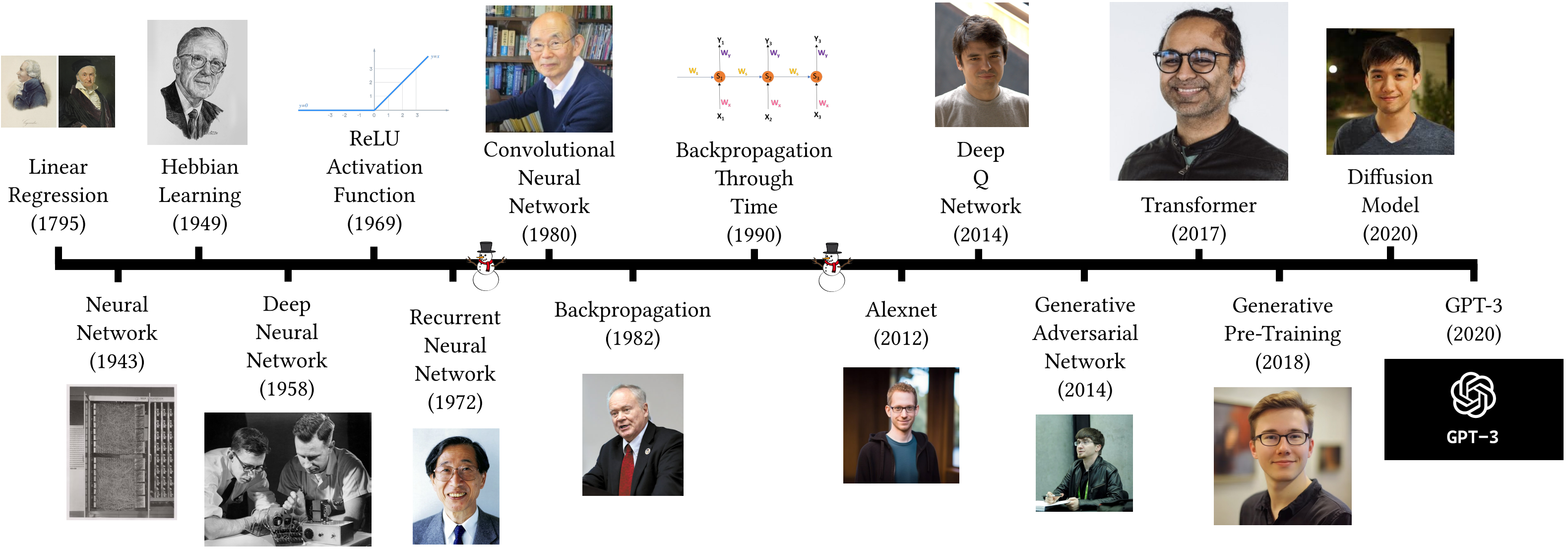

Neural networks share many similarities with linear regression

Linear Regression

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Let us start with regression

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Example Problem

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

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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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- *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

Example Problem

Task: Given your education, predict your life expectancy

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Approach: Learn the parameters θ such that

$$f(x, \theta) = y; \quad x \in X, y \in Y$$

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

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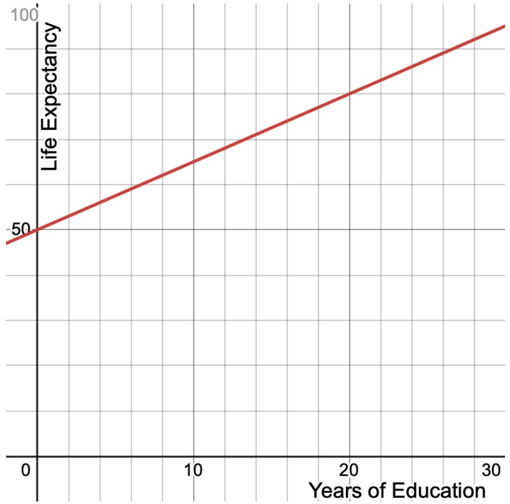
$$f(x, \boldsymbol{\theta}) = f\left(x, \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}\right) = \theta_1 x + \theta_0$$



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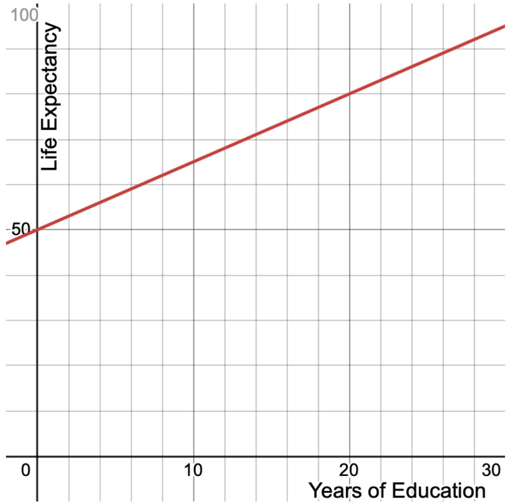

Now, we need to find the parameters $\boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_0 \end{bmatrix}$ that makes $f(x, \boldsymbol{\theta}) = y$

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Loss Function

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

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

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

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

Loss Function

We compute the loss using the **loss function**

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The loss function tells us how close $f(x, \boldsymbol{\theta})$ is to y

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

Loss Function

Let’s derive the error function

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

f(x) should predict y

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Move y to LHS

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Move y to LHS

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

Square for minimization

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f(x) should predict y

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

Move y to LHS

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

Square for minimization

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

Loss Function

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

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

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

Question: Will this $\mathcal{L}$ give us a good prediction for all possible x?

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Question: Will this $\mathcal{L}$ give us a good prediction for all possible x?

Answer: No! We only consider a single datapoint x_i, y_i. We want to learn $\boldsymbol{\theta}$ for the entire dataset, for all $x \in X, y \in Y$

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When $\mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta})$ is small, then $f(x, \boldsymbol{\theta}) \approx y$ for the whole dataset!

Linear Regression

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Here is our loss function:

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Let us state this more formally

Optimization

Our objective is to **minimize** the loss, using $\arg\min$

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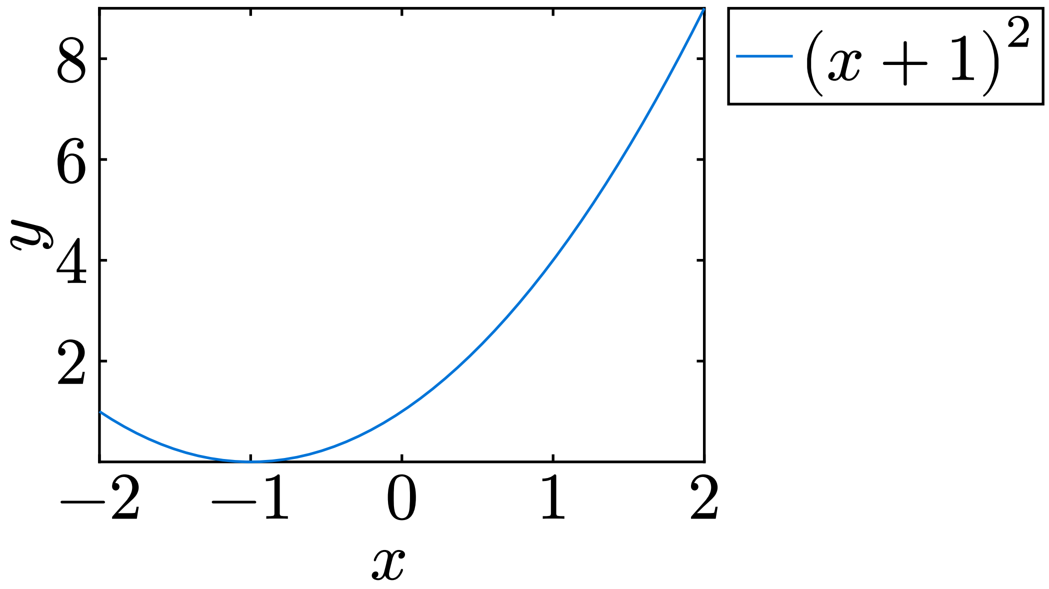
What is $\arg\min_x (x+1)^2$



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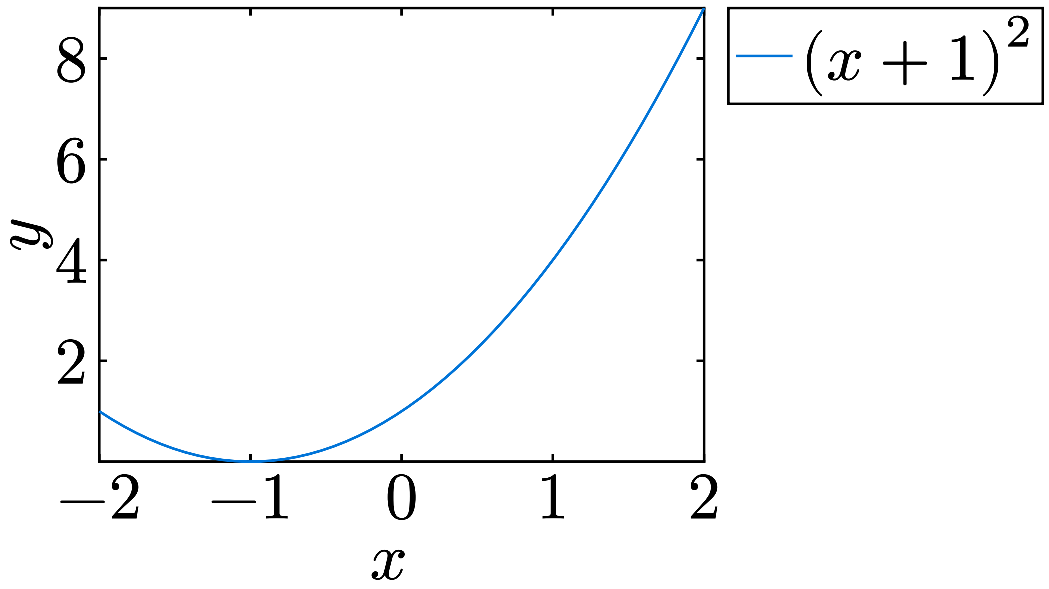

Answer: $\arg\min_x (x+1)^2 = -1$, where $f(x) = 0$

Optimization

Formally, our objective is to find the arg min of the loss

$$\begin{aligned}\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{\theta}) &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \text{error}(f(x_i, \boldsymbol{\theta}), y_i) \\ &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} (f(x_i, \boldsymbol{\theta}) - y_i)^2\end{aligned}$$

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We will go over the steps to find $\boldsymbol{\theta}$

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

Optimization

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

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

Optimization

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

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

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(Magic!) We can find the parameters that minimize $\mathcal{L}$

Optimization

To summarize:

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Linear Regression

Back to the example...

Linear Regression

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Task: Given your education, predict your life expectancy

Linear Regression

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

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You will be doing this in your first assignment!

Linear Regression

Plot the datapoints $(x_1, y_1), (x_2, y_2), ...$

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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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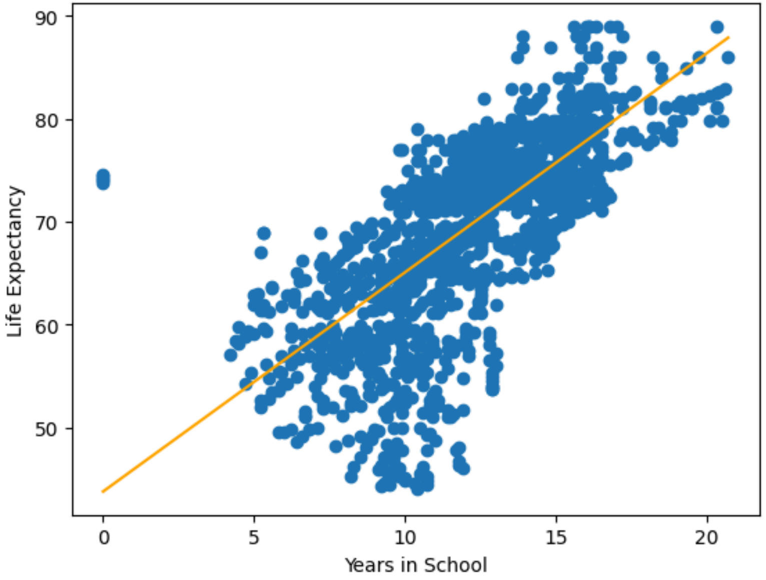

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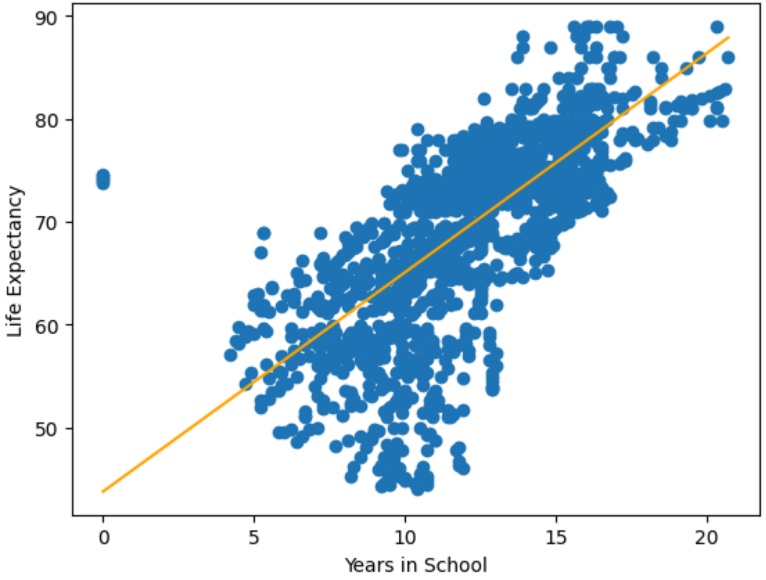

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Relax

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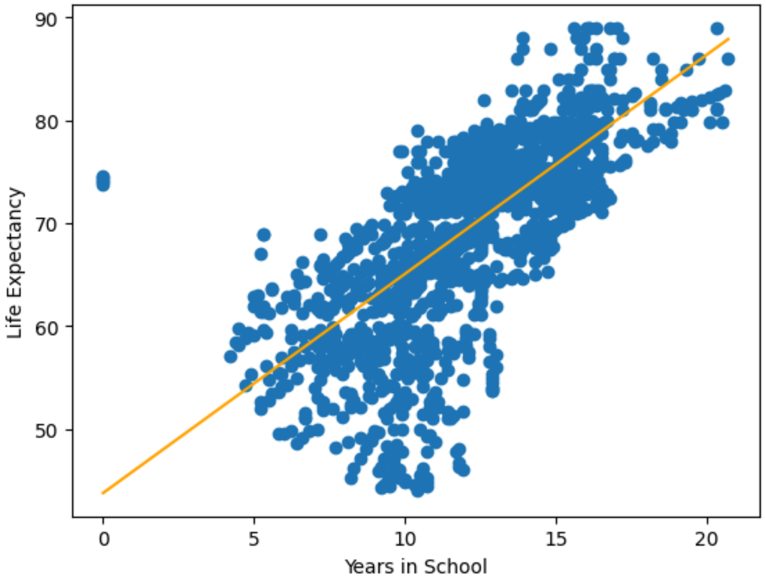

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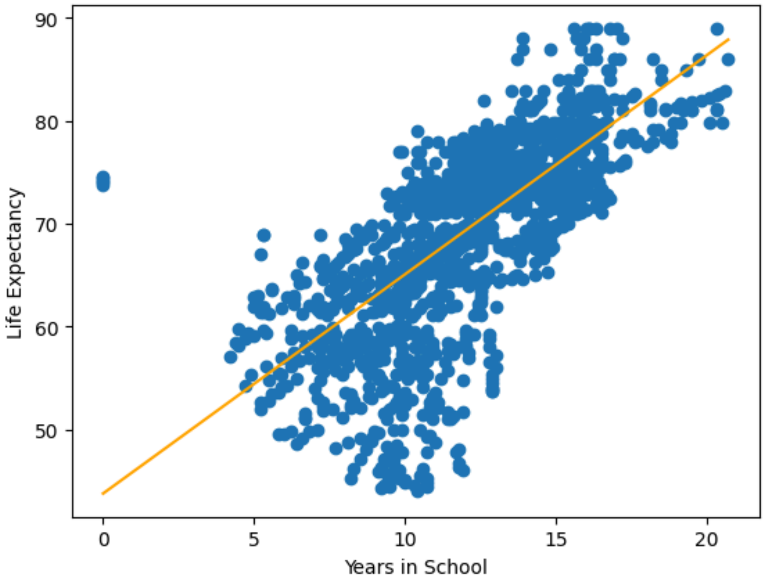
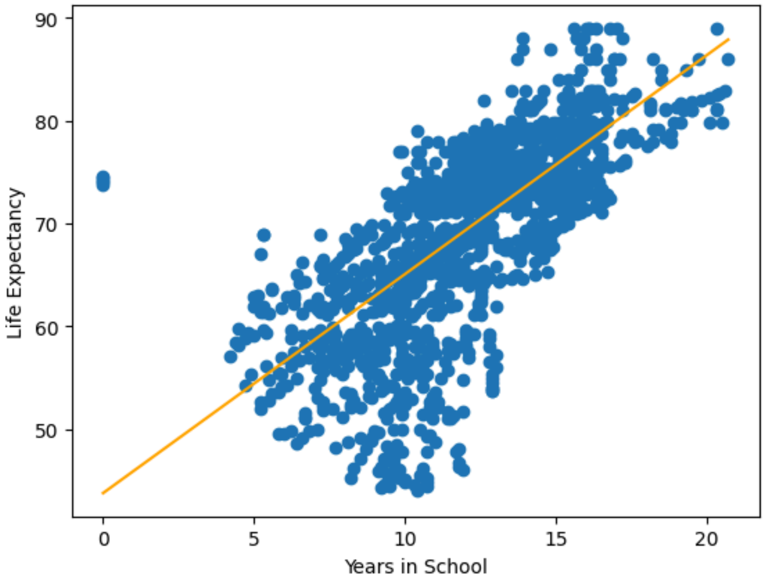


We figured out linear regression!

Linear Regression



We figured out linear regression!

But can we do better?

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Does the data look linear?

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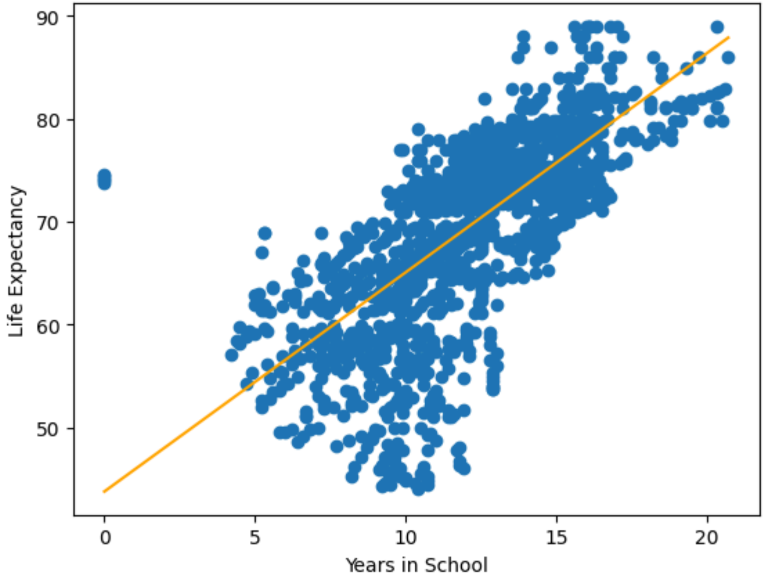

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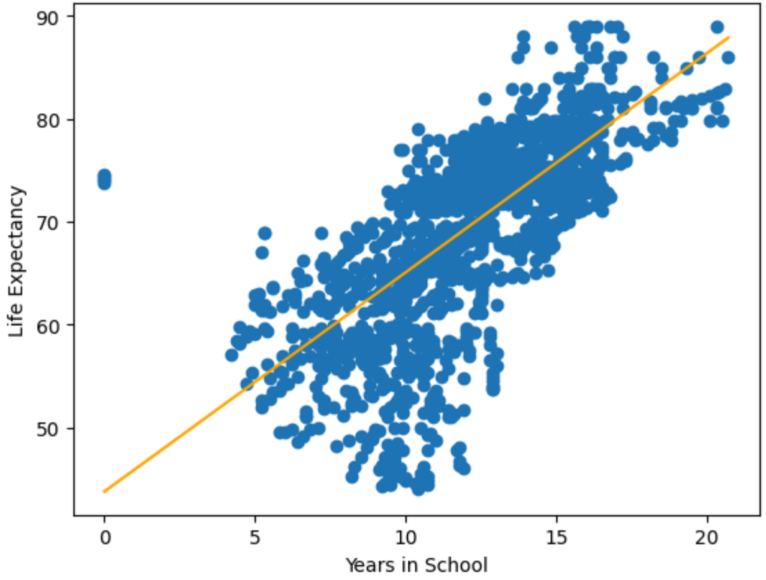

Or maybe more logarithmic?

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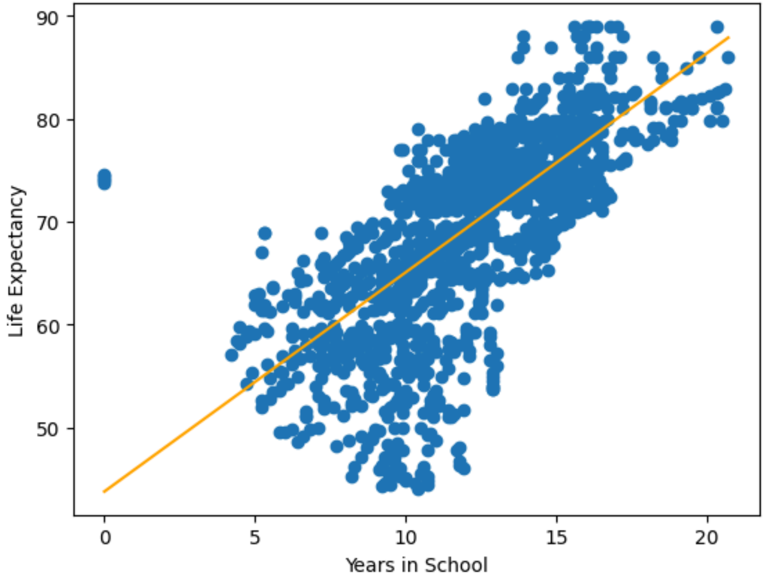

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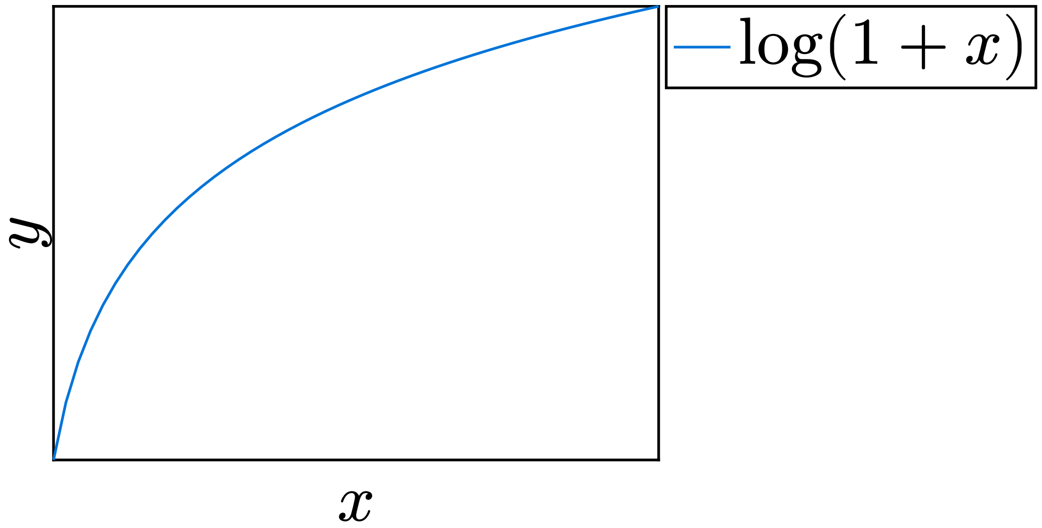

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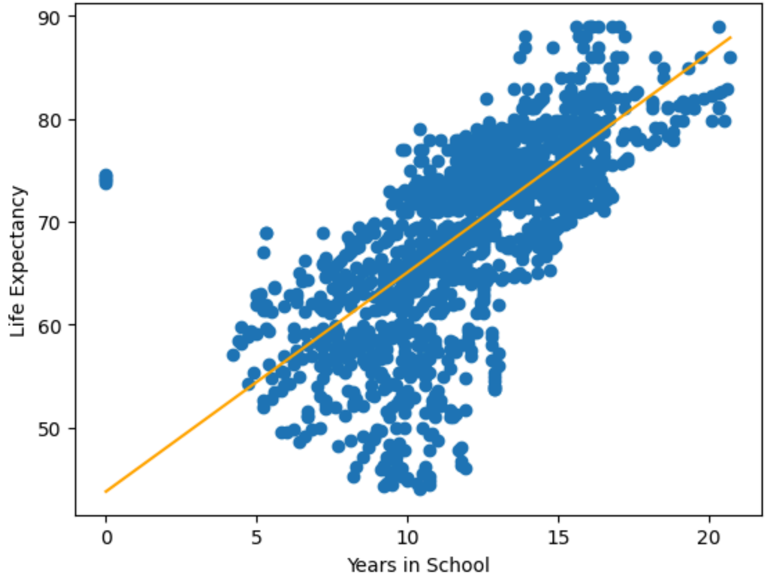

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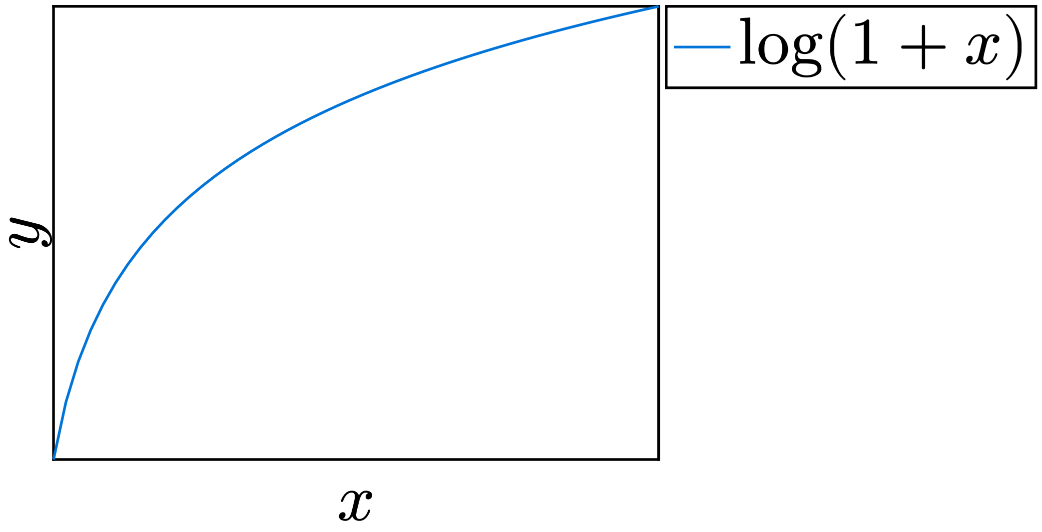

However, linear regression must be linear!

Nonlinear Regression

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

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

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

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

Nonlinear Regression

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...

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

Nonlinear Regression

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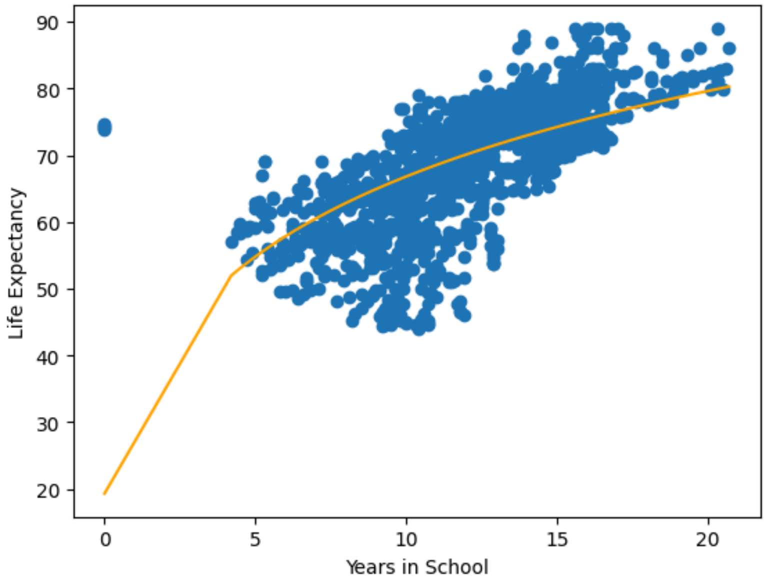
New function...

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

Same solution...

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

Nonlinear Regression



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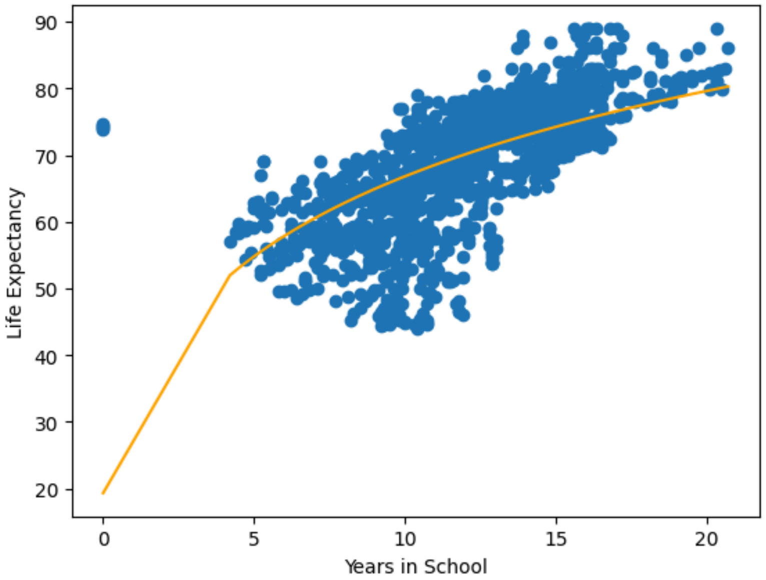
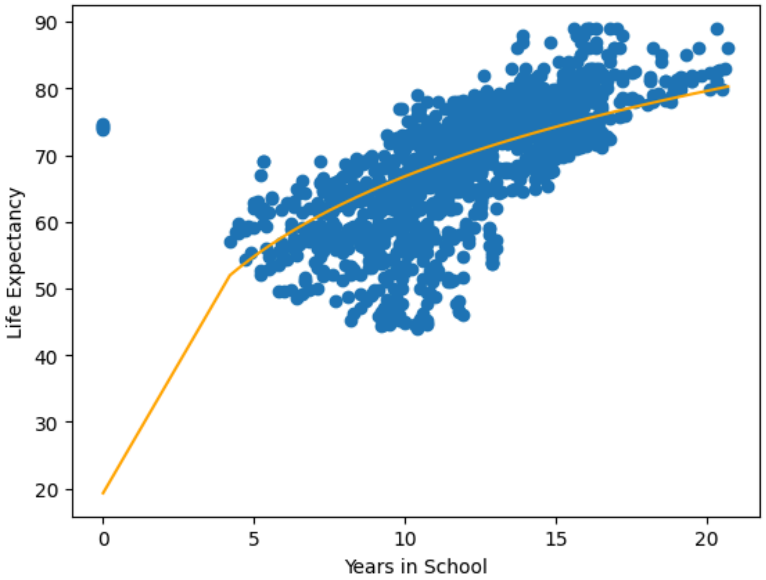


Better, but still not perfect

Nonlinear Regression



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Can we do even better?

Nonlinear Regression

What about polynomials?

Nonlinear Regression

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

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Can we extend linear regression to polynomials?

Nonlinear Regression

Expand x to a multi-dimensional input space...

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Expand x to a multi-dimensional input space...

$$\boldsymbol{X}_D = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \Rightarrow \boldsymbol{X}_D = \begin{bmatrix} x_1^n & x_1^{n-1} & \dots & x_1 & 1 \\ x_2^n & x_2^{n-1} & \dots & x_2 & 1 \\ \vdots & \vdots & \ddots & & \\ x_n & x_n^{n-1} & \dots & x_n & 1 \end{bmatrix}$$

And add some new parameters...

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

Nonlinear Regression

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

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

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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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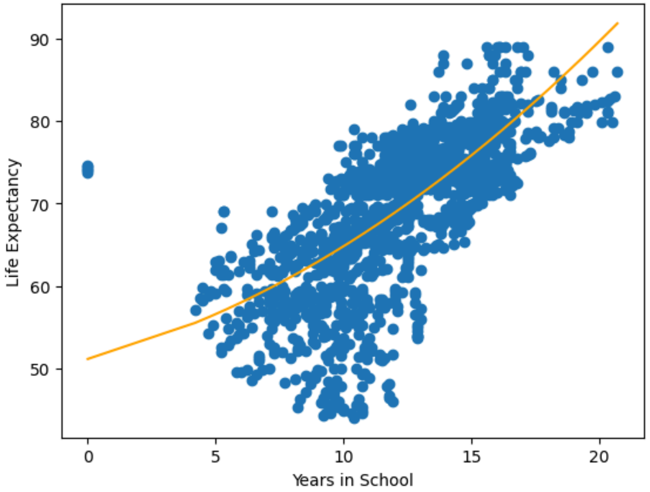
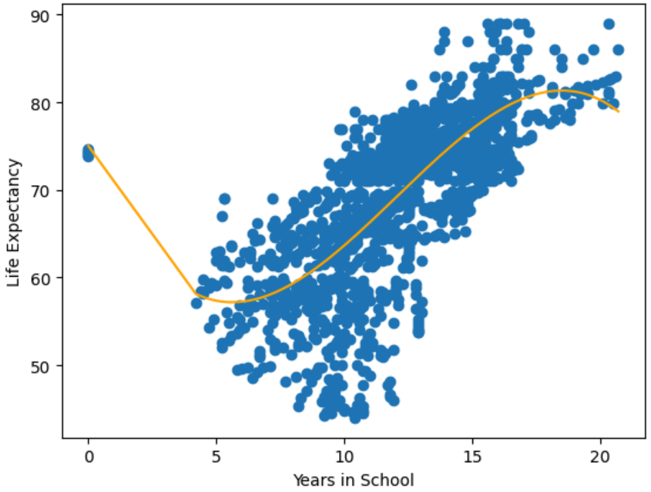
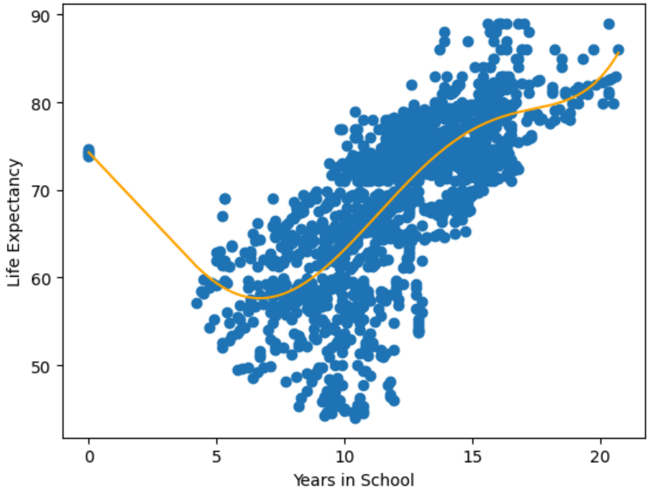


$n = 2$



$n = 3$



$n = 5$

Overfitting

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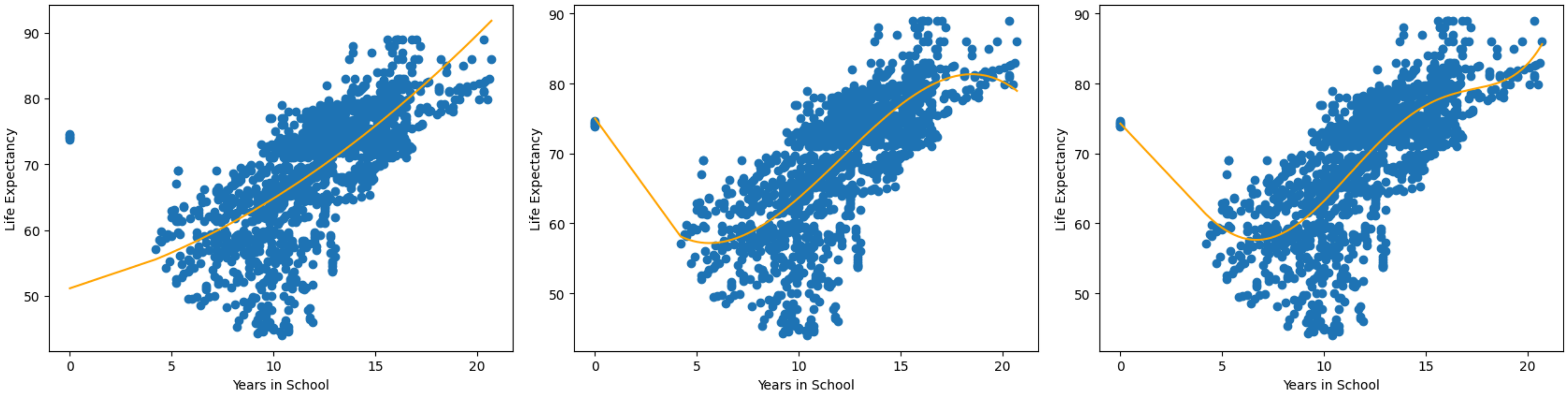
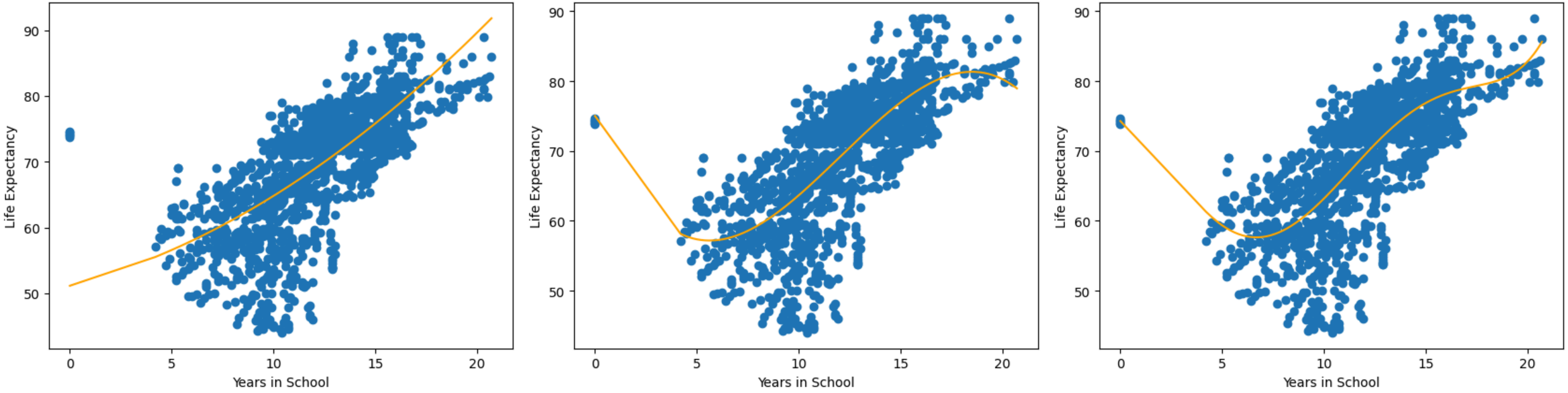


$n = 2$ $\qquad$ $n = 3$ $\qquad$ $n = 5$

Pick the n with the smallest loss

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

Overfitting



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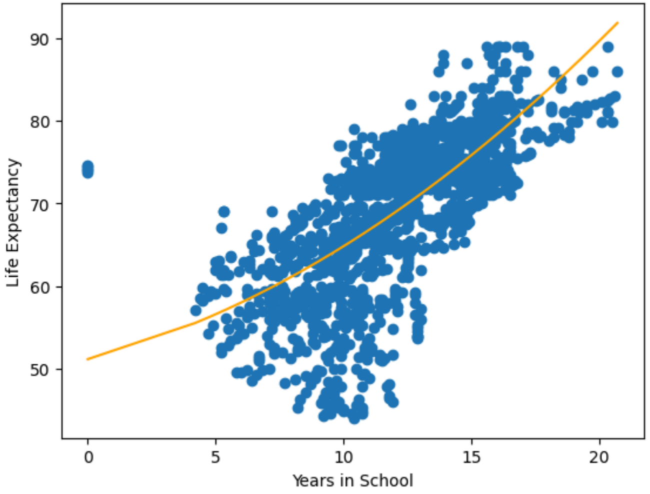
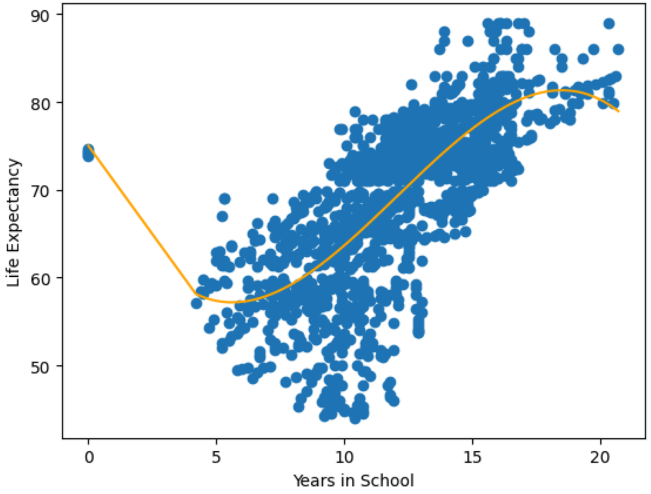
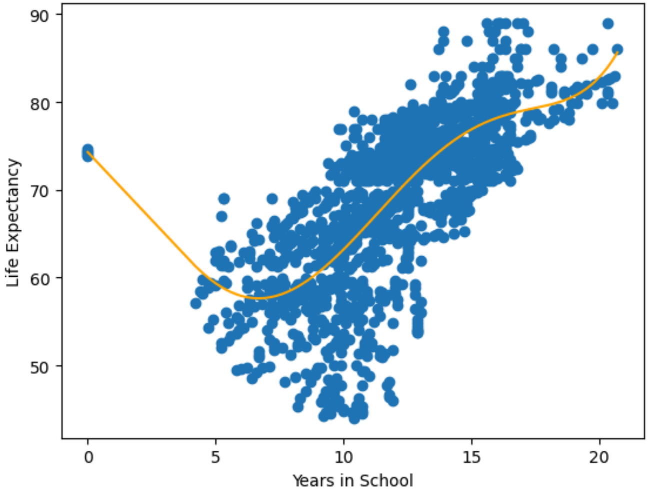
Question: Which n do you think has the smallest loss?

Overfitting







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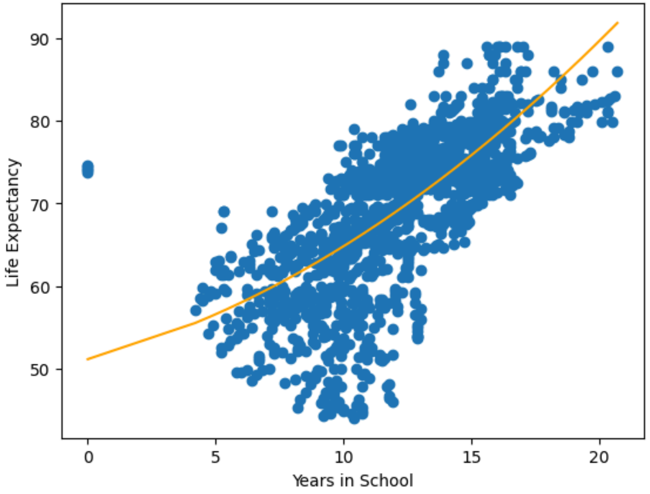
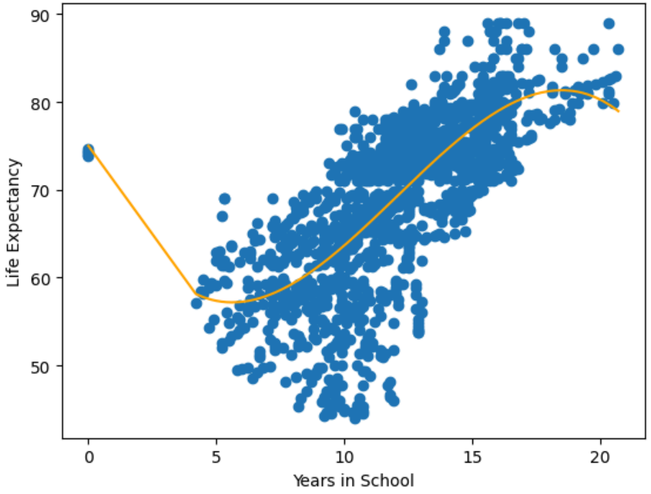
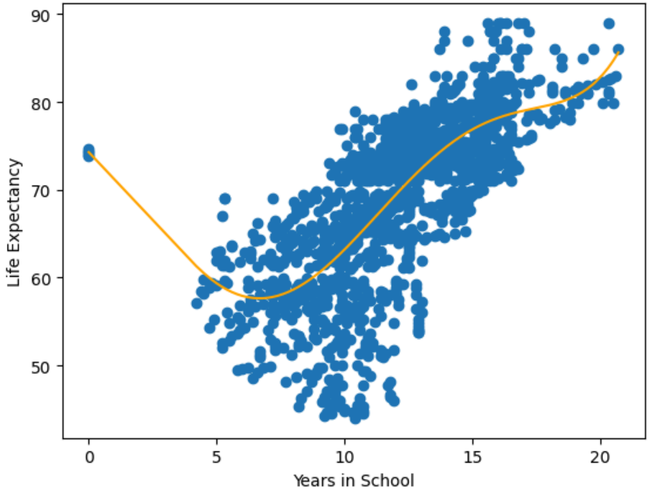
Question: Which n do you think has the smallest loss?

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

Overfitting







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

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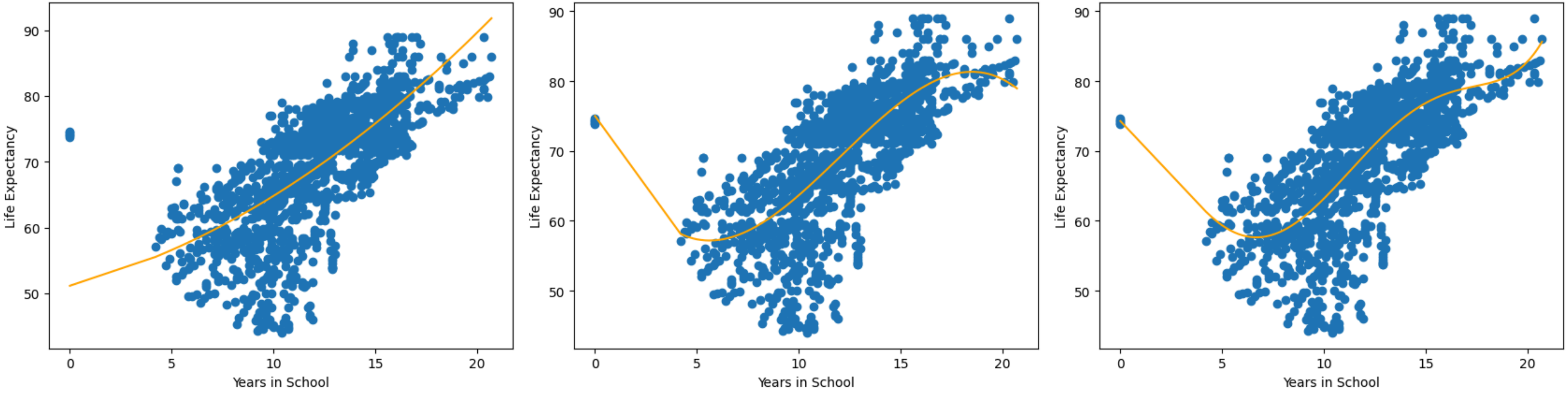

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We will only use our model for new data (we already have the y for a known x)!

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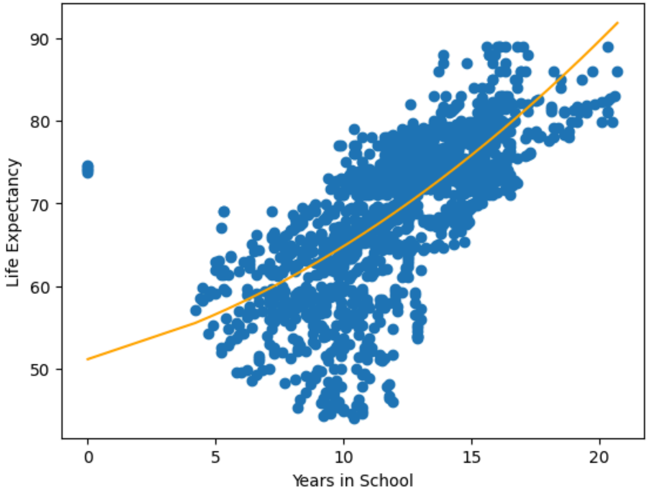

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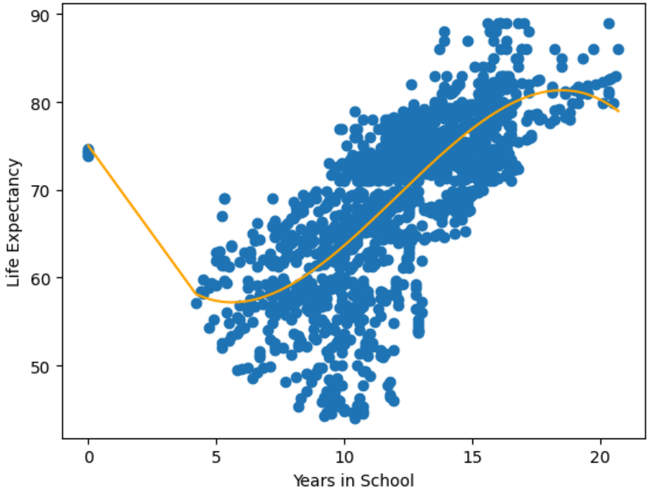

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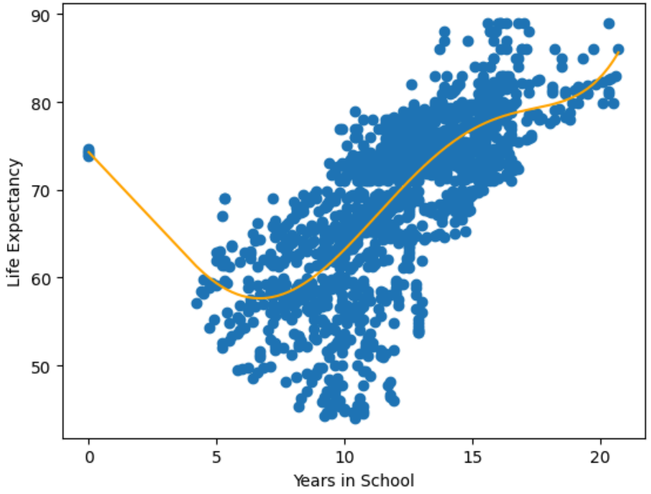

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Answer: Compute the loss on unseen data!

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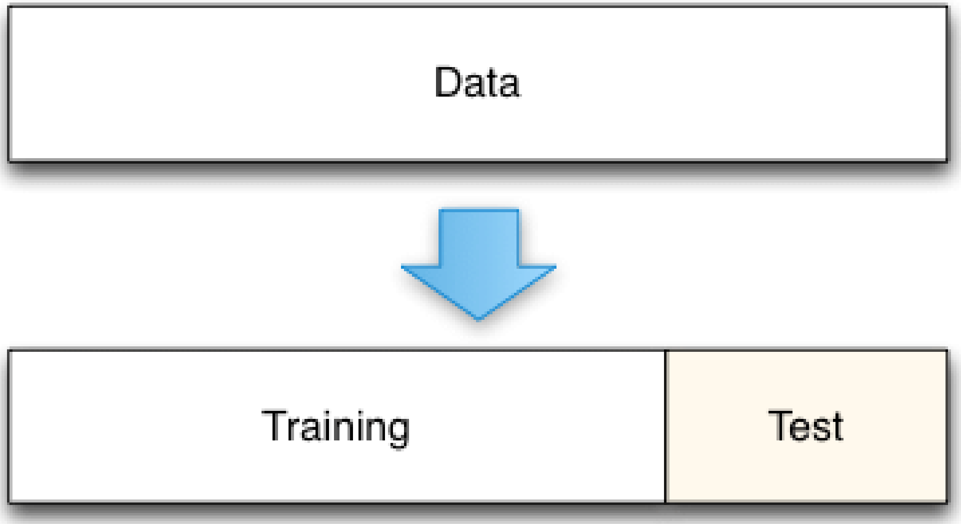

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Note: The model must never see the testing dataset during training. This is very important!

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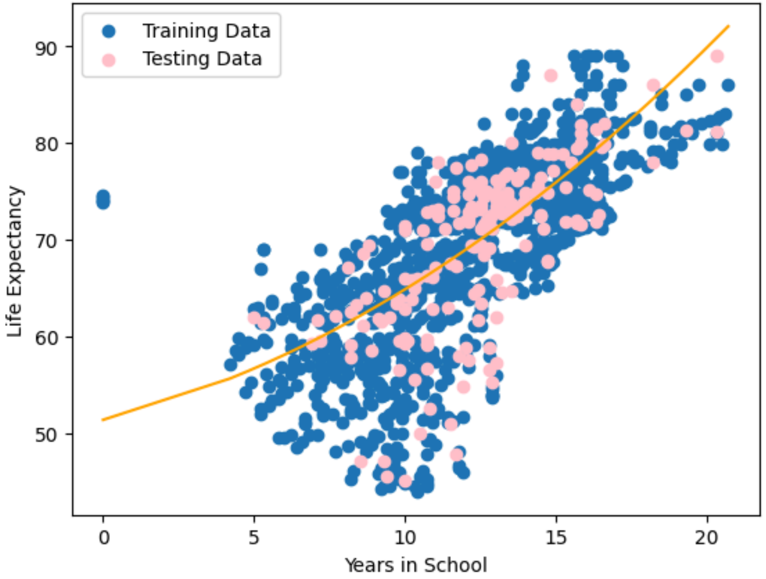

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$$\mathcal{L}(\boldsymbol{X}_{\text{train}}, \boldsymbol{y}_{\text{train}}, \boldsymbol{\theta}) \qquad\qquad \mathcal{L}(\boldsymbol{X}_{\text{test}}, \boldsymbol{y}_{\text{test}}, \boldsymbol{\theta})$$

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We use separate training and testing datasets on **all** machine learning models, not just linear regression

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Everything you need is in the lecture notes

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https://colab.research.google.com/drive/1I6YgapkfaU71RdOotaTPLYdX9WflV1me