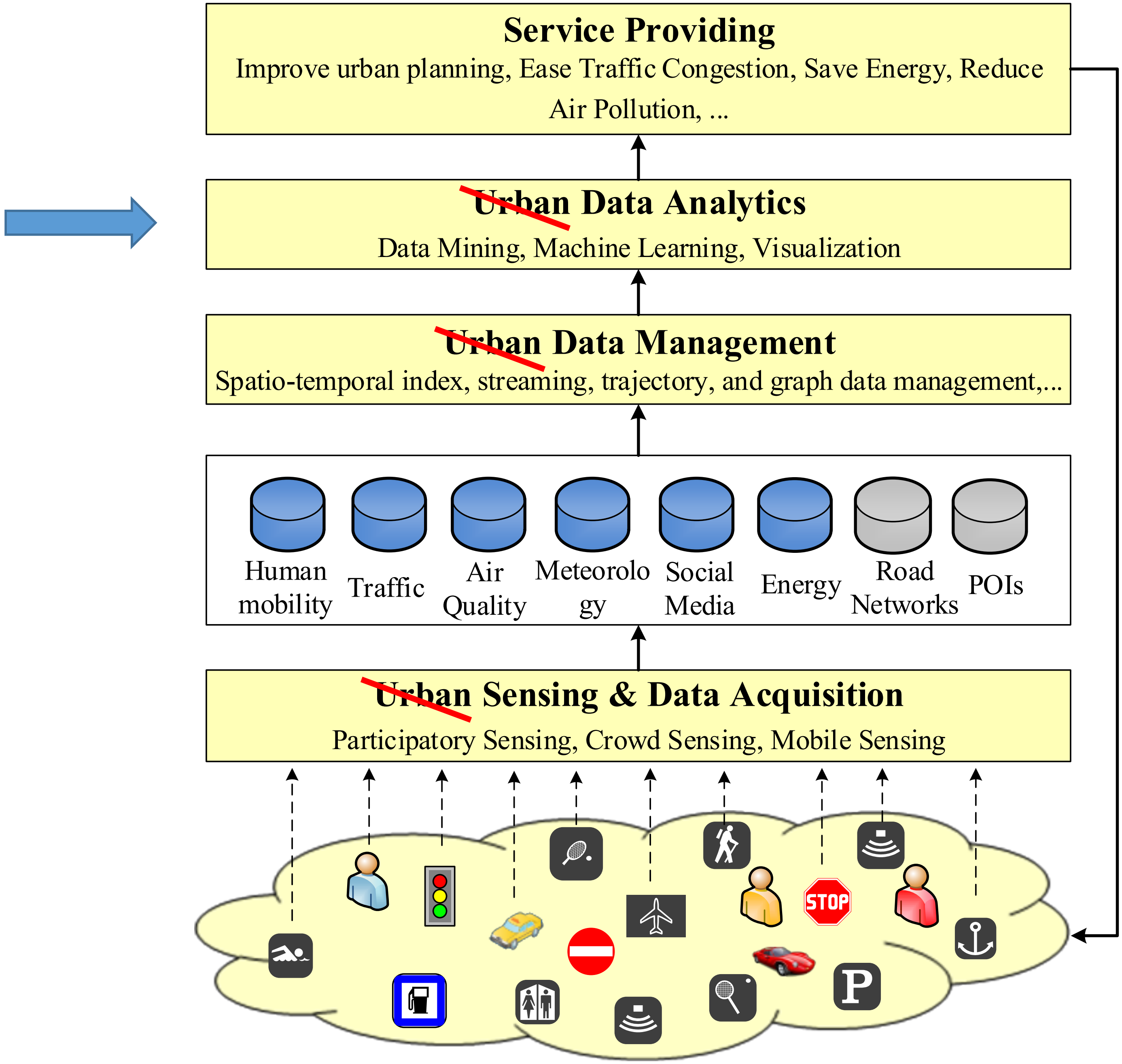
Welcome to

DS3010:
DS-III: Computational Data Intelligence
Machine Learning Introduction

Prof. Yanhua Li

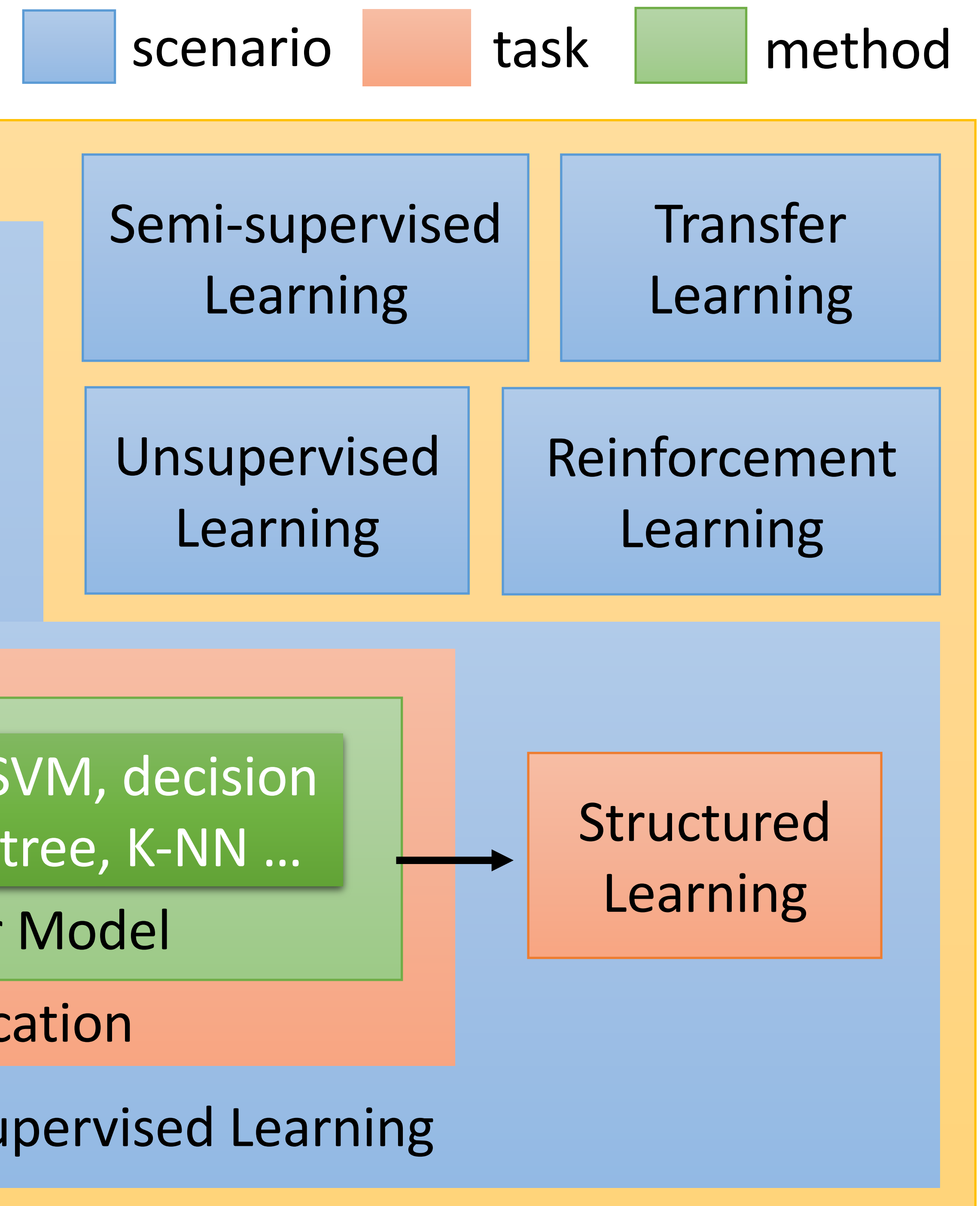
Time: 11:00am – 12:50pm M & R
Location: HL 114
D-term 2022

Data pipeline



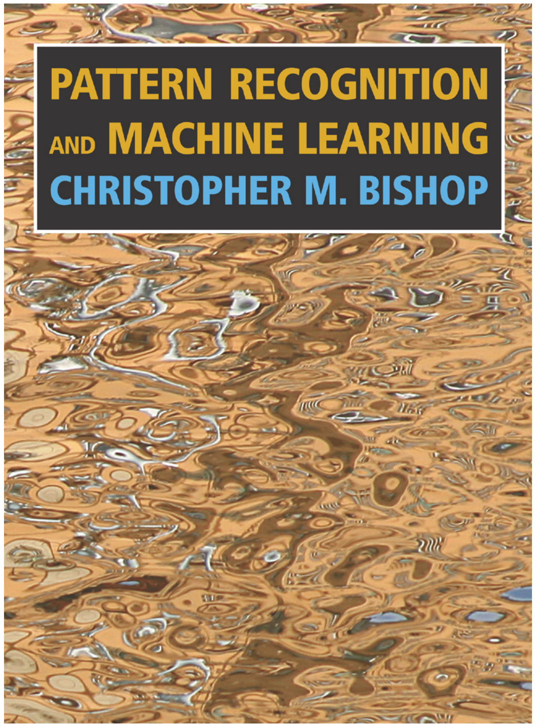
Urban Computing: concepts, methodologies, and applications.
Zheng, Y., et al. *ACM transactions on Intelligent Systems and Technology*.

Learning Map



References

Regression



Bishop: Chapter 1.1

Regression: Output a scalar

- Stock Market Forecast

$f($  $) =$ Dow Jones Industrial Average at tomorrow

- Self-driving Car

$f($  $) =$ Degree to turning the steering wheel

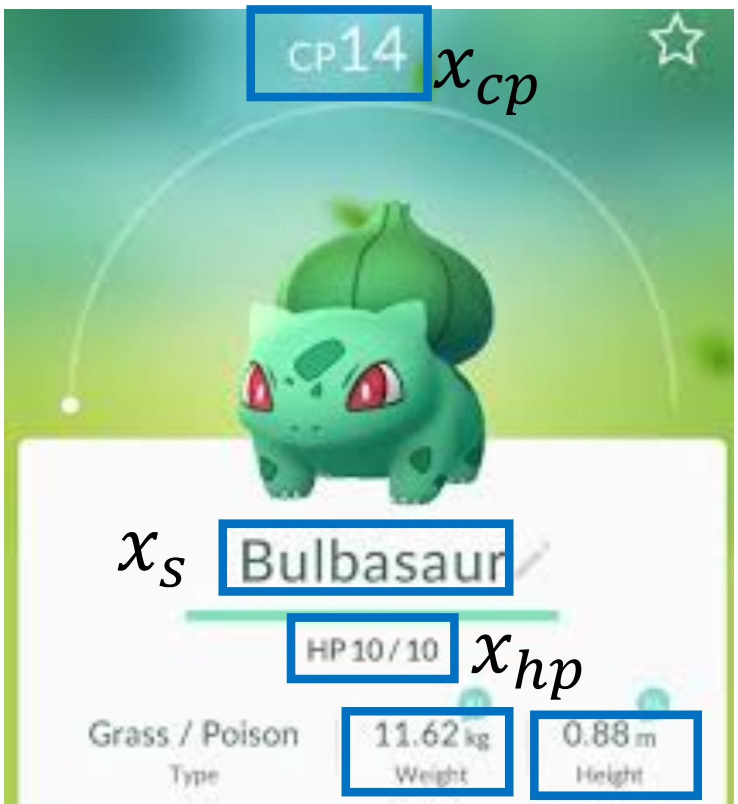
- Recommendation

$f($ Customer A Item B $) =$ Chance of purchase

Example Application

- Estimating the Combat Power (CP) of a pokemon after evolution

$f($



x_{cp} x_s x_{hp} x_w x_h

x

$) =$ CP after evolution y

Step 1: Model

w and b are parameters
(can be any value)

$y = b + w \cdot x_{cp}$

A set of function

Model

$f_1, f_2 \cdots$

f_1: $y = 10.0 + 9.0 \cdot x_{cp}$

f_2: $y = 9.8 + 9.2 \cdot x_{cp}$

f_3: $y = -0.8 - 1.2 \cdot x_{cp}$

…… infinite

$f($

$x) =$ CP after evolution y

x_i: $x_{cp}, x_{hp}, x_w, x_h \ldots$

Linear model: $y = b + \sum w_i x_i$

feature

w_i: weight, b: bias

Step 2: Goodness of Function

$y = b + w \cdot x_{cp}$

A set of function

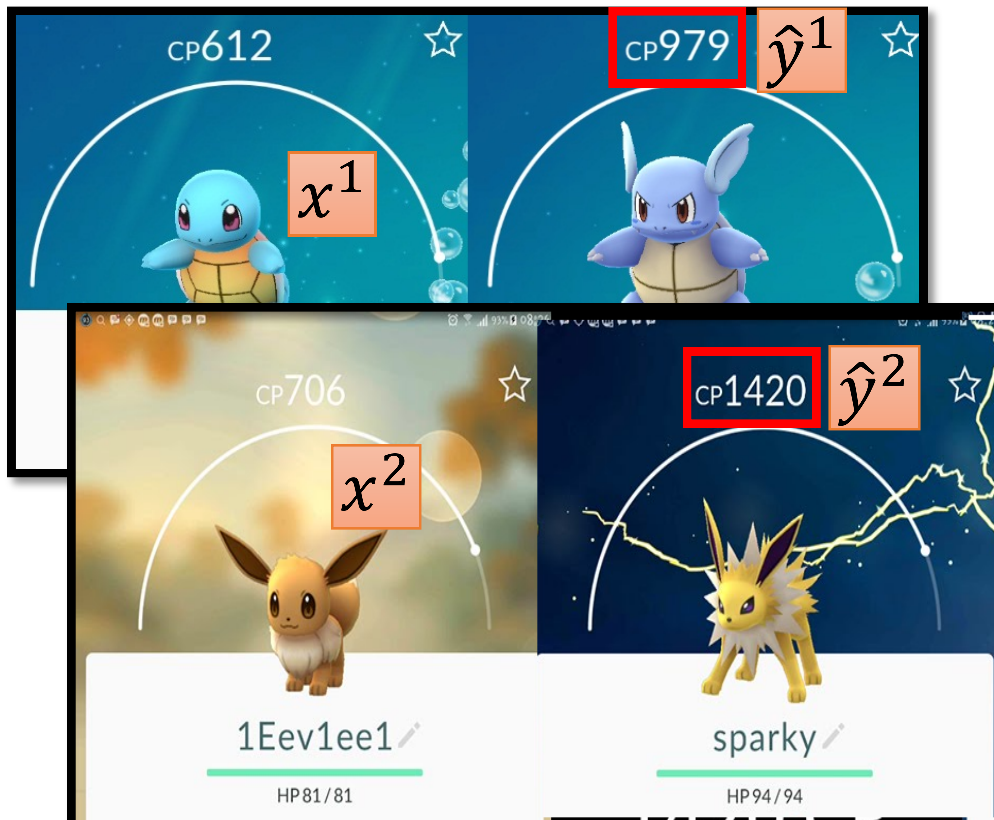
Model

$f_1, f_2 \cdots$

Training Data

function input:

function Output (scalar):



Step 2: Goodness of Function

Training Data:
10 pokemons

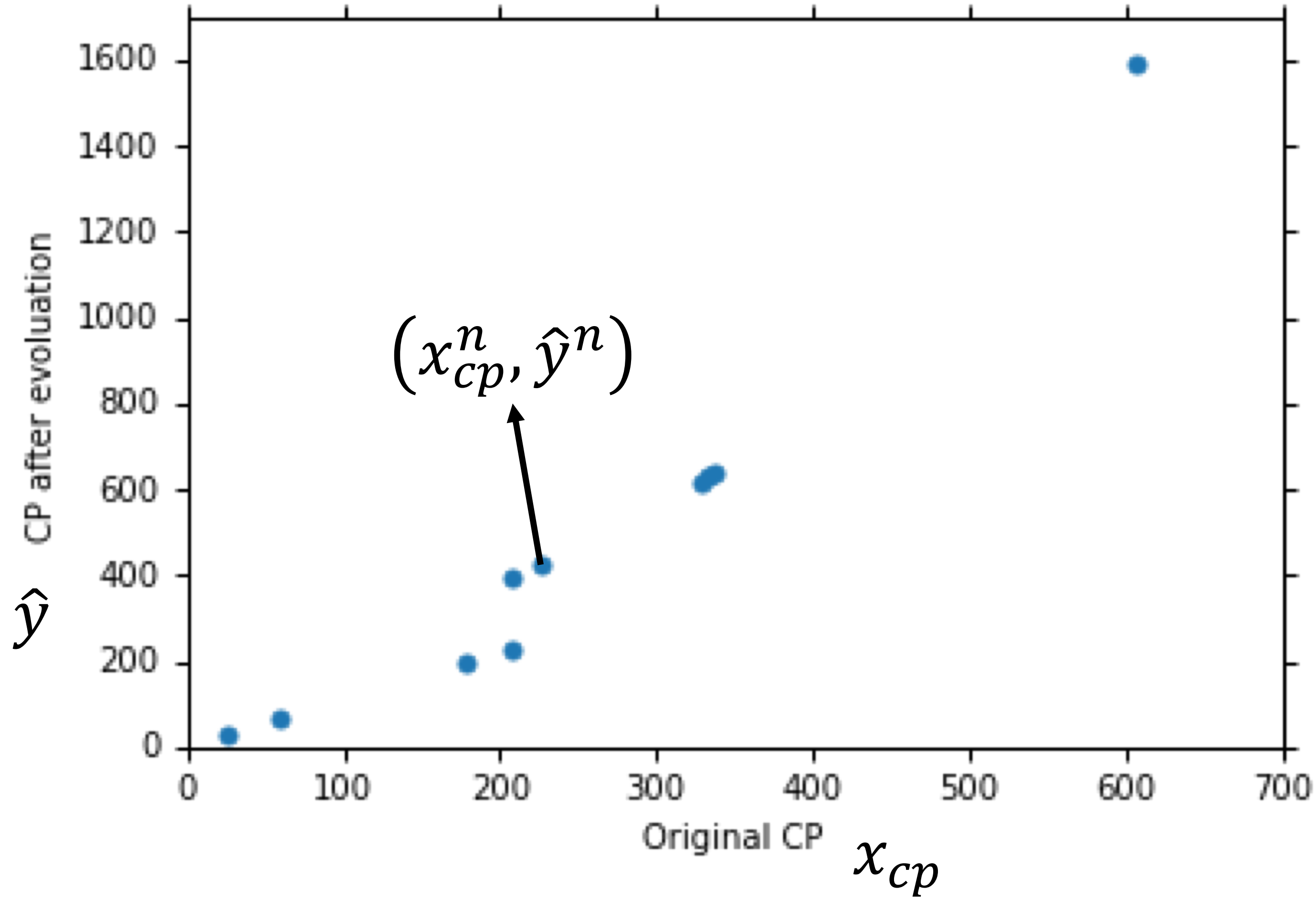
$(x^1, \hat{y}^1)$

$(x^2, \hat{y}^2)$

⋮

$(x^{10}, \hat{y}^{10})$

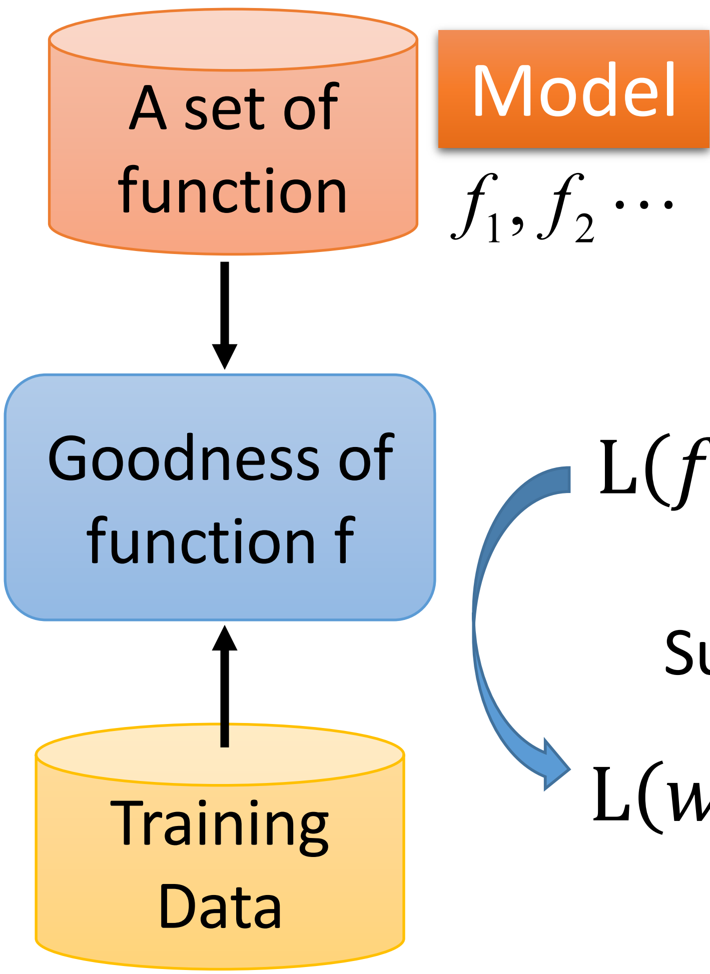
This is real data.



Source: https://www.openintro.org/book/statdata/index.php?data=pokemon

Step 2: Goodness of Function

$y = b + w \cdot x_{cp}$



Loss function L:

Input: a function, output: how bad it is

Estimation error

$$L(f) = \sum_{n=1}^{10} \boxed{\left(\hat{y}^n - f\left(x_{cp}^n\right)\right)^2}$$

Sum over examples

Estimated y based on input function

$$L(w, b) = \sum_{n=1}^{10} \left(\hat{y}^n - \left(b + w \cdot x_{cp}^n\right)\right)^2$$

Step 2: Goodness of Function

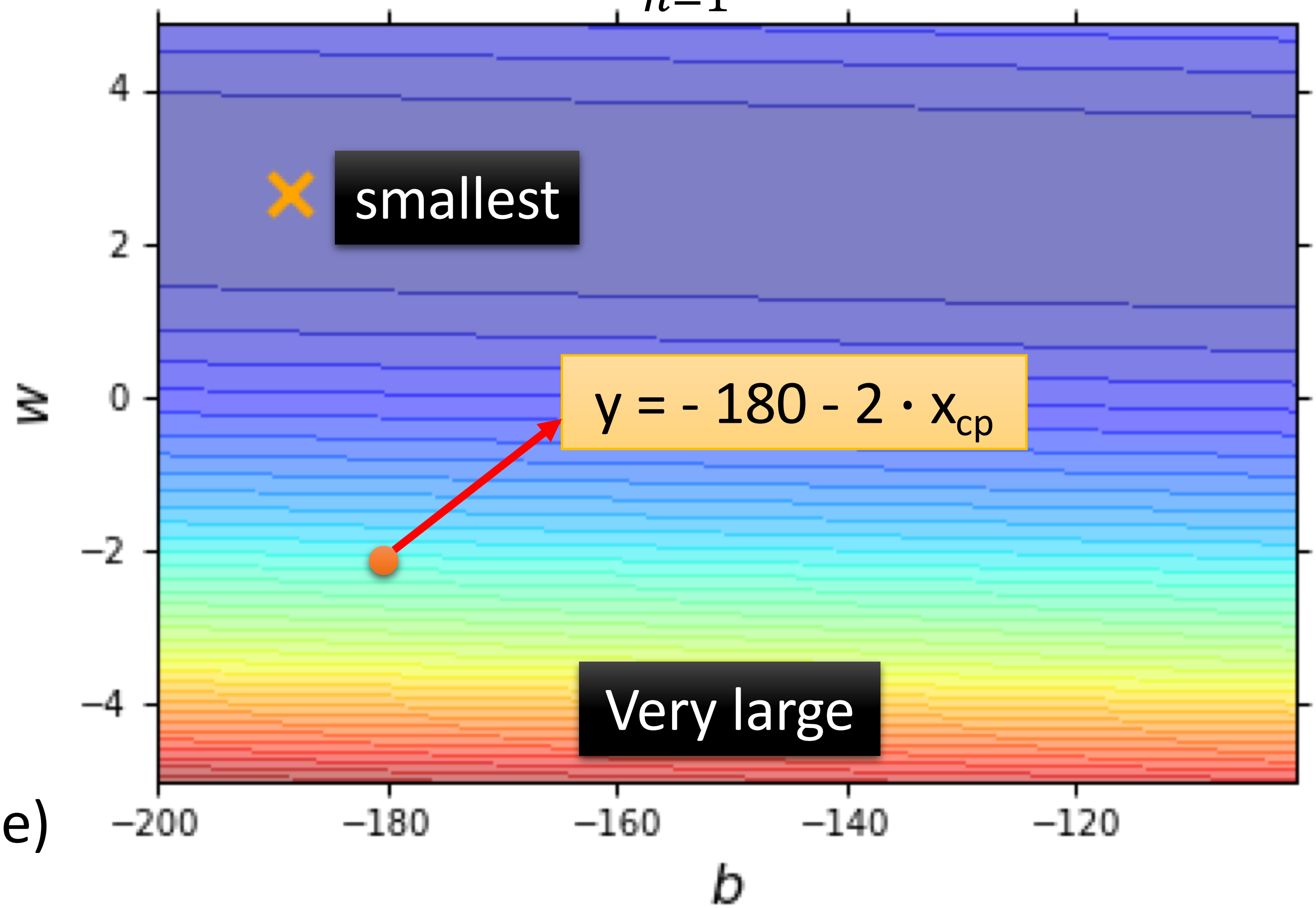
- Loss Function

$$L(w, b) = \sum_{n=1}^{10} \left(\hat{y}^n - \left(b + w \cdot x_{cp}^n \right) \right)^2$$

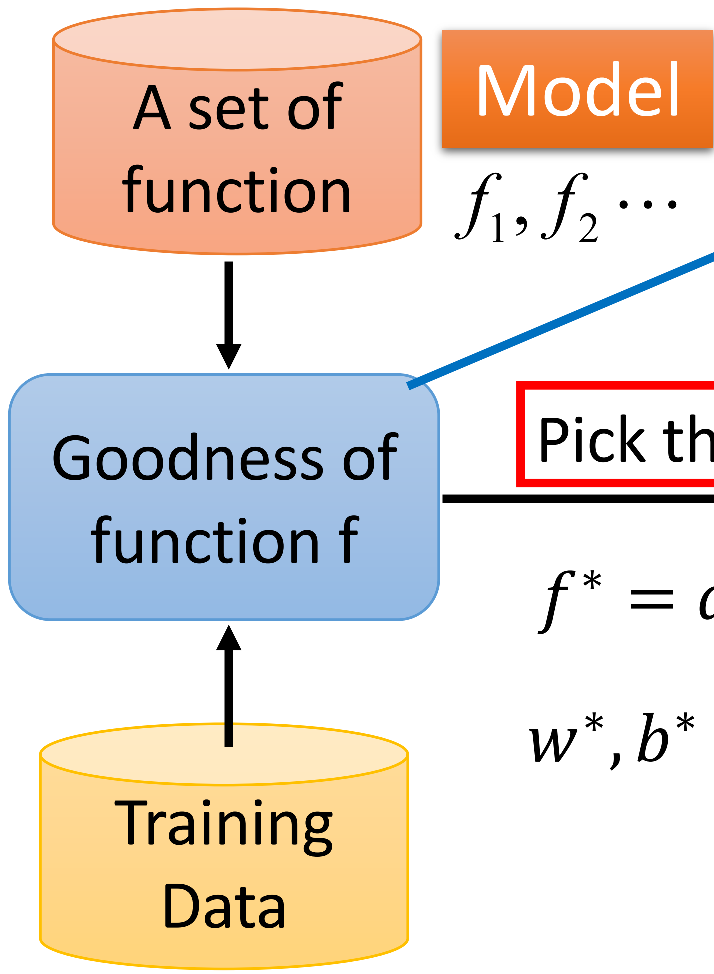
Each point in the figure is a function

The color represents $L(w, b)$.

(true example)



Step 3: Best Function



$$L(w, b) = \sum_{n=1}^{10} \left(\hat{y}^n - \left(b + w \cdot x_{cp}^n \right) \right)^2$$

Pick the "Best" Function

$$f^* = arg \min_f L(f)$$

$$w^*, b^* = arg \min_{w,b} L(w, b)$$

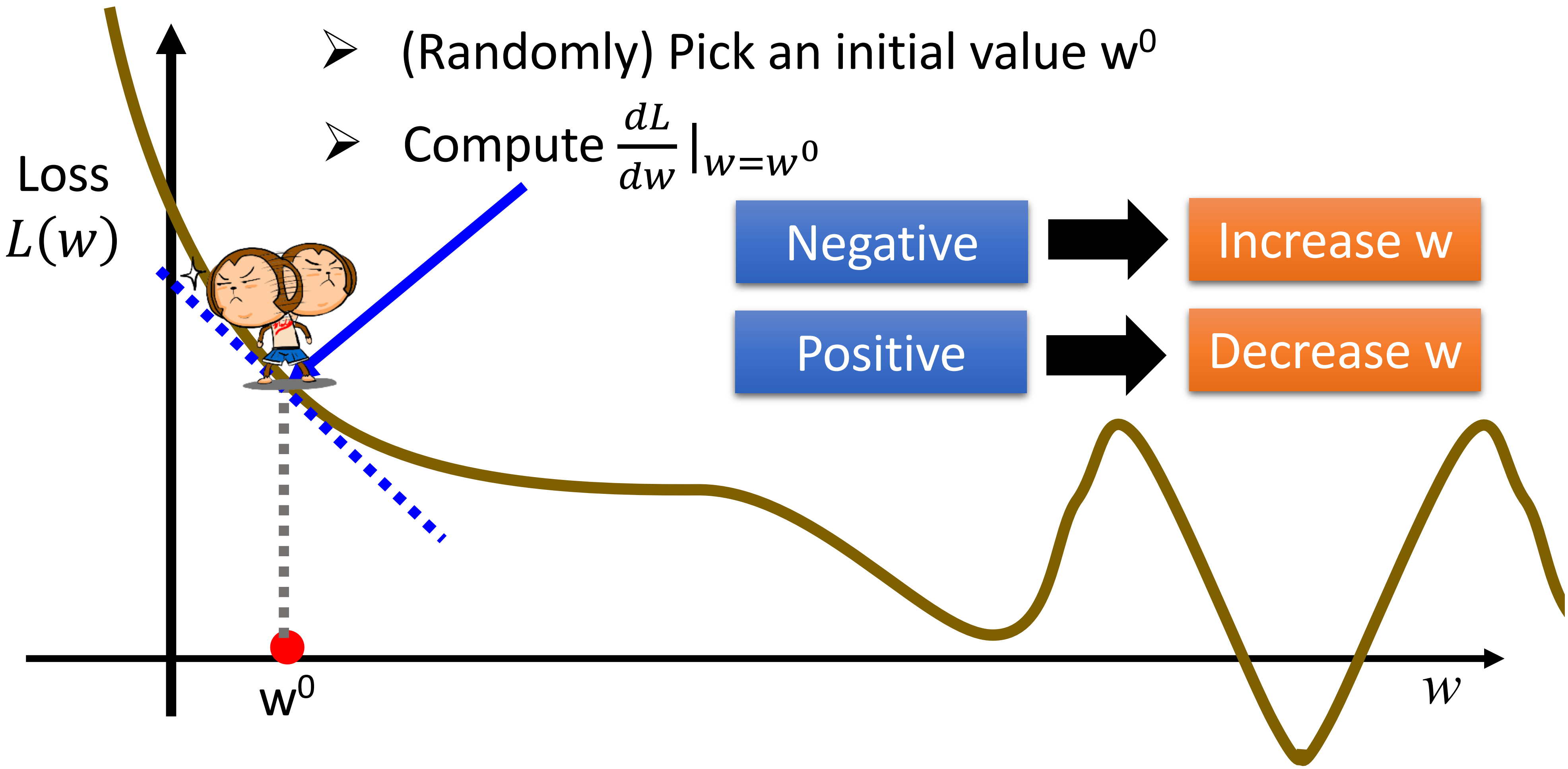
$$= arg \min_{w,b} \sum_{n=1}^{10} \left(\hat{y}^n - \left(b + w \cdot x_{cp}^n \right) \right)^2$$

Gradient Descent

Step 3: Gradient Descent

$$w^* = arg \min_w L(w)$$

- Consider loss function $L(w)$ with one parameter w:
  - (Randomly) Pick an initial value w^0
  - Compute $\frac{dL}{dw}|_{w=w^0}$

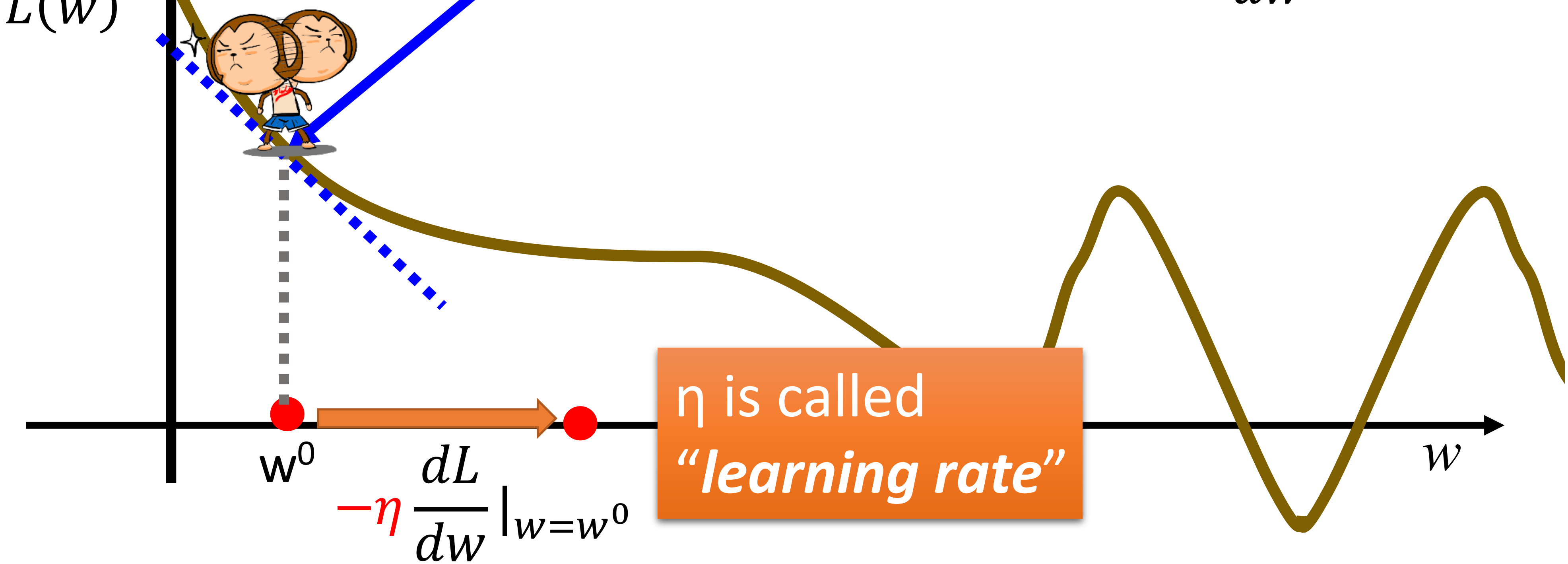


Step 3: Gradient Descent

$$w^* = arg \min_w L(w)$$

- Consider loss function $L(w)$ with one parameter w:
  - ➢ (Randomly) Pick an initial value w^0
  - ➢ Compute $\frac{dL}{dw}|_{w=w^0}$

$$w^1 \leftarrow w^0 - \eta \frac{dL}{dw}|_{w=w^0}$$

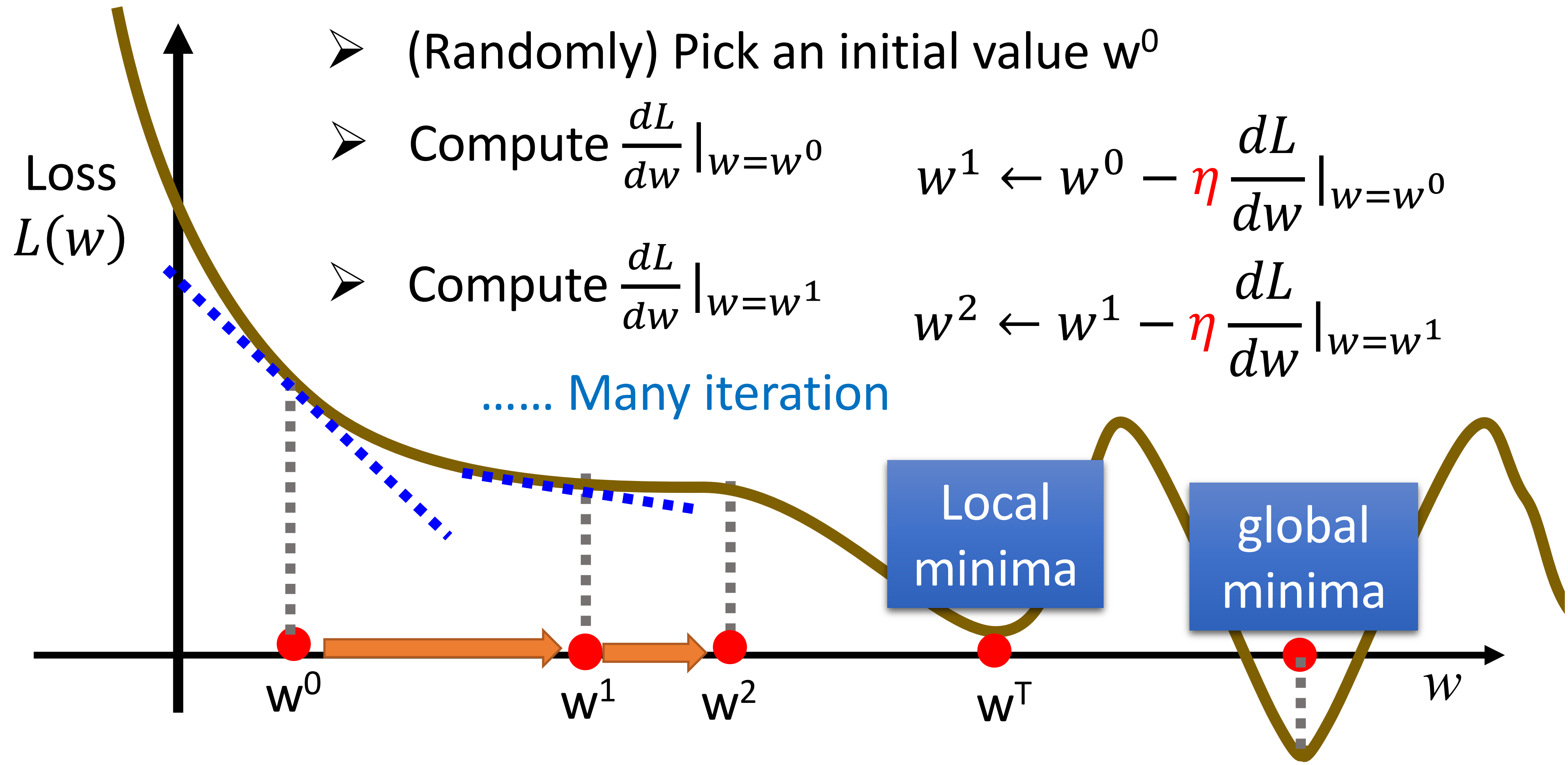


Step 3: Gradient Descent

$$w^* = arg\min_w L(w)$$

- Consider loss function $L(w)$ with one parameter w:
  - (Randomly) Pick an initial value w^0
  - Compute $\frac{dL}{dw}|_{w=w^0}$ $\quad w^1 \leftarrow w^0 - \eta\frac{dL}{dw}|_{w=w^0}$
  - Compute $\frac{dL}{dw}|_{w=w^1}$ $\quad w^2 \leftarrow w^1 - \eta\frac{dL}{dw}|_{w=w^1}$

…… Many iteration



Step 3: Gradient Descent

$$\begin{bmatrix} \frac{\partial L}{\partial w} \\ \frac{\partial L}{\partial b} \end{bmatrix}_{\text{gradient}}$$

- How about two parameters? $w^*, b^* = arg \min_{w,b} L(w, b)$

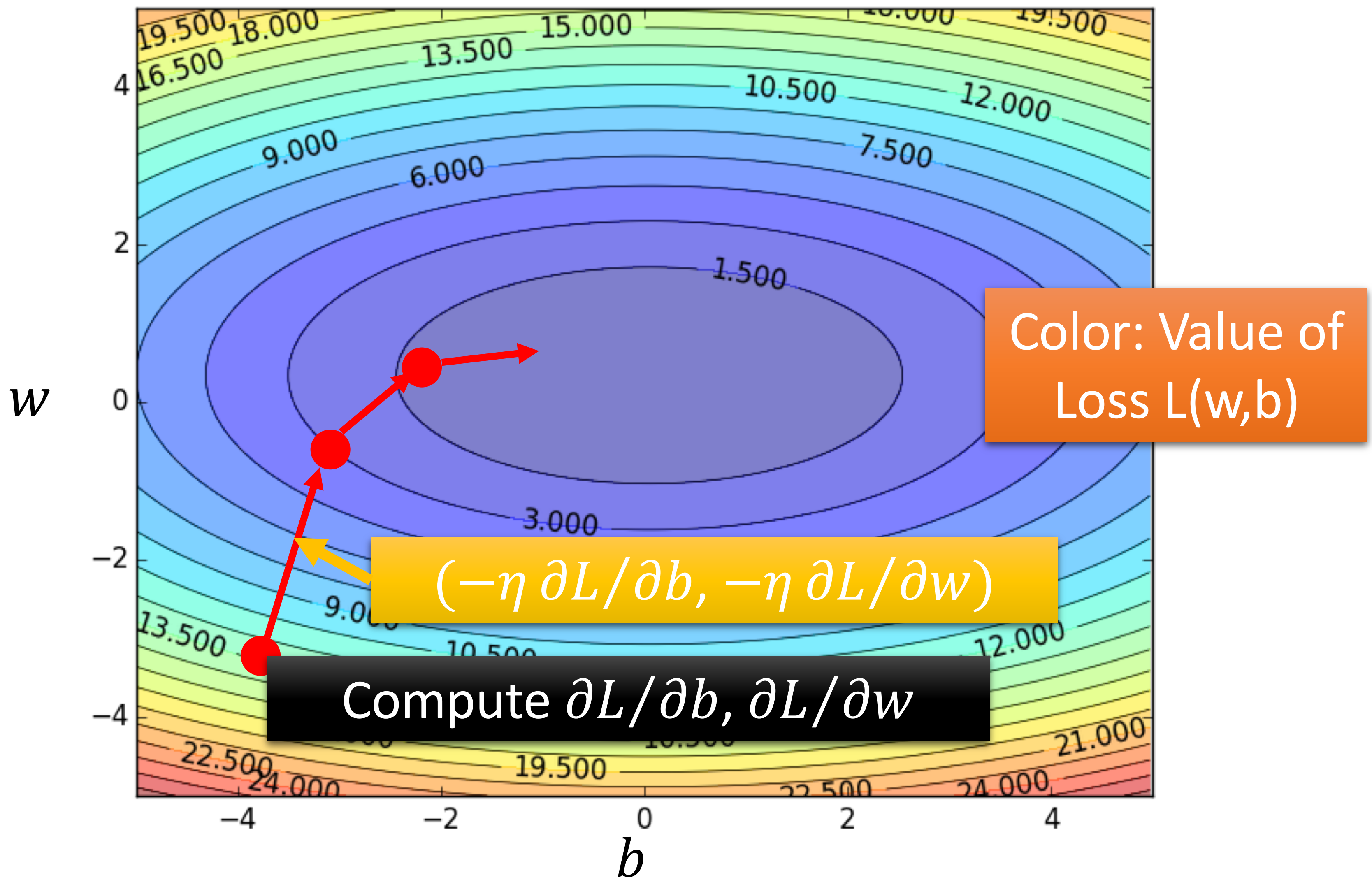
  - (Randomly) Pick an initial value w^0, b^0
  - Compute $\frac{\partial L}{\partial w}|_{w=w^0,b=b^0}, \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$

$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \qquad b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

  - Compute $\frac{\partial L}{\partial w}|_{w=w^1,b=b^1}, \frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$

$$w^2 \leftarrow w^1 - \eta \frac{\partial L}{\partial w}|_{w=w^1,b=b^1} \qquad b^2 \leftarrow b^1 - \eta \frac{\partial L}{\partial b}|_{w=w^1,b=b^1}$$

Step 3: Gradient Descent



Step 3: Gradient Descent

- When solving:

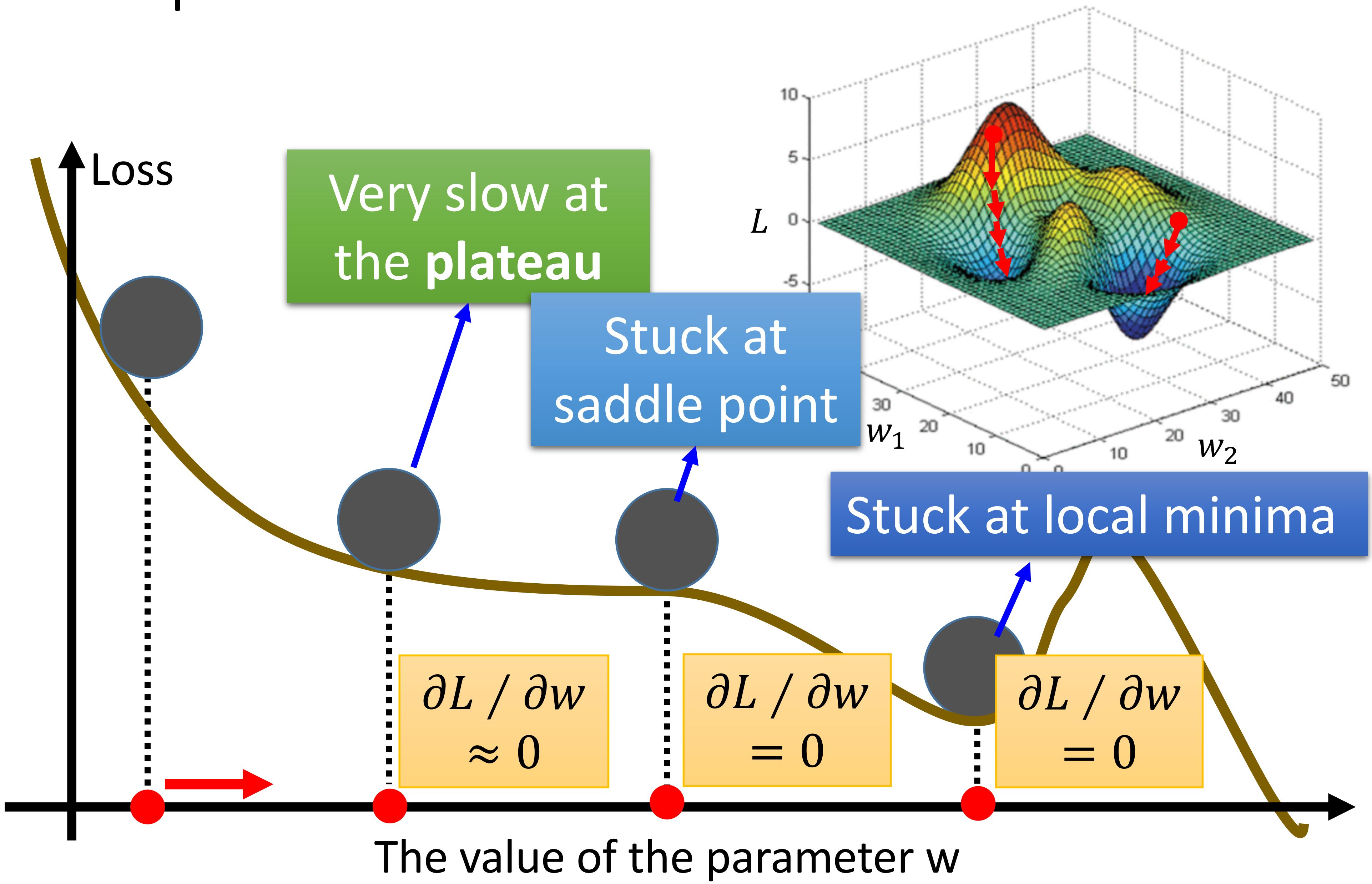
$$\theta^* = \arg\min_{\theta} L(\theta) \quad \text{by gradient descent}$$

- Each time we update the parameters, we obtain θ that makes $L(\theta)$ smaller.

$$L(\theta^0) > L(\theta^1) > L(\theta^2) > \cdots$$

Is this statement correct?

Step 3: Gradient Descent



Step 3: Gradient Descent

- Formulation of $\partial L / \partial w$ and $\partial L / \partial b$

$$L(w,b) = \sum_{n=1}^{10} \left(\hat{y}^n - \left(b + \underline{w \cdot x_{cp}^n} \right) \right)^2$$

$$\frac{\partial L}{\partial w} =? \sum_{n=1}^{10} 2 \left(\hat{y}^n - \left(b + w \cdot x_{cp}^n \right) \right)$$

$$\frac{\partial L}{\partial b} =?$$

Step 3: Gradient Descent

- Formulation of $\partial L / \partial w$ and $\partial L / \partial b$

$$L(w,b) = \sum_{n=1}^{10}\left(\hat{y}^n - \left(b + w \cdot x_{cp}^n\right)\right)^2$$

$$\frac{\partial L}{\partial w} =? \sum_{n=1}^{10} 2\left(\hat{y}^n - \left(b + w \cdot x_{cp}^n\right)\right)\left(-x_{cp}^n\right)$$

$$\frac{\partial L}{\partial b} =? \sum_{n=1}^{10} 2\left(\hat{y}^n - \left(b + w \cdot x_{cp}^n\right)\right)$$

Step 3: Gradient Descent

How's the results?

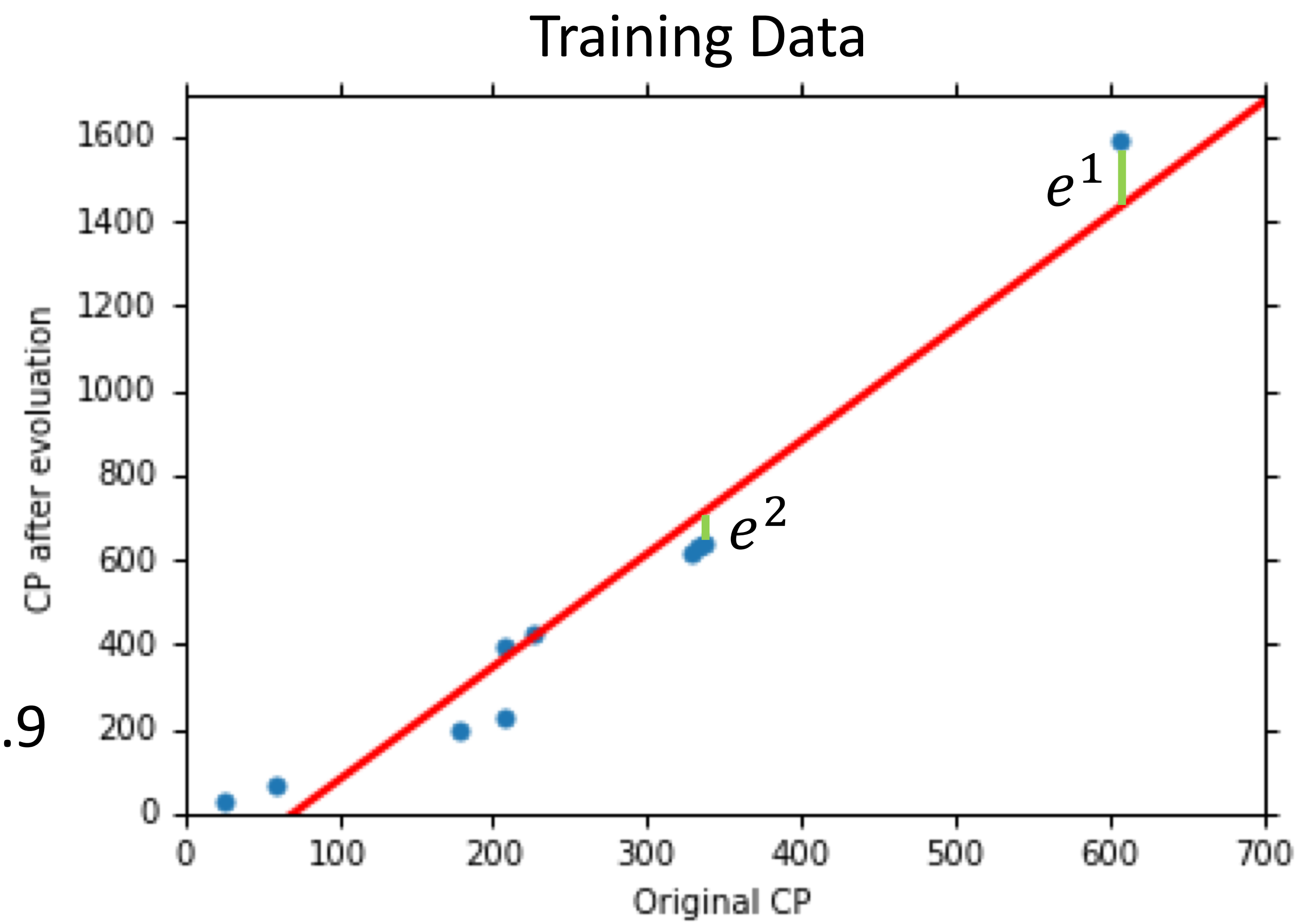
$y = b + w \cdot x_{cp}$

b = -188.4

w = 2.7

Average Error on Training Data

$$= \frac{1}{10} \sum_{n=1}^{10} e^n = 31.9$$



How's the results?
- Generalization

What we really care about is the error on new data (testing data)

$y = b + w \cdot x_{cp}$

b = -188.4

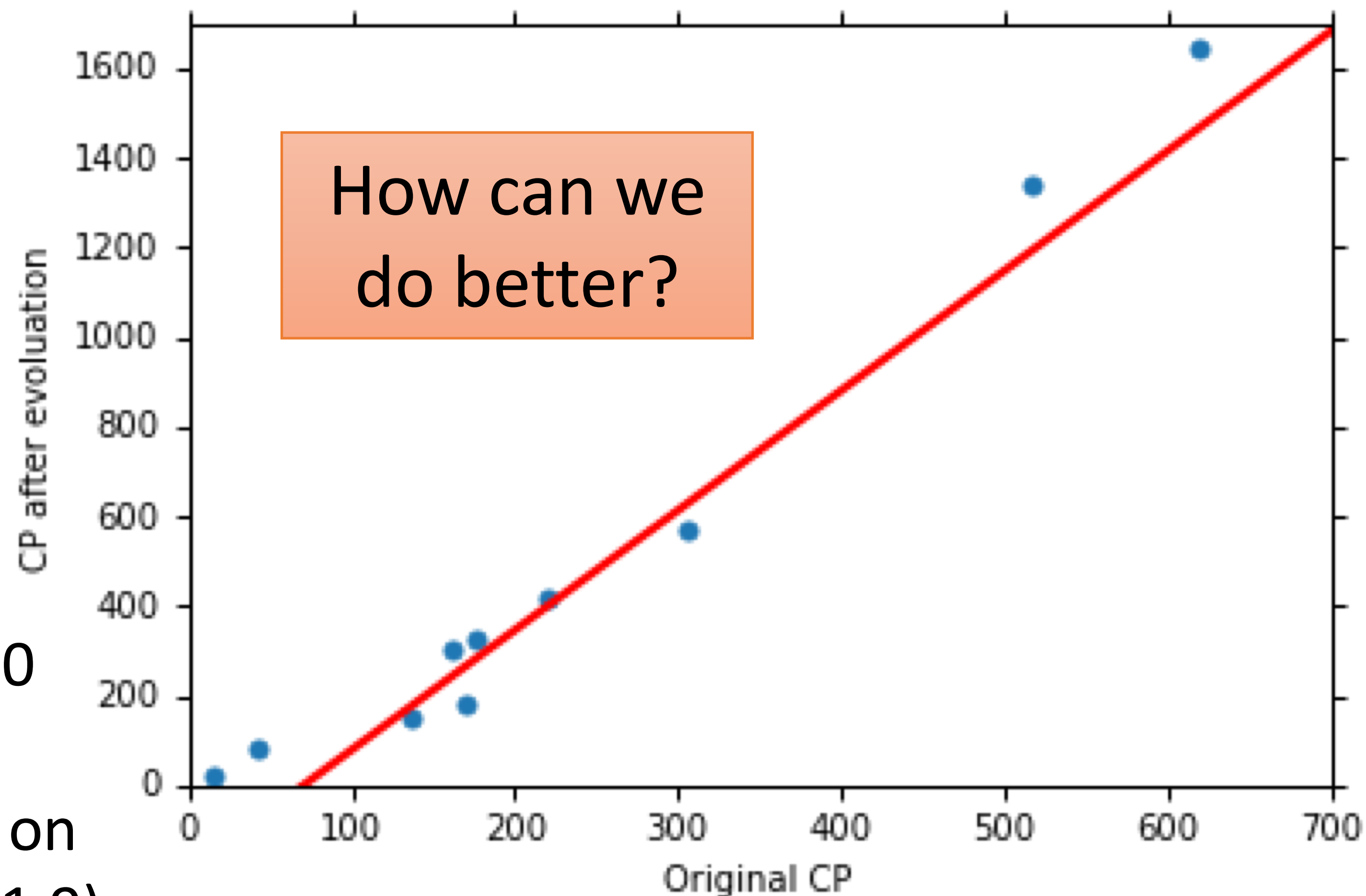
w = 2.7

Average Error on Testing Data

$$= \frac{1}{10}\sum_{n=1}^{10} e^n = 35.0$$

> Average Error on Training Data (31.9)

Another 10 pokemons as testing data



Selecting another Model

$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$$

Best Function

$b = -10.3$

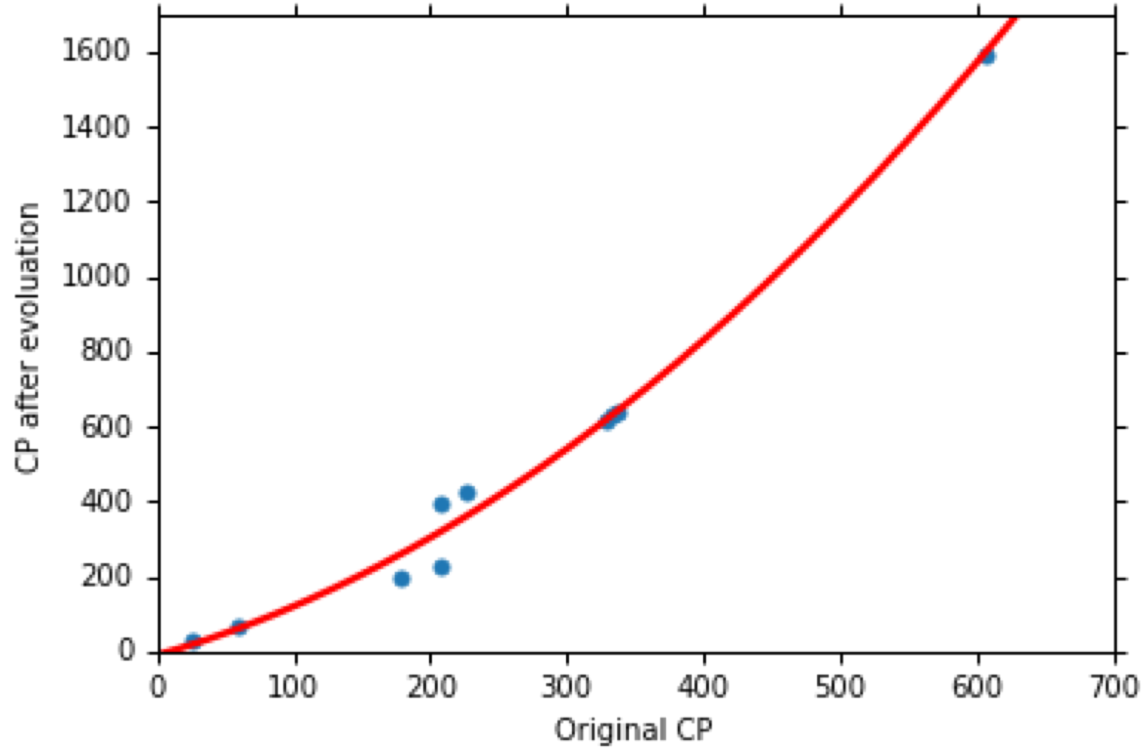
$w_1 = 1.0$, $w_2 = 2.7 \times 10^{-3}$

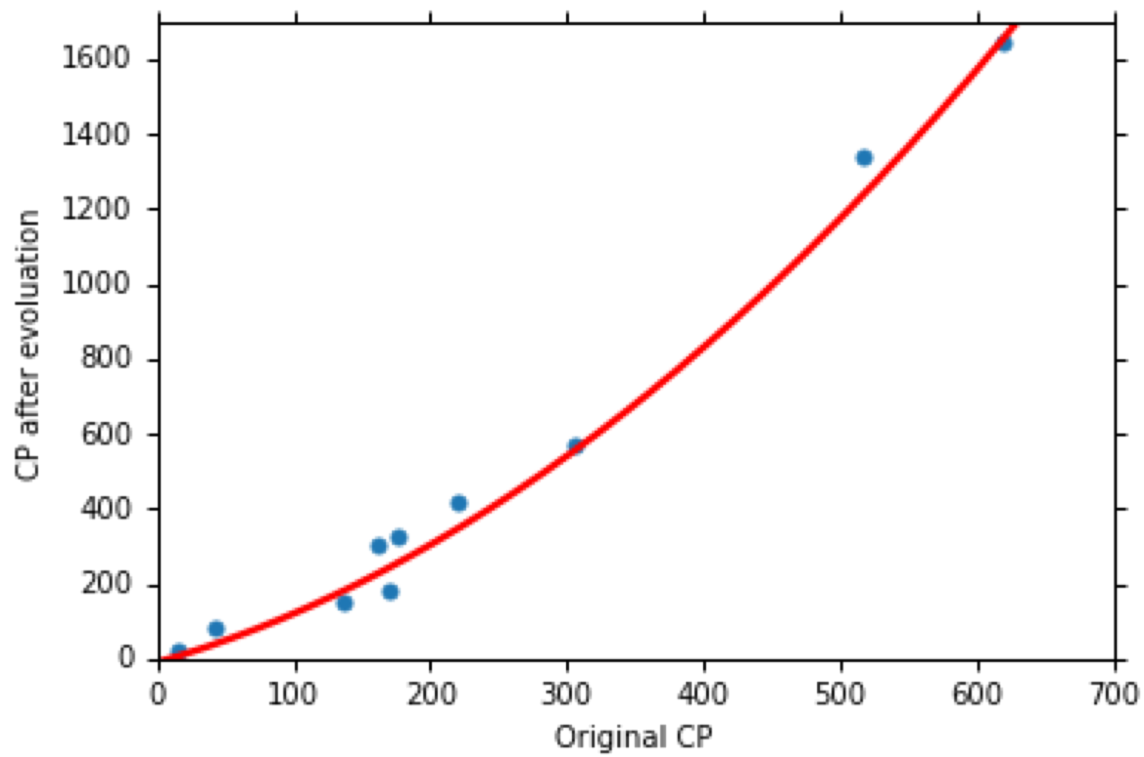
Average Error = 15.4

Testing:

Average Error = 18.4

Better! Could it be even better?





Selecting another Model

$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$$

Best Function

$b = 6.4$, $w_1 = 0.66$

$w_2 = 4.3 \times 10^{-3}$

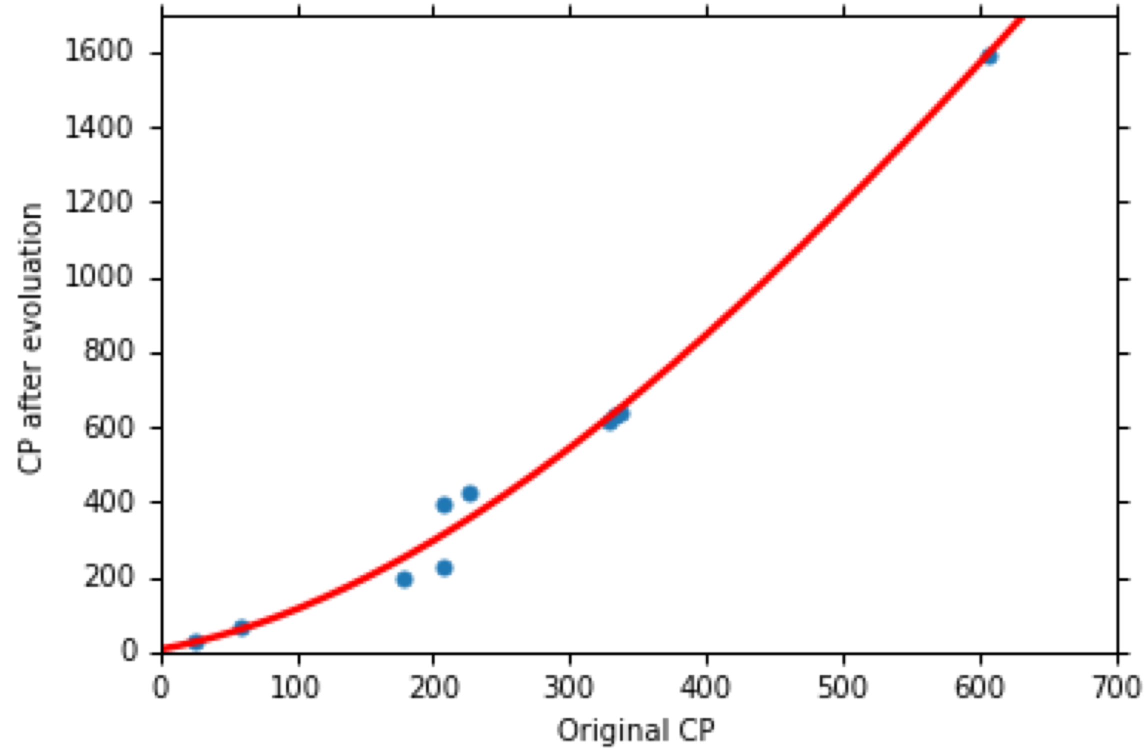
$w_3 = -1.8 \times 10^{-6}$

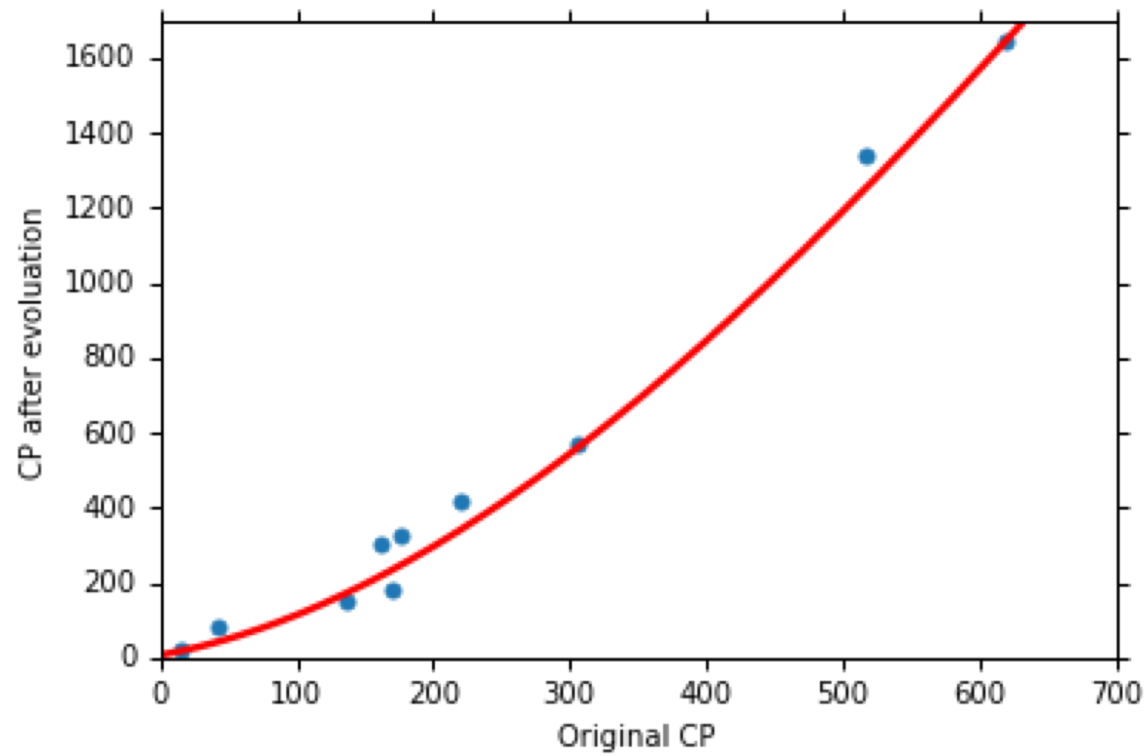
Average Error = 15.3

Testing:

Average Error = 18.1

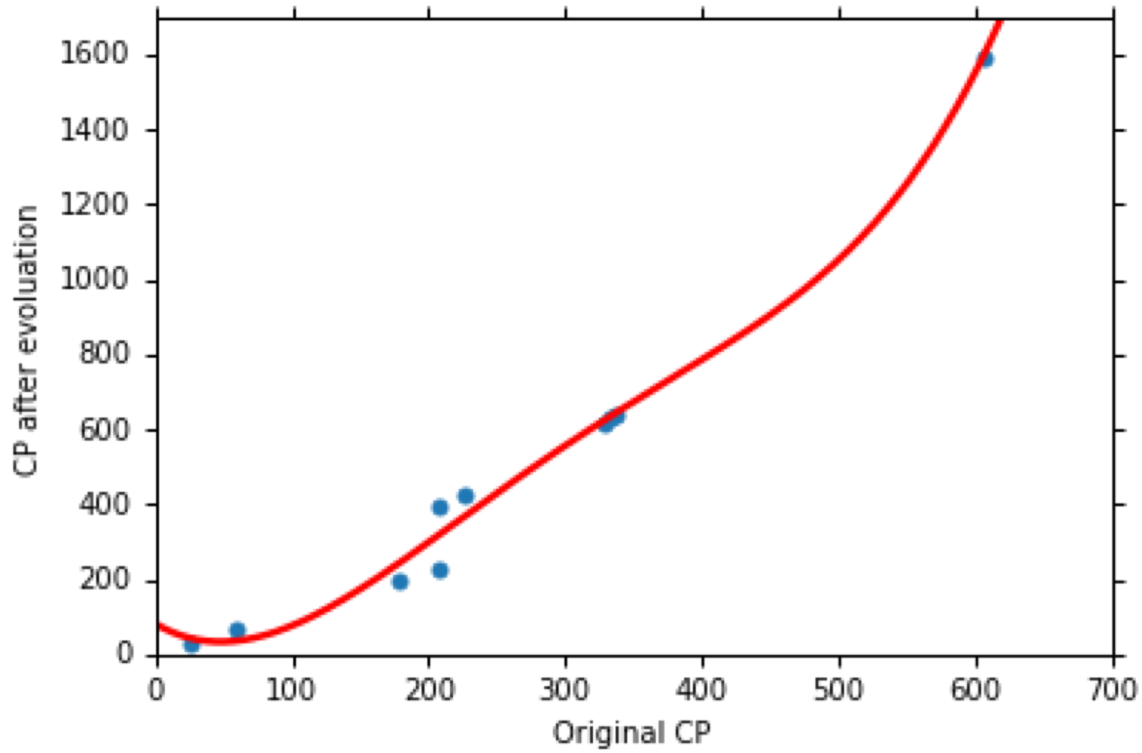
Slightly better.
How about more complex model?





Selecting another Model

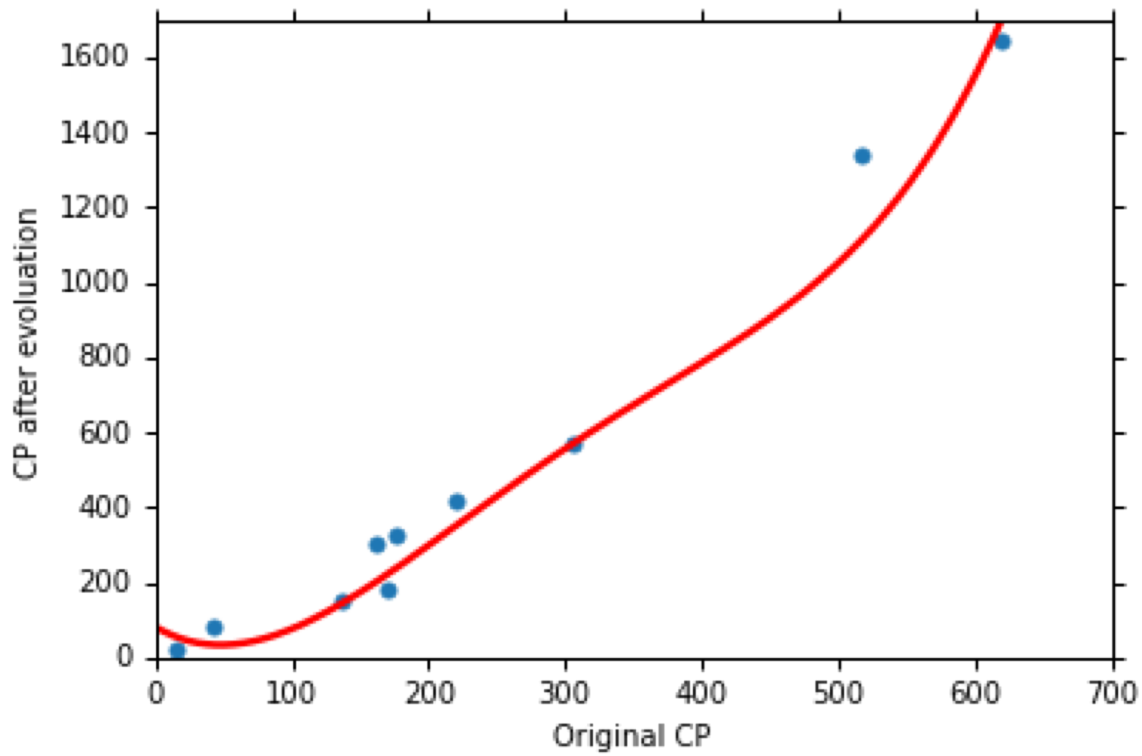
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$$



Best Function

Average Error = 14.9

Testing:

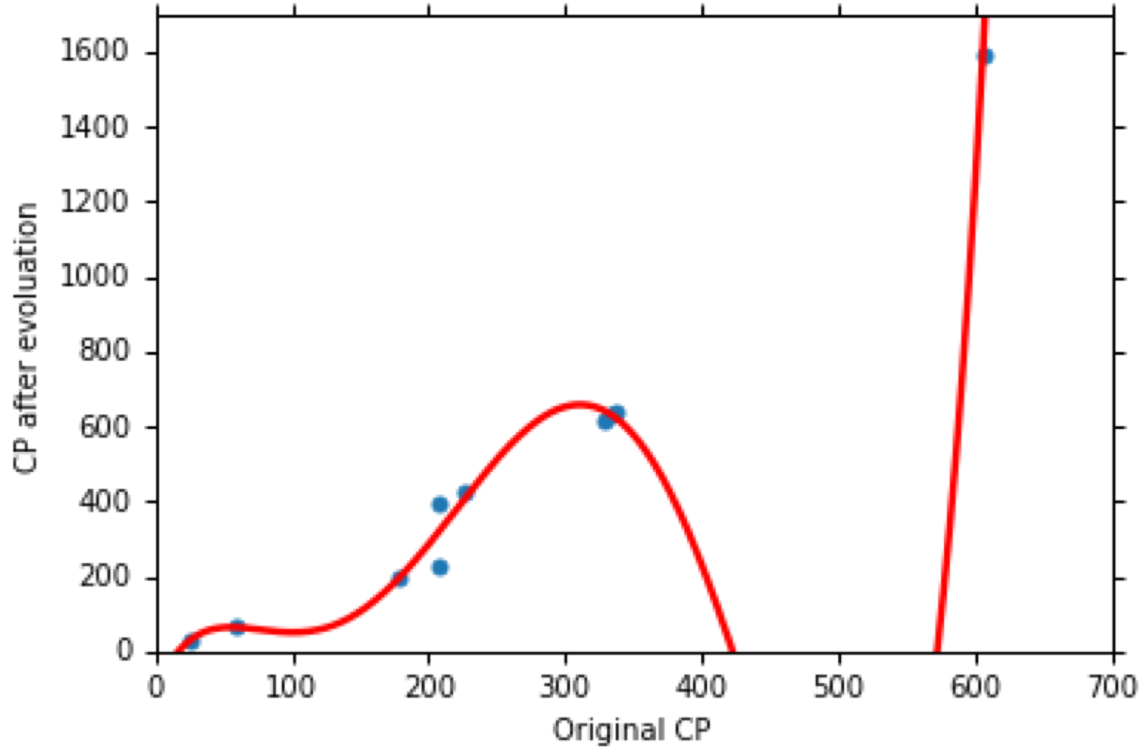


Average Error = 28.8

The results become worse ...

Selecting another Model

$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$



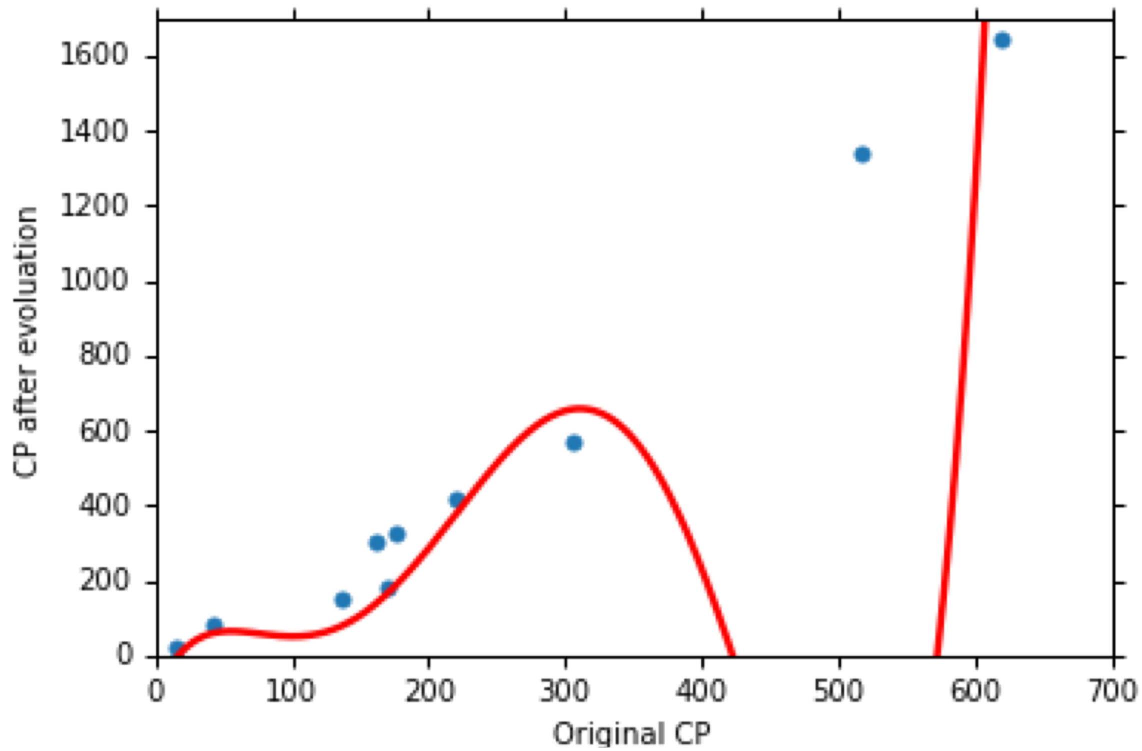
Best Function

Average Error = 12.8

Testing:

Average Error = 232.1

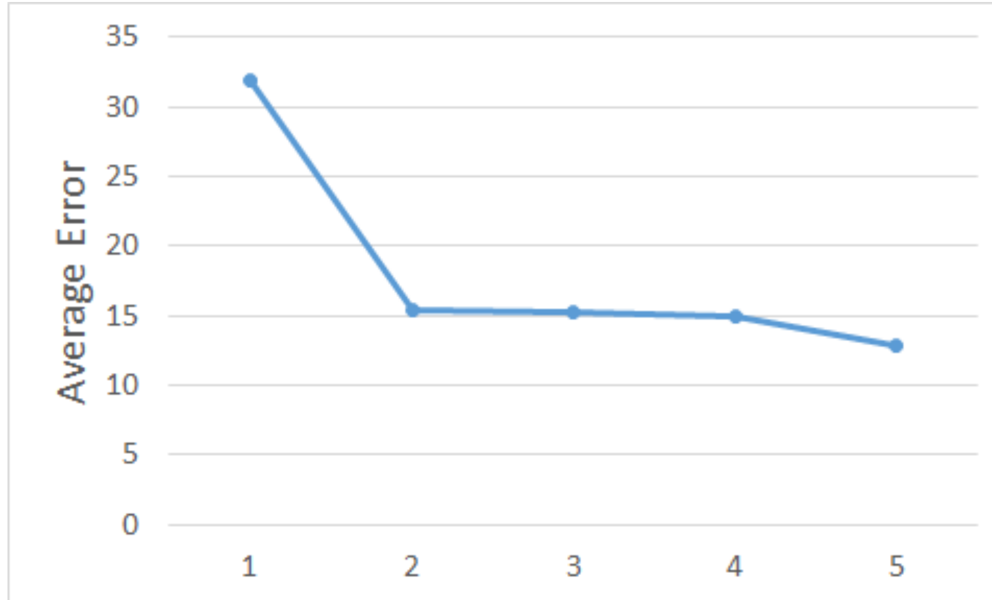
The results are so bad.

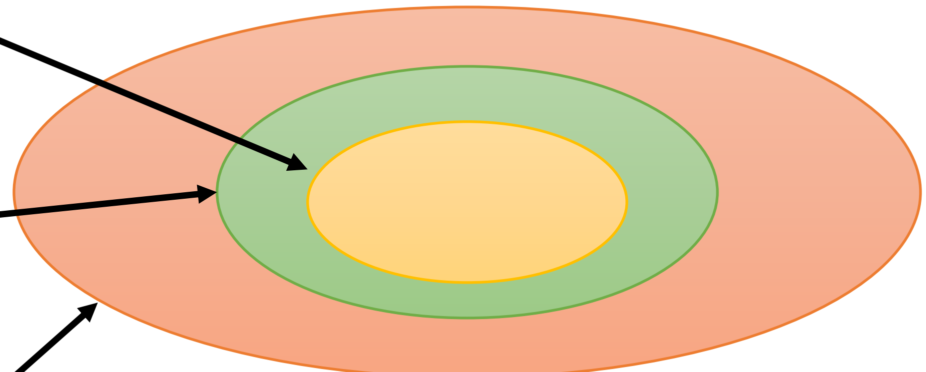


Model Selection

1. $y = b + w \cdot x_{cp}$
2. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$
3. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$
4. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$
5. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$

Training Data

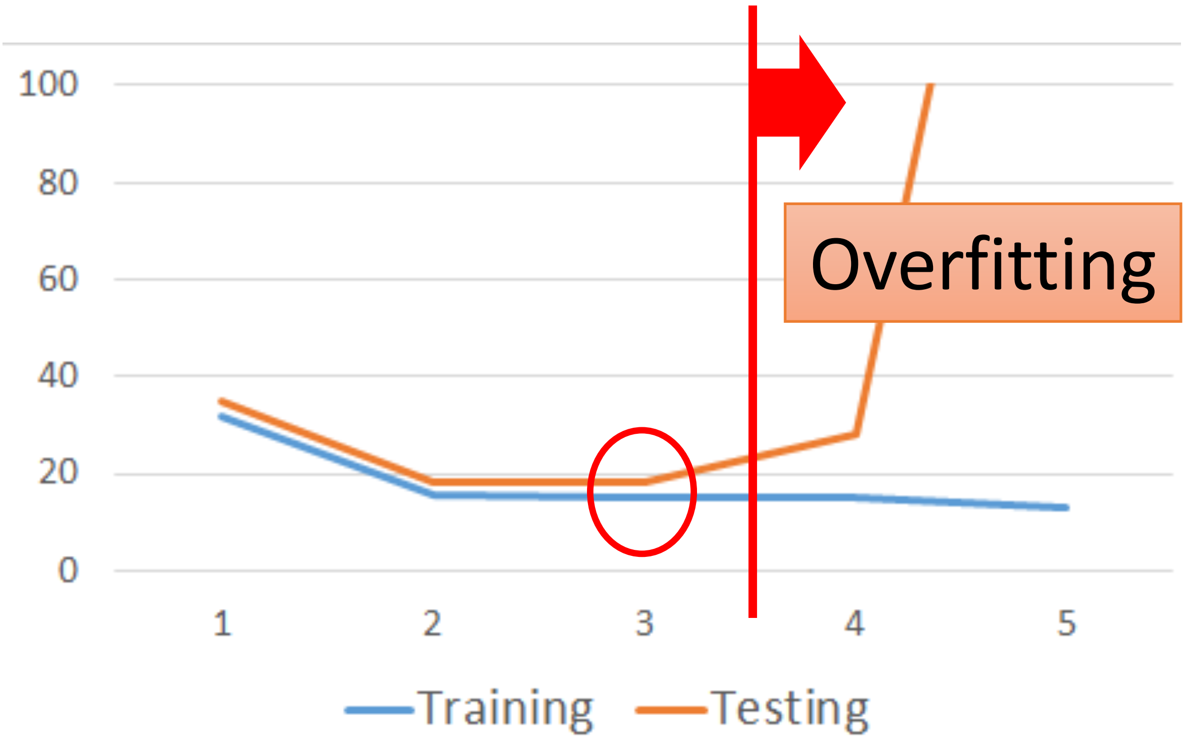




A more complex model yields lower error on training data.

If we can truly find the best function

Model Selection

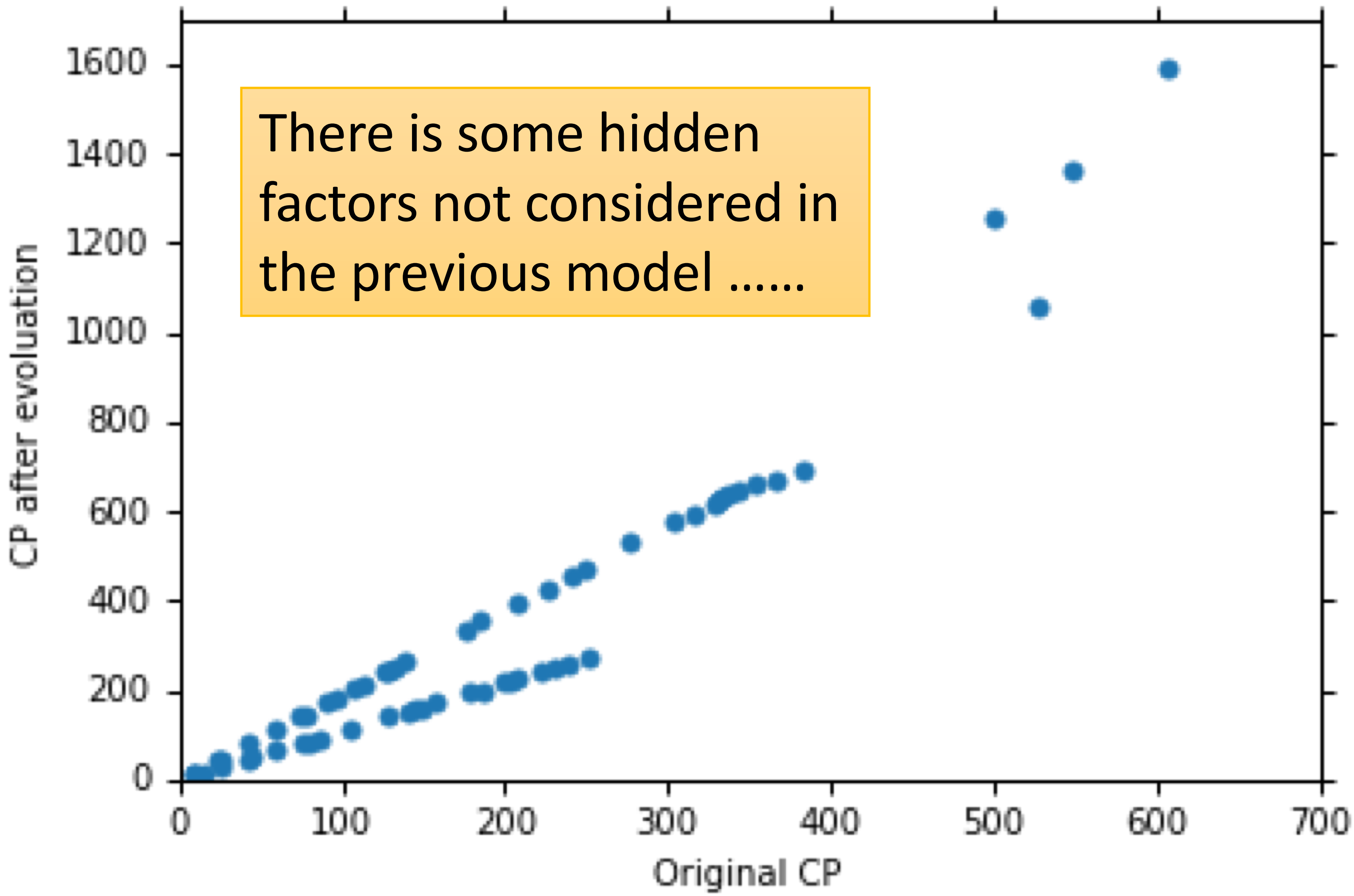


	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

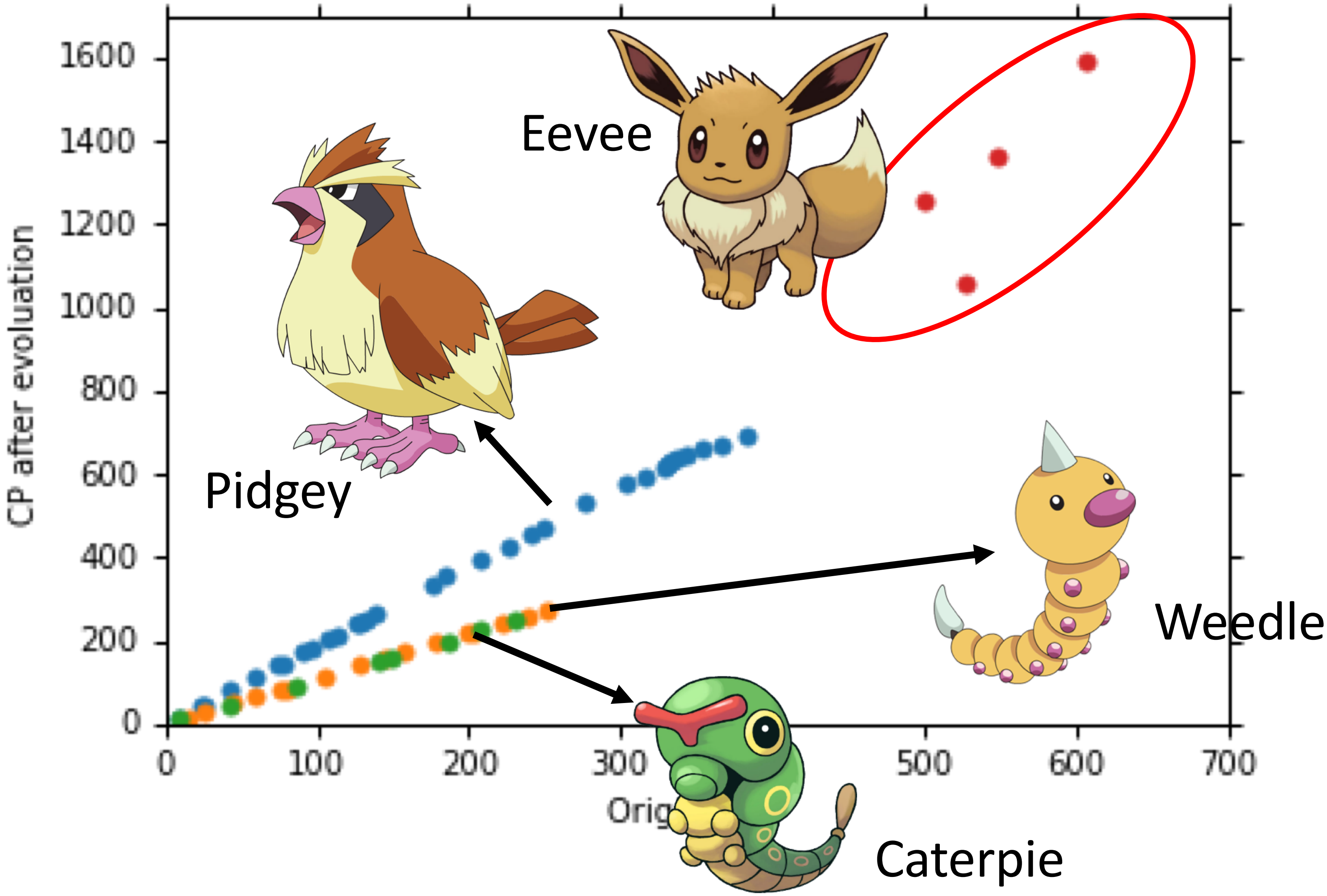
A more complex model does not always lead to better performance on ***testing data***.

This is ***Overfitting***. ➡ Select suitable model

Let’s collect more data



What are the hidden factors?



Back to step 1: Redesign the Model

$$y = b + \sum w_i x_i$$

Linear model?

x_s = species of x

x

If x_s = Pidgey: $y = b_1 + w_1 \cdot x_{cp}$

If x_s = Weedle: $y = b_2 + w_2 \cdot x_{cp}$

If x_s = Caterpie: $y = b_3 + w_3 \cdot x_{cp}$

If x_s = Eevee: $y = b_4 + w_4 \cdot x_{cp}$

y

Back to step 1: Redesign the Model

$$y = b + \sum w_i \boxed{x_i}$$

Linear model?

$y = b_1 \cdot$ 1

$+w_1 \cdot$ 1 x_{cp}

$+b_2 \cdot$ 0

$+w_2 \cdot$ 0

$+b_3 \cdot$ 0

$+w_3 \cdot$ 0

$+b_4 \cdot$ 0

$+w_4 \cdot$ 0

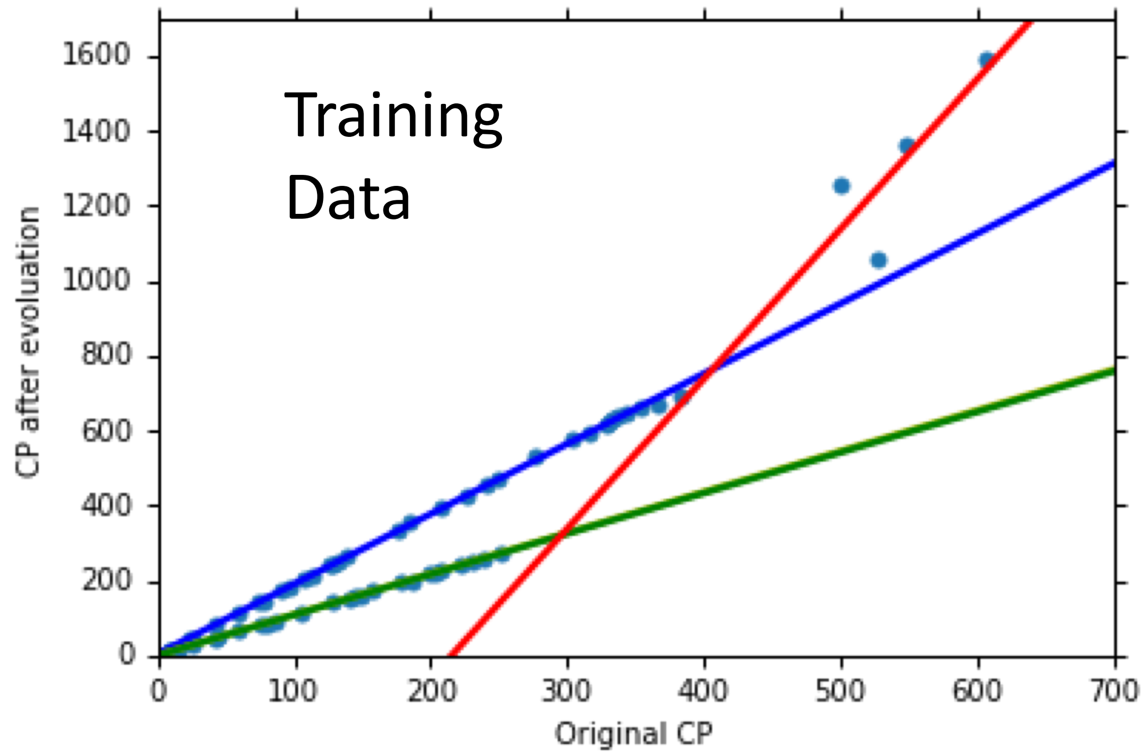
$\delta(x_s =$ Pidgey$)$

$$\begin{cases} =1 & \text{If } x_s = \text{Pidgey} \\ =0 & \text{otherwise} \end{cases}$$

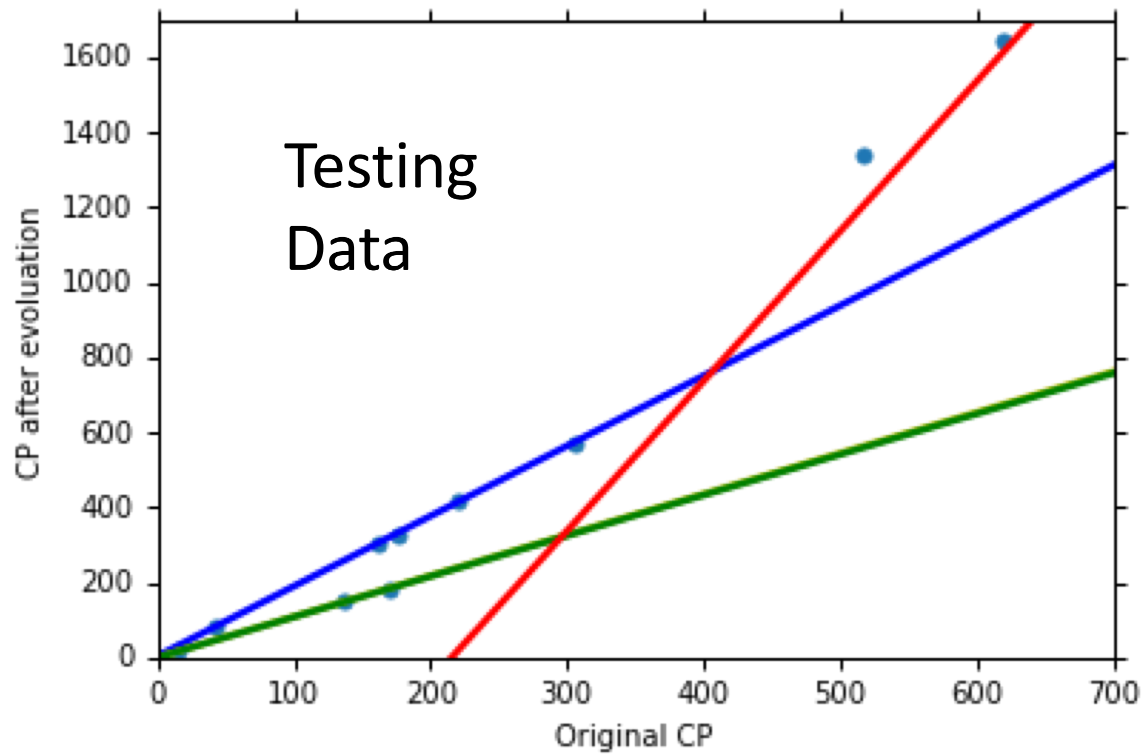
If $x_s =$ Pidgey

$$y = b_1 + w_1 \cdot x_{cp}$$

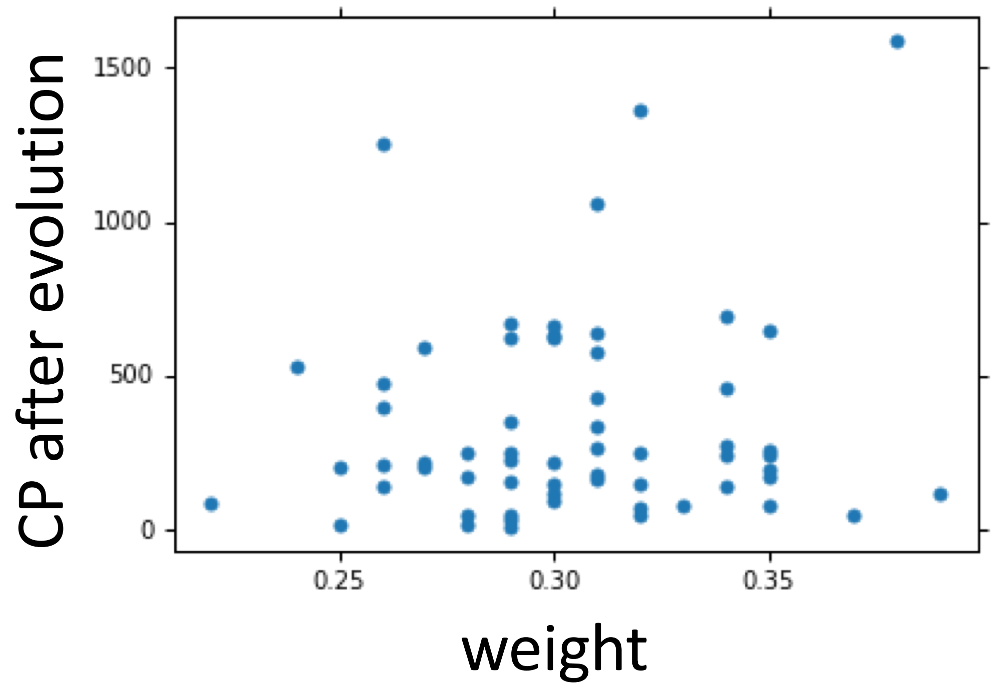
Average error = 3.8

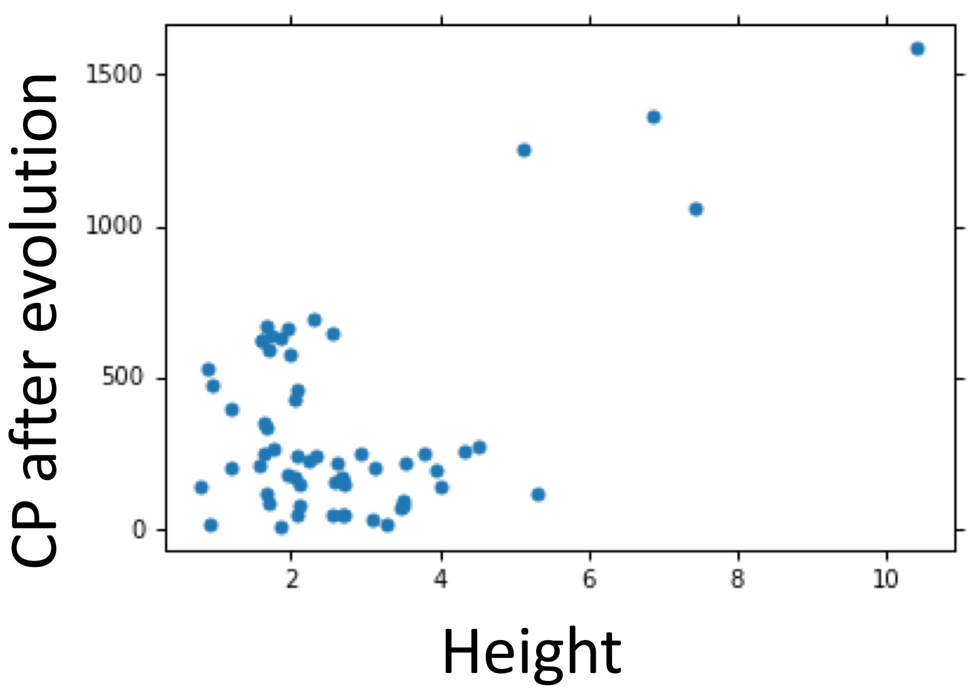


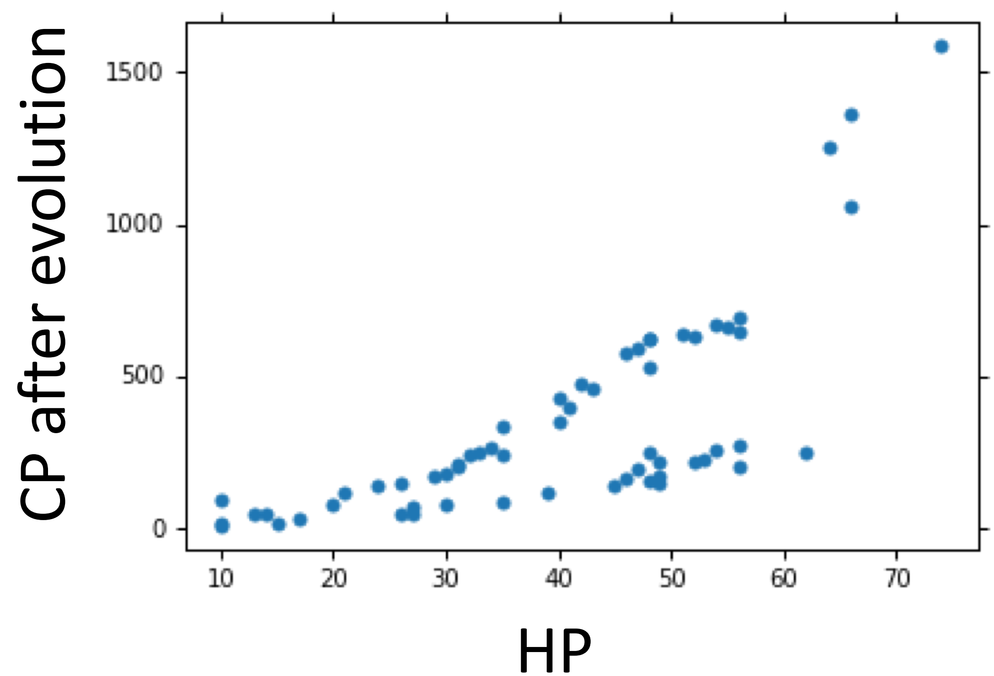
Average error = 14.3



Are there any other hidden factors?







Back to step 1: Redesign the Model Again

x

If $x_s =$ Pidgey: $$y' = b_1 + w_1 \cdot x_{cp} + w_5 \cdot (x_{cp})^2$$

If $x_s =$ Weedle: $$y' = b_2 + w_2 \cdot x_{cp} + w_6 \cdot (x_{cp})^2$$

If $x_s =$ Caterpie: $$y' = b_3 + w_3 \cdot x_{cp} + w_7 \cdot (x_{cp})^2$$

If $x_s =$ Eevee: $$y' = b_4 + w_4 \cdot x_{cp} + w_8 \cdot (x_{cp})^2$$

$$y = y' + w_9 \cdot x_{hp} + w_{10} \cdot (x_{hp})^2$$
$$+ w_{11} \cdot x_h + w_{12} \cdot (x_h)^2 + w_{13} \cdot x_w + w_{14} \cdot (x_w)^2$$

y

Training Error = 1.9

Testing Error = 102.3

Overfitting!

Back to step 2: Regularization

$$y = b + \sum w_i x_i$$

The functions with smaller w_i are better

$$L = \sum_n \left(\hat{y}^n - \left(b + \sum w_i x_i \right) \right)^2 \boxed{+\lambda \sum (w_i)^2}$$

- Smaller w_i means … smoother

$$y = b + \sum w_i x_i$$

$$y + \sum w_i \Delta x_i = b + \sum w_i (x_i + \Delta x_i)$$

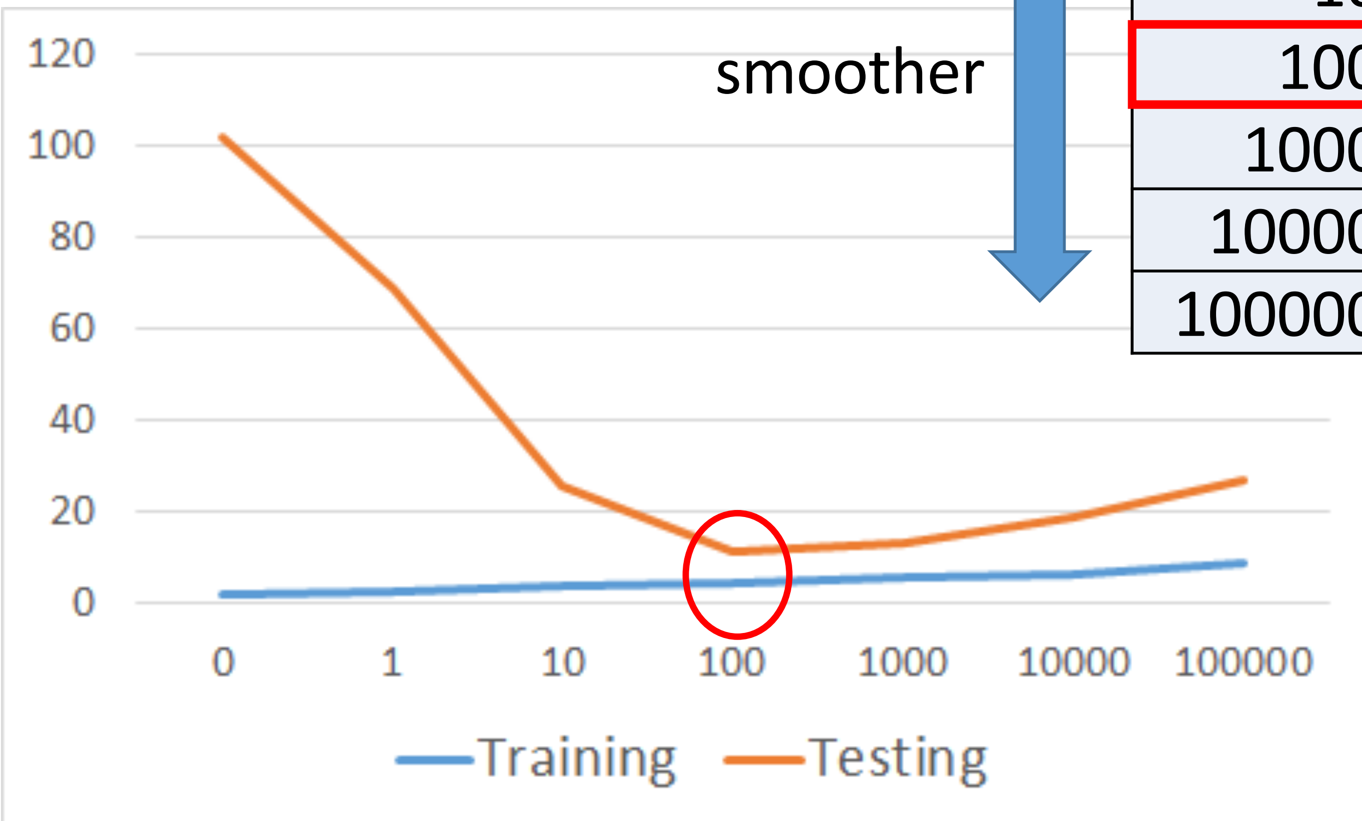
- We believe smoother function is more likely to be correct

Do you have to apply regularization on bias?

Regularization

λ	Training	Testing
0	1.9	102.3
1	2.3	68.7
10	3.5	25.7
100	4.1	11.1
1000	5.6	12.8
10000	6.3	18.7
100000	8.5	26.8

smoother



How smooth?

Select λ obtaining the best model

- Training error: larger λ, considering the training error less
- We prefer smooth function, but don't be too smooth.

Questions?