Regression

Hung-yi Lee
李宏毅

Regression: Output a scalar

Regression 問題的「函式範圍」屬於 Linear！也就是找到一個 Linear Function 來解決 Regression 問題

- Stock Market Forecast

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

- Self-driving Car

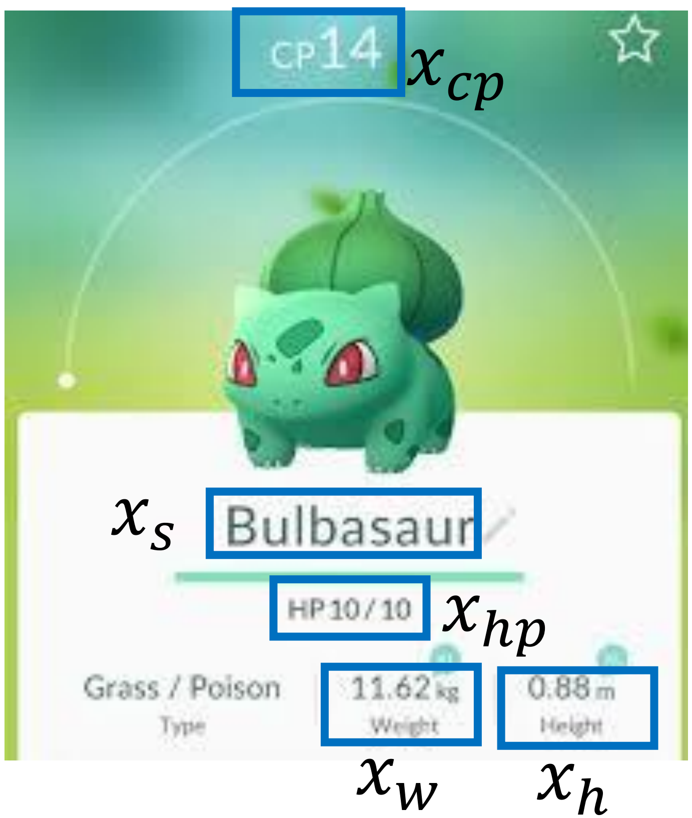
$f($  $) =$ 方向盤角度

- Recommendation

$f($ 使用者 A 商品 B $) =$ 購買可能性

Example Application

- Estimating the Combat Power (CP) of a pokemon after evolution 輸入一隻寶可夢 => 輸出進化後的 CP

$f($ 

x $) =$ CP after evolution y

機器學習第一步：建立一個 Model => 定義一個 Function Set (限制函式的範圍)

Step 1: Model

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

A set of function

Model

$f_1, f_2 \cdots$

w and b are parameters (can be any value)

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

feature

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

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

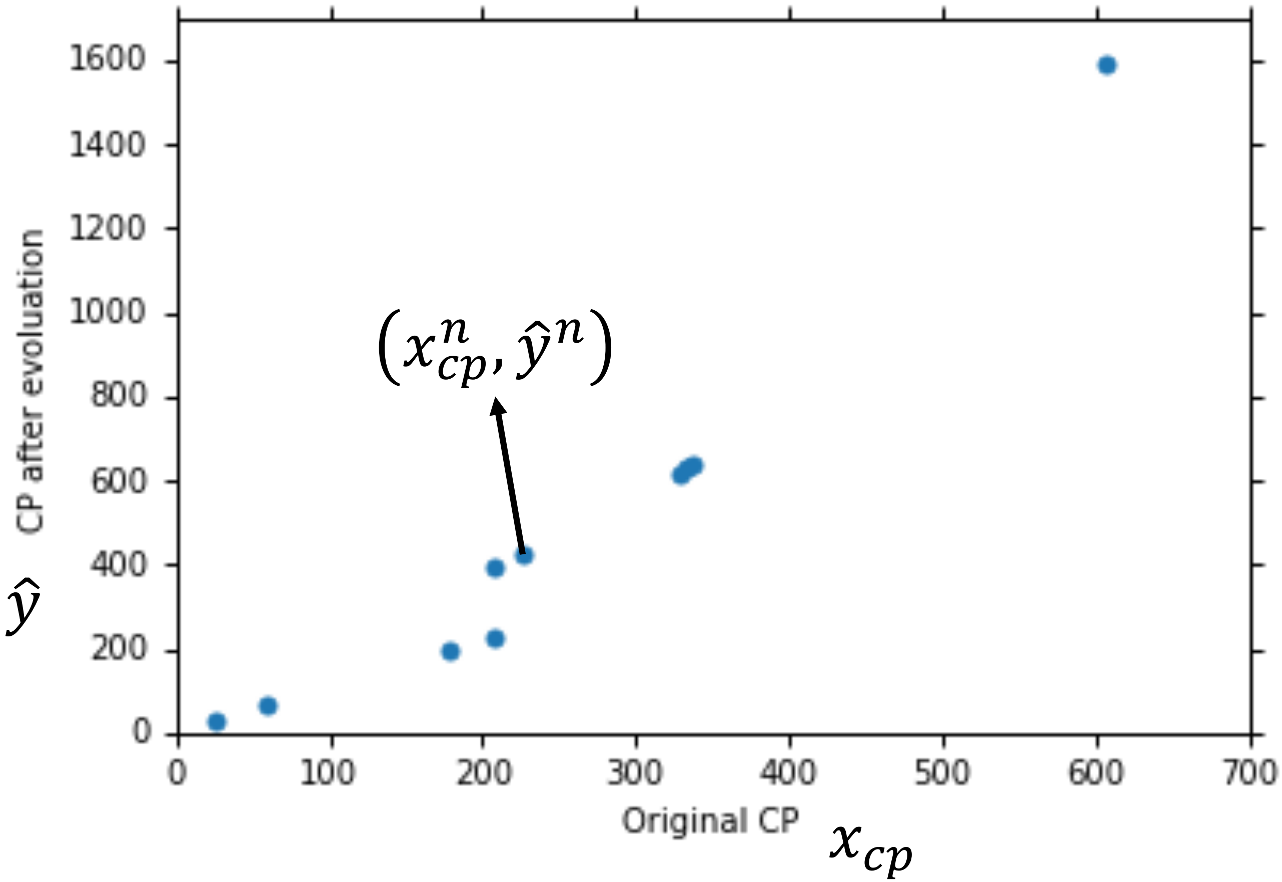
$(x^1, \hat{y}^1)$

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

⋮

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

This is real data.

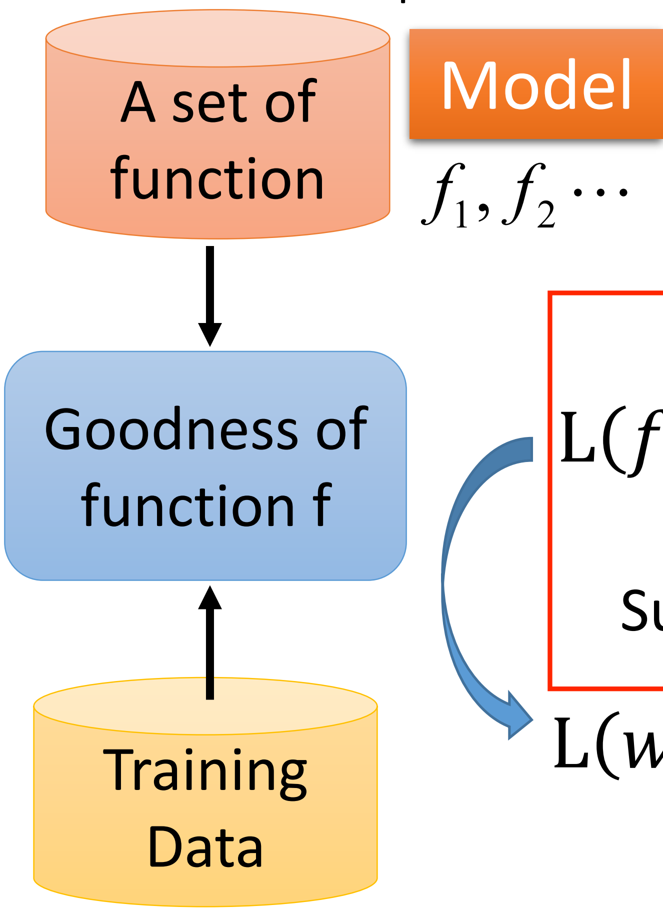


Source: https://www.openintro.org/stat/data/?data=pokemon

機器學習第二步：建立一個「特別的 Function」來評定 Function Set 中 Function 的好壞 => 特別的 Function：Loss Function

Step 2: Goodness of Function

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



Loss function L:

Input: a function, output: how bad it is

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

Estimation error

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

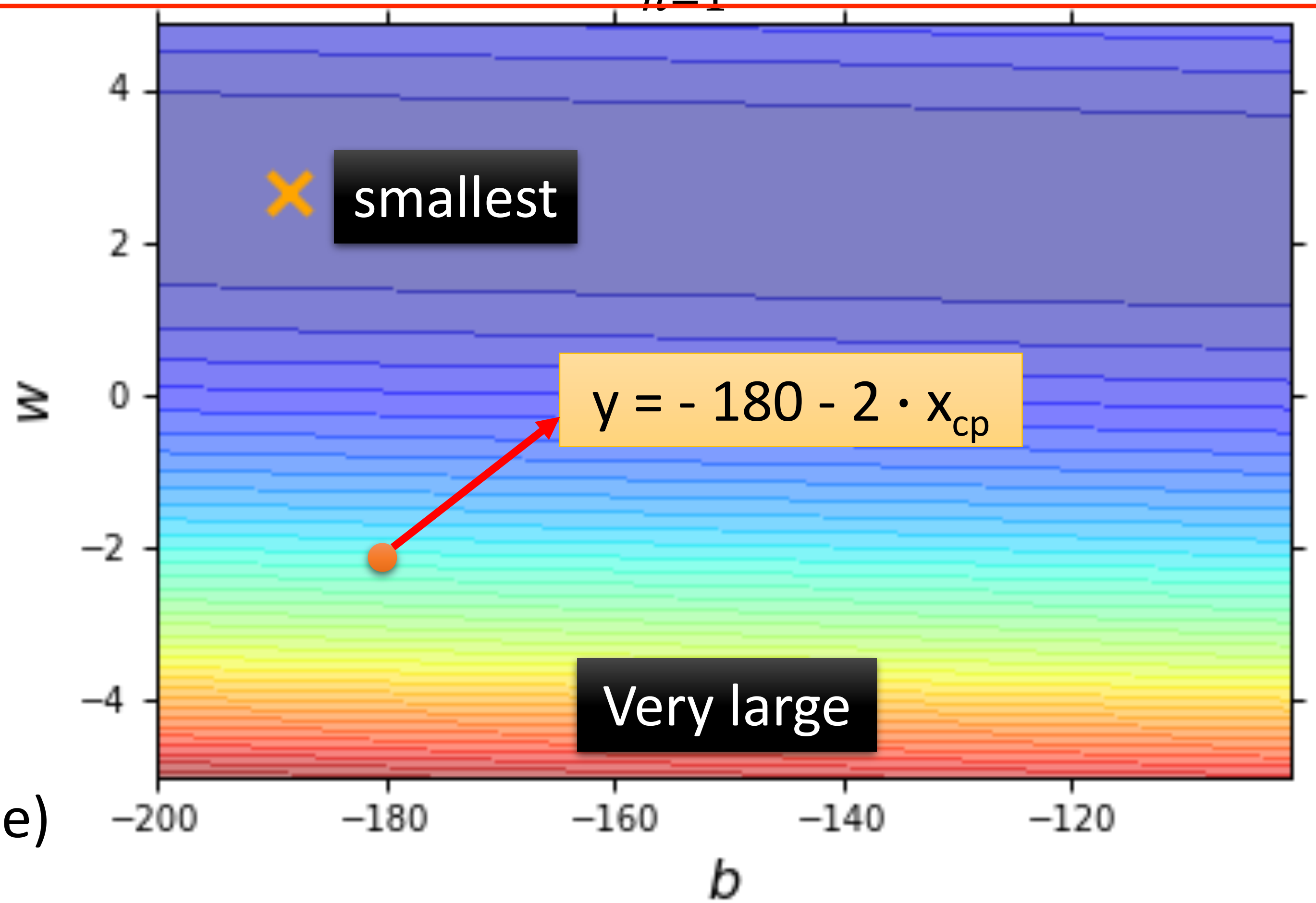
- Loss Function

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

Each point in the figure is a function

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

(true example)



機器學習第三步：利用 Loss Function 從 Function Set 中找到「最好」的 Function

Step 3: Best Function

A set of function

Model

$f_1, f_2 \cdots$

Goodness of function f

Training Data

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

Pick the "Best" Function

$$\boxed{f^*} = arg \min_f L(f)$$

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

最好的 Function

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

Gradient Descent

從前頁可知：要利用 Loss Function 從 Function Set 中找到最好的 Function => Loss(F) ＝ Loss(w, b) 最小！要如何改變 w 與 b 才能得到最小的 Loss ？ => 透過 Gradient Descent

http://chico386.pixnet.net/album/photo/171572850

Step 3: Gradient Descent

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

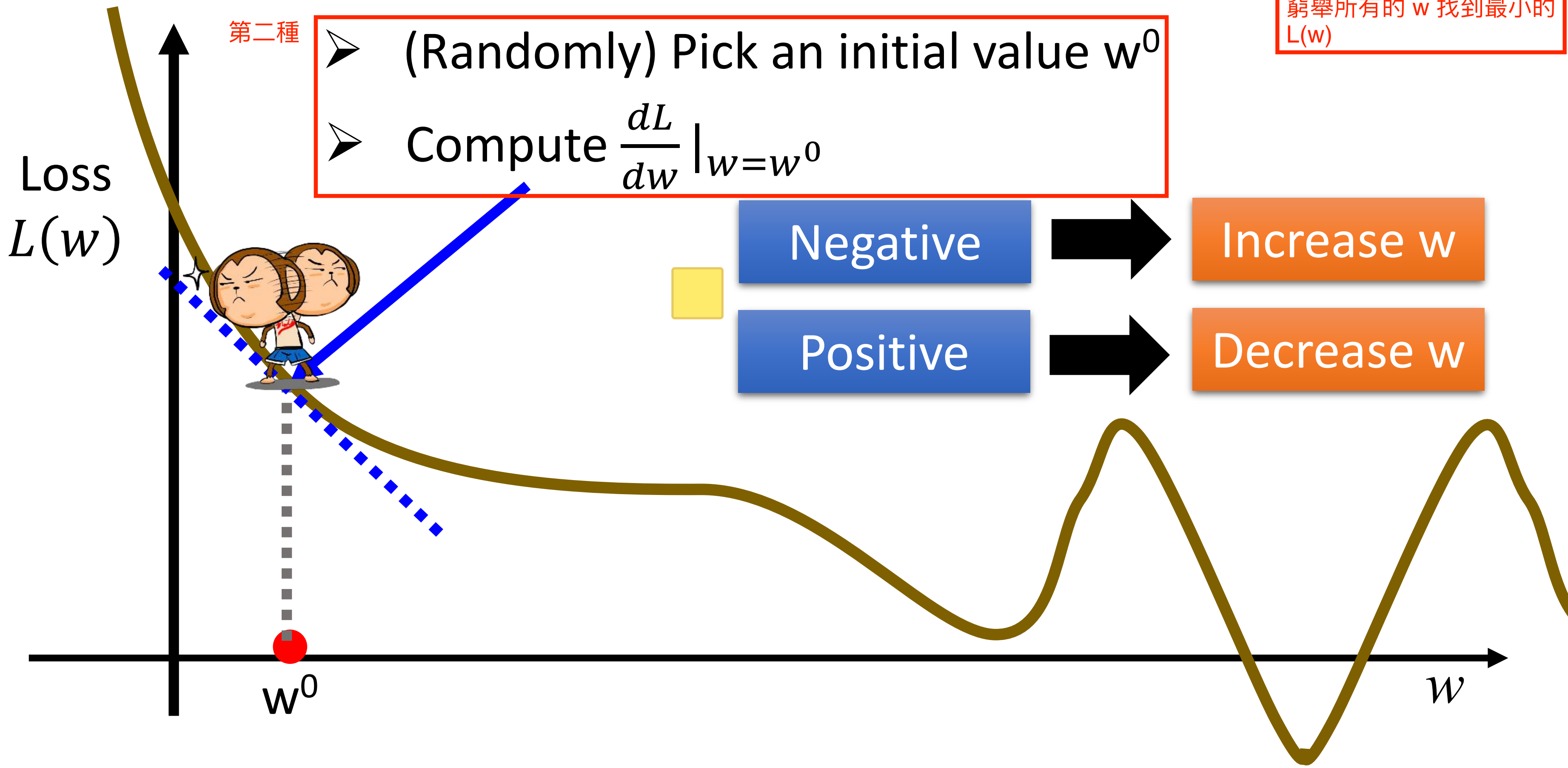
- Consider loss function $L(w)$ with one parameter w:

第一種

窮舉所有的 w 找到最小的 L(w)

第二種

- ➢ (Randomly) Pick an initial value w^0
- ➢ Compute $\frac{dL}{dw}|_{w=w^0}$



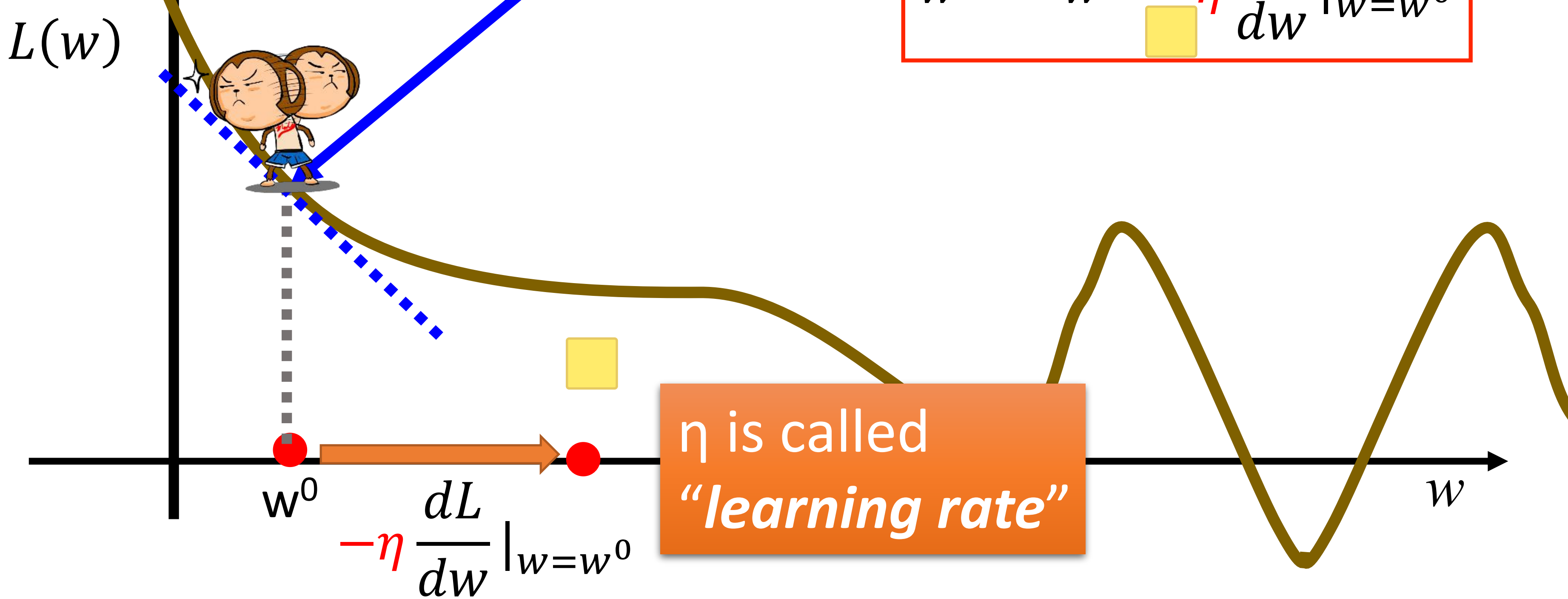
http://chico386.pixnet.net/album/photo/171572850

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 $\frac{dL}{dw}|_{w=w^0}$

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



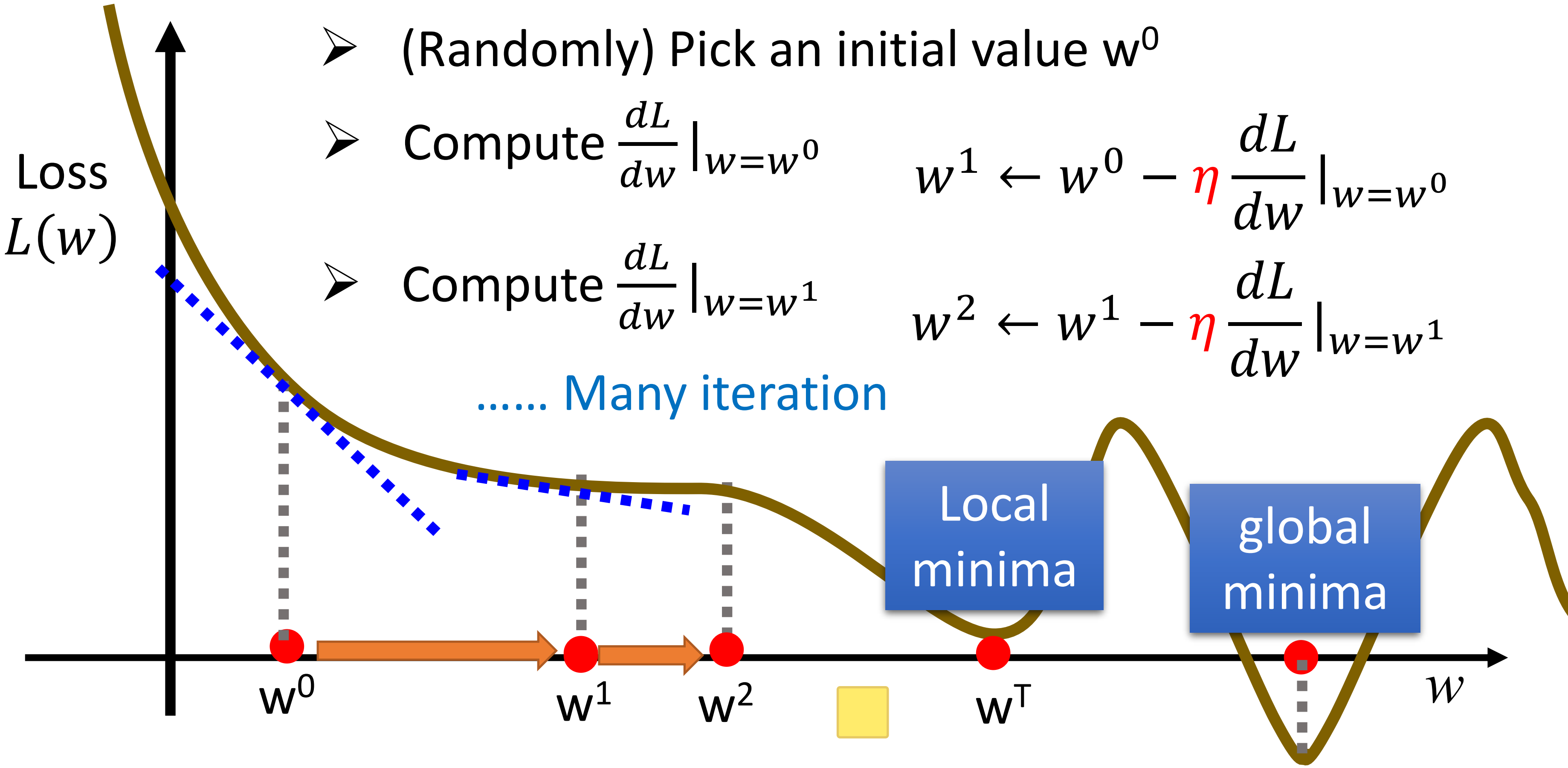
Step 3: Gradient Descent

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

- Consider loss function $L(w)$ with one parameter w:

  - ➢ (Randomly) Pick an initial value w^0
  - ➢ Compute $\frac{dL}{dw}|_{w=w^0}$ $\qquad w^1 \leftarrow w^0 - \eta \frac{dL}{dw}|_{w=w^0}$
  - ➢ Compute $\frac{dL}{dw}|_{w=w^1}$ $\qquad w^2 \leftarrow w^1 - \eta \frac{dL}{dw}|_{w=w^1}$

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

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

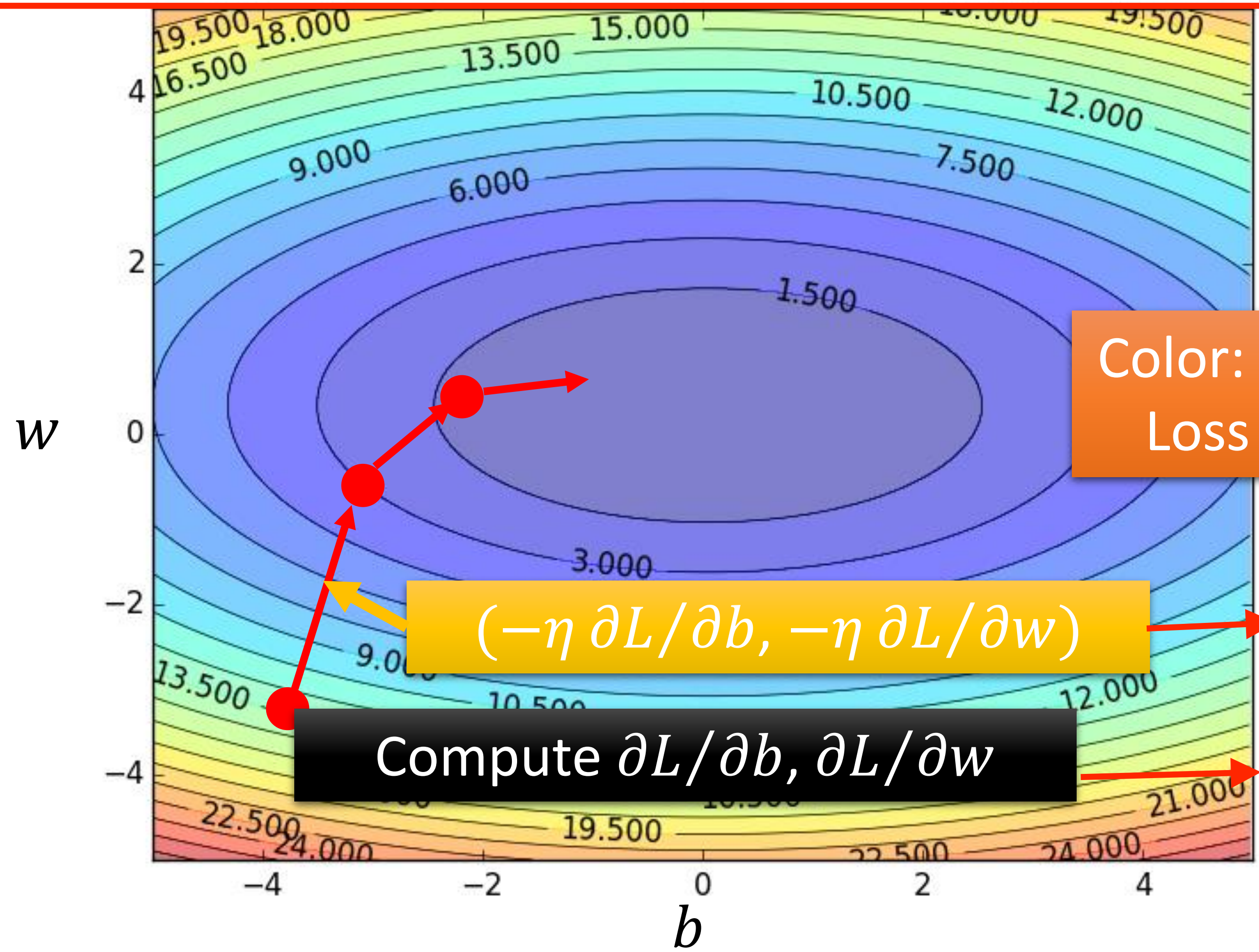
$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \qquad b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

  - 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

將「兩個參數」的 Loss Function 的 Gradient Descent 視覺化！



參數更新的大小

計算切線斜率

Step 3: Gradient Descent

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

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

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

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

How’s the results?

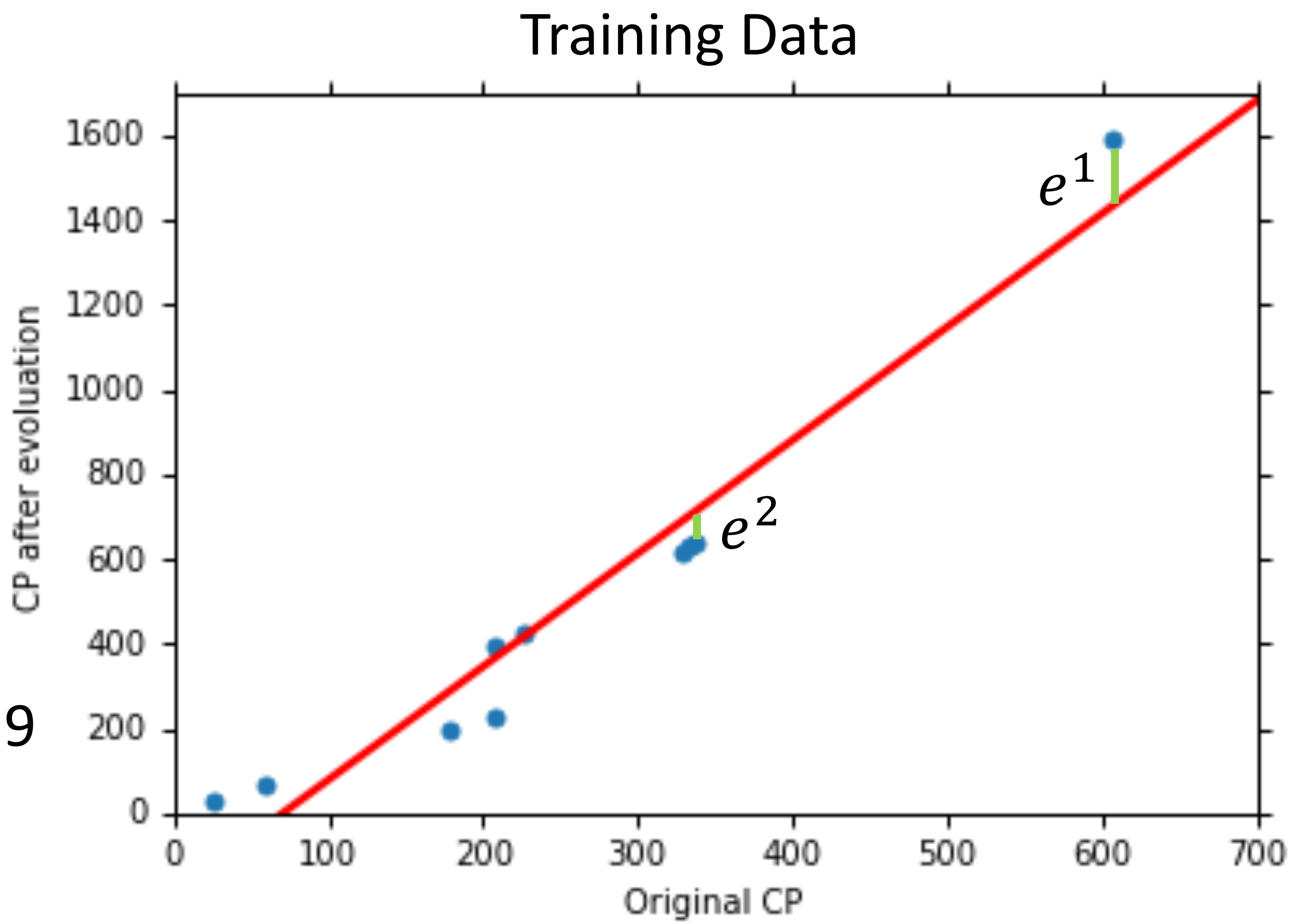
$y = b + w \cdot x_{cp}$

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

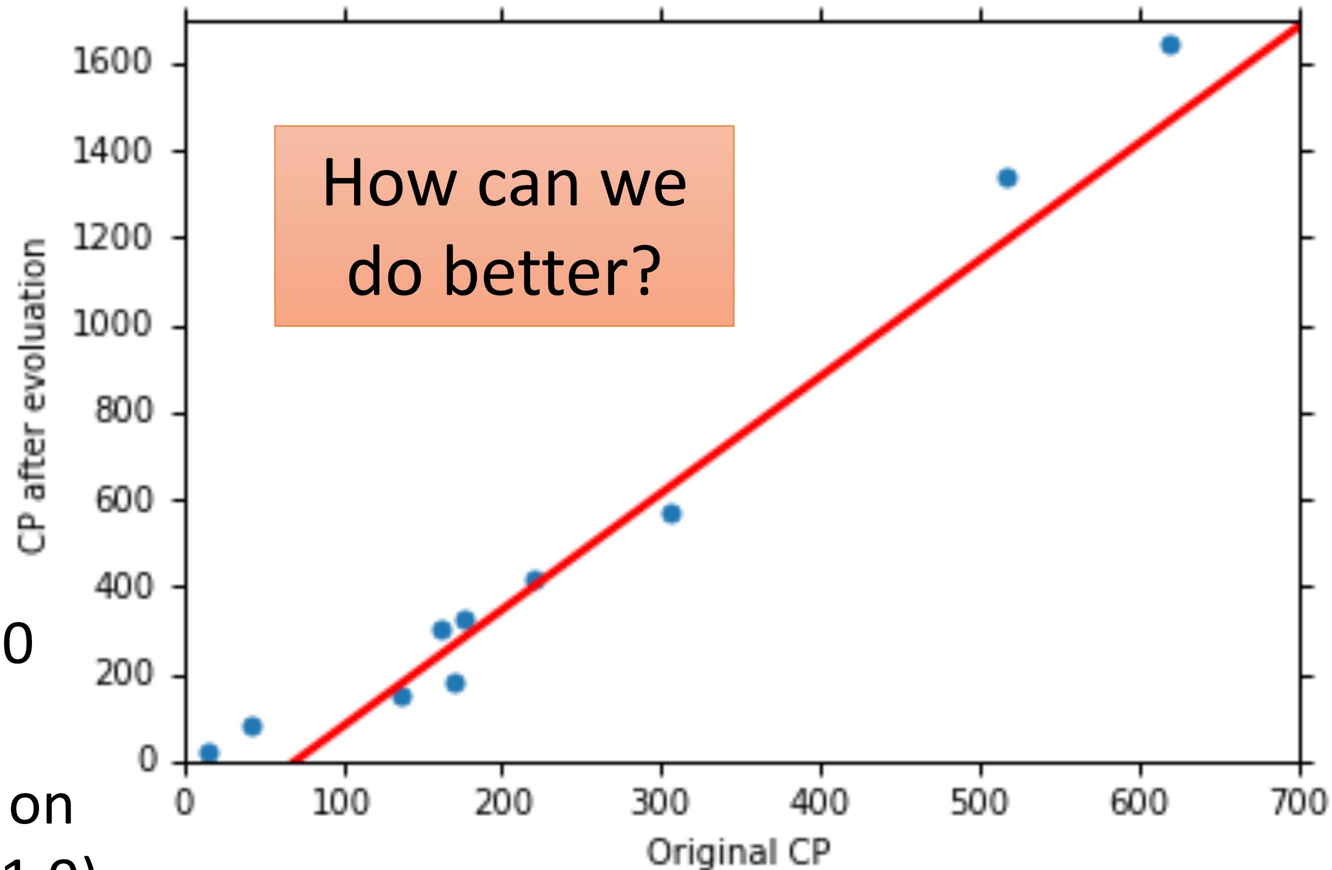
w = 2.7

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

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

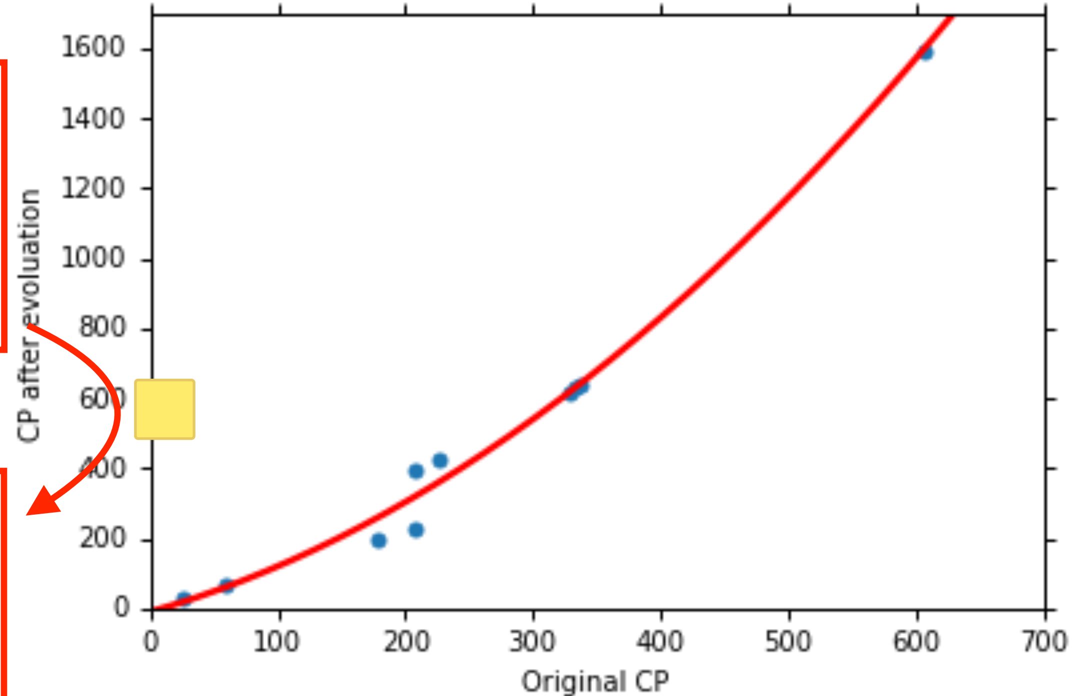
重新定義一個 Function Set

Best Function

$b = -10.3$

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

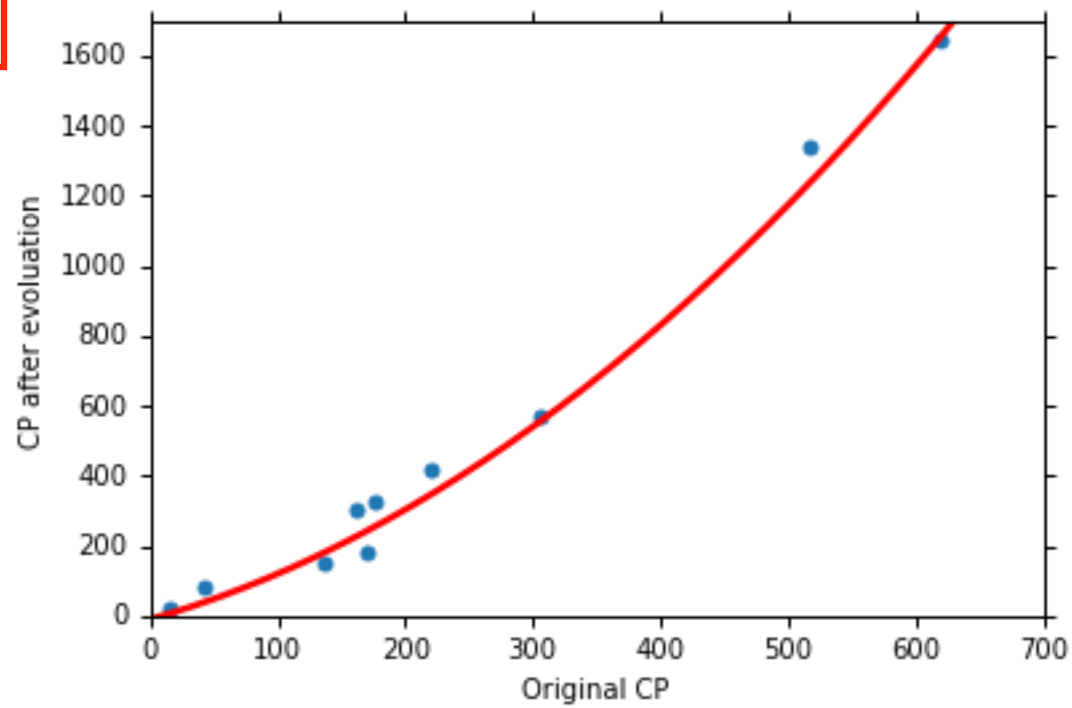
Average Error = 15.4



Testing:

Average Error = 18.4

Better! Could it be even better?



Selecting another Model

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

重新定義一個 Function Set => 項數更多

Best Function

$b = 6.4$, $w_1 = 0.66$

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

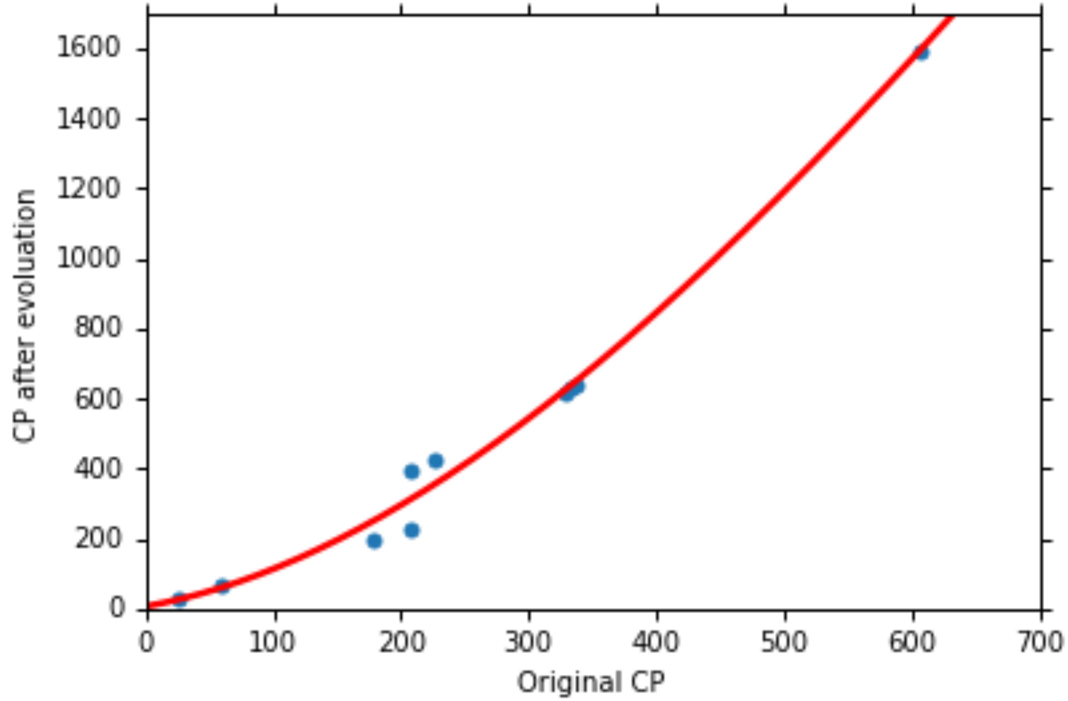
$w_3 = -1.8 \times 10^{-6}$

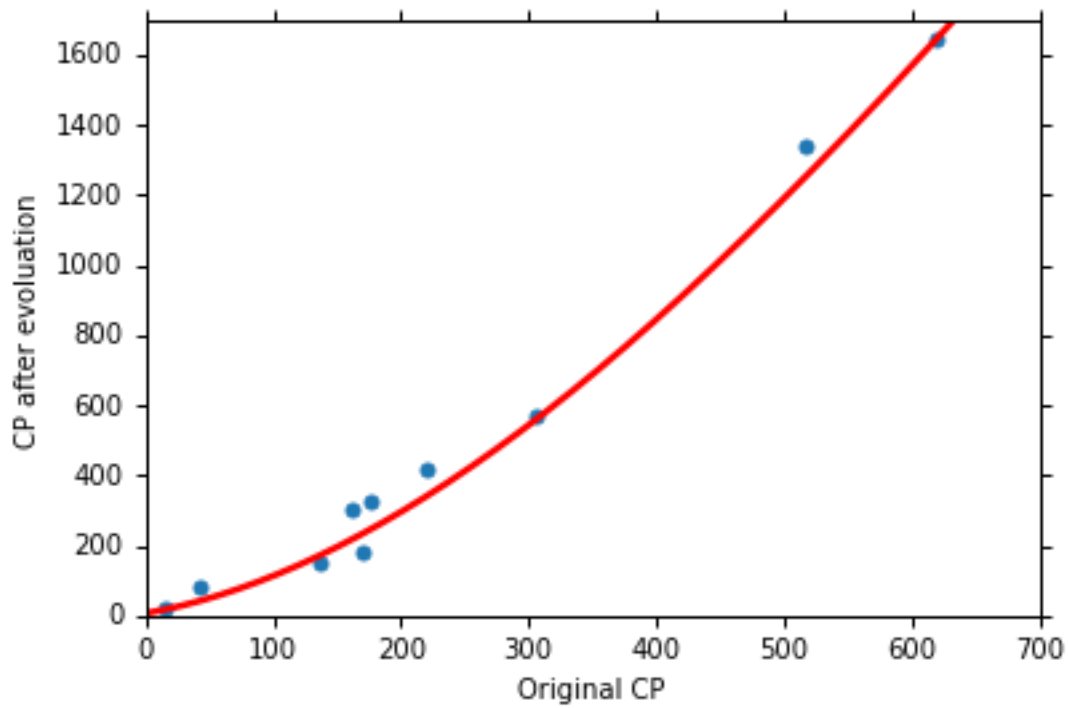
Average Error = 15.3

Testing:

Average Error = 18.1

Slightly better.
How about more complex model?





Selecting another Model

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

重新定義一個 Function Set => 項數更多

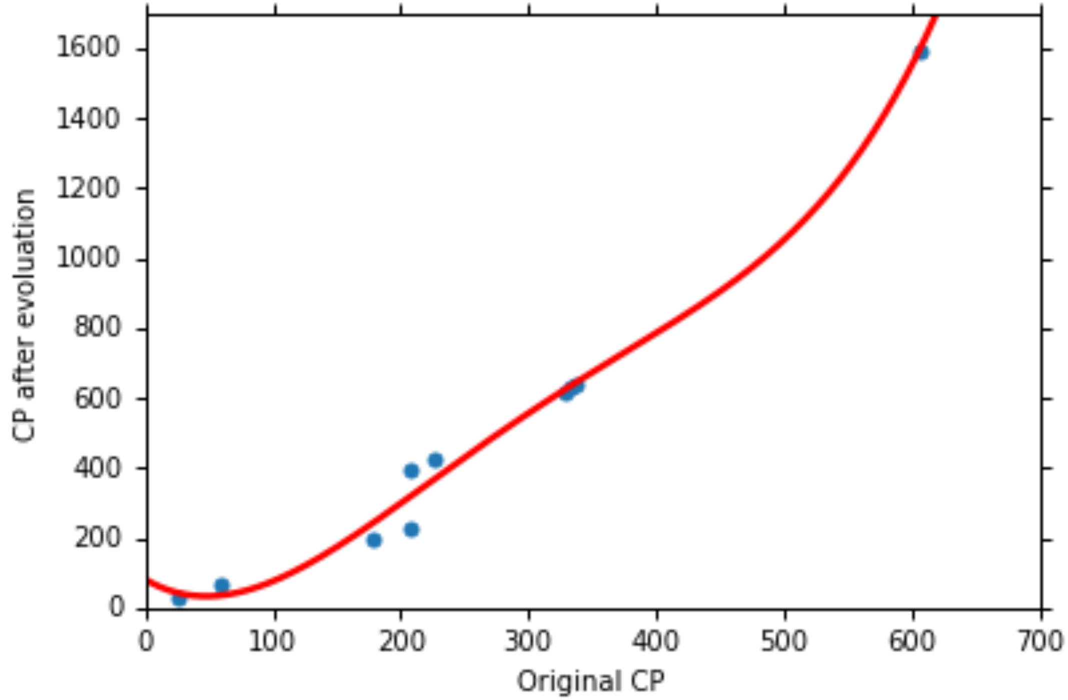
Best Function

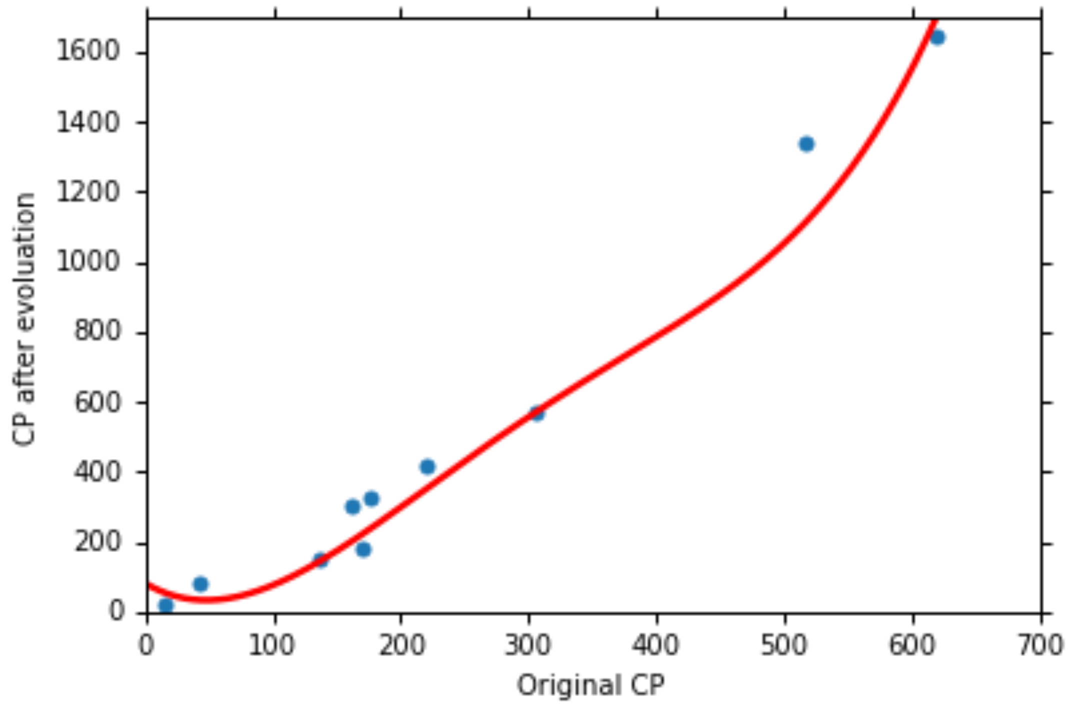
Average Error = 14.9

Testing:

Average Error = 28.8

The results become worse ...

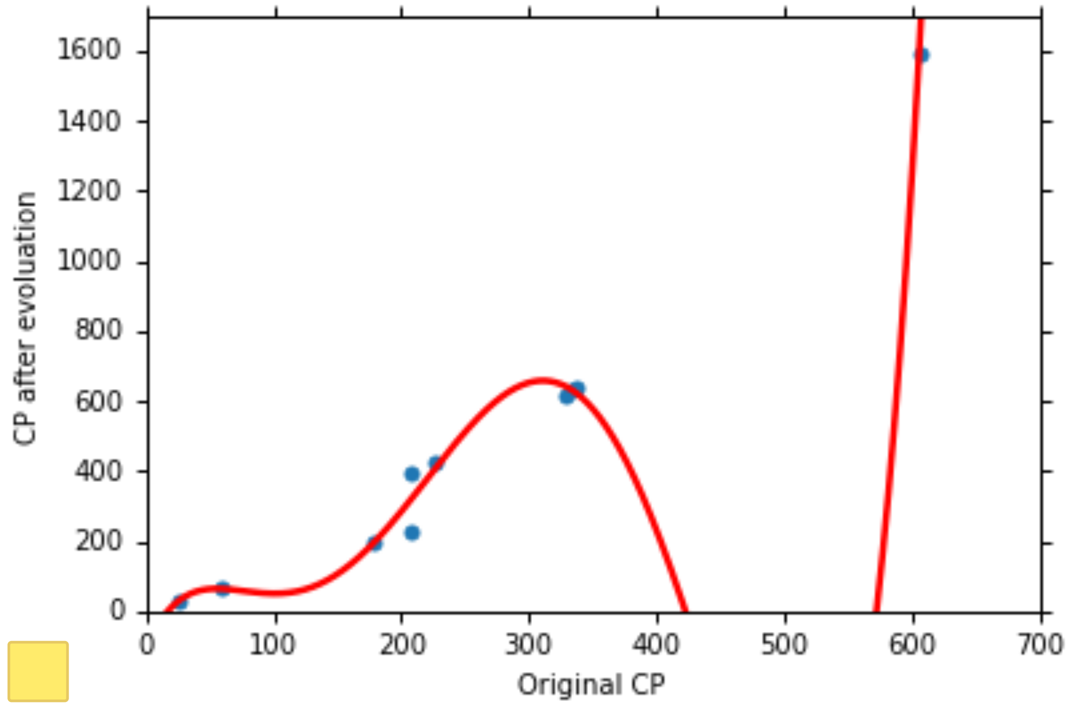




Selecting another Model

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

重新定義一個 Function Set => 項數更多



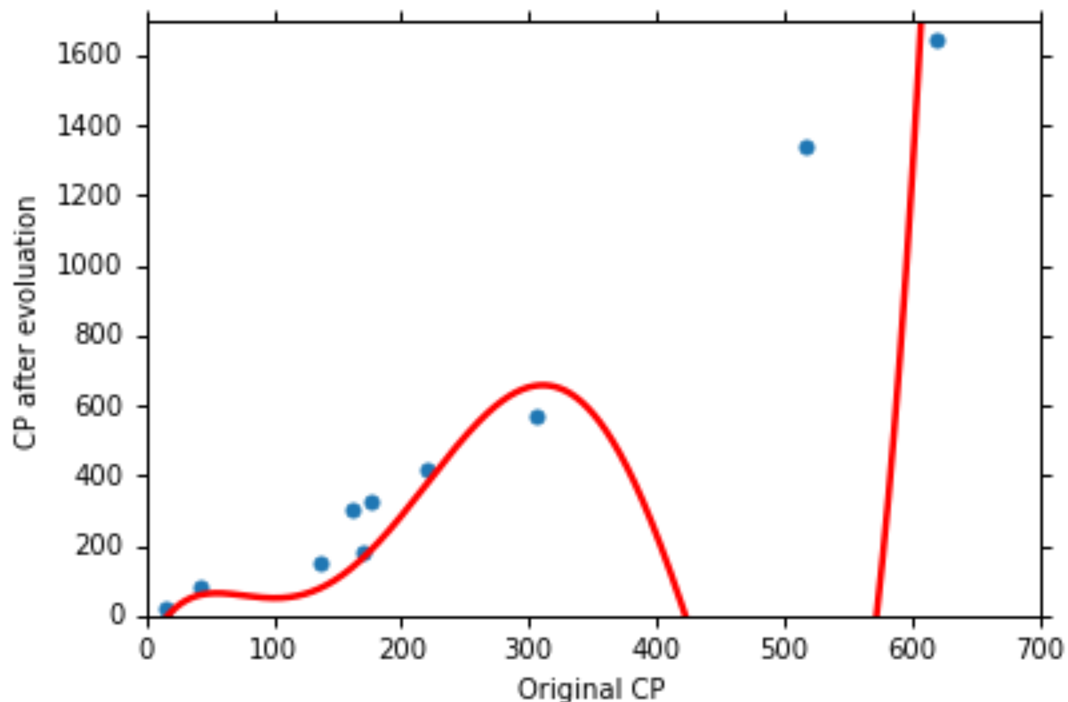
Best Function

Average Error = 12.8

Testing:

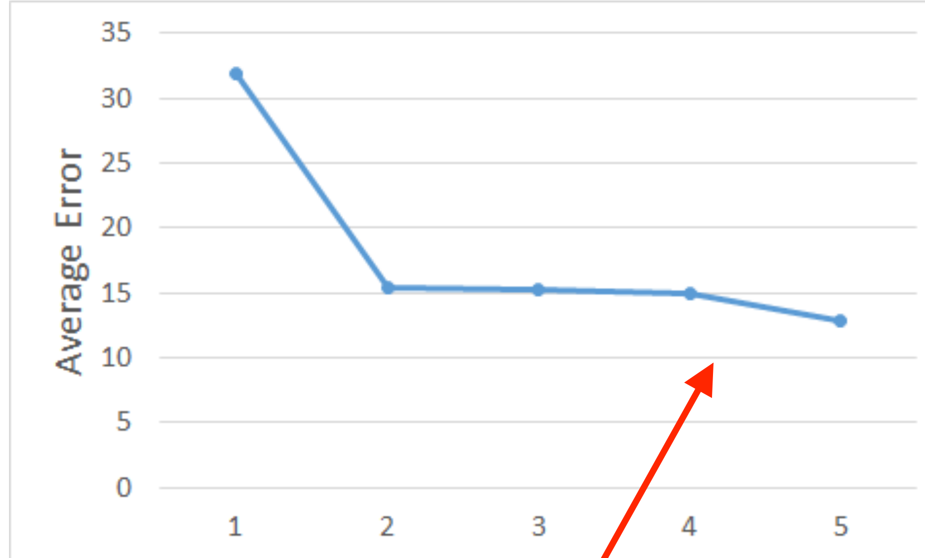
Average Error = 232.1

The results are so bad.

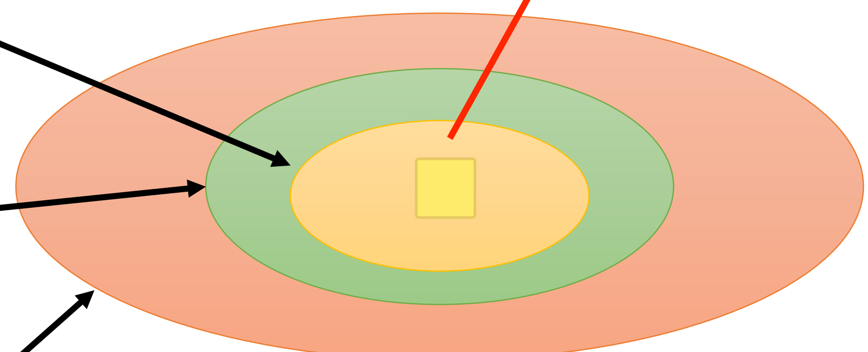


Model Selection

Training Data



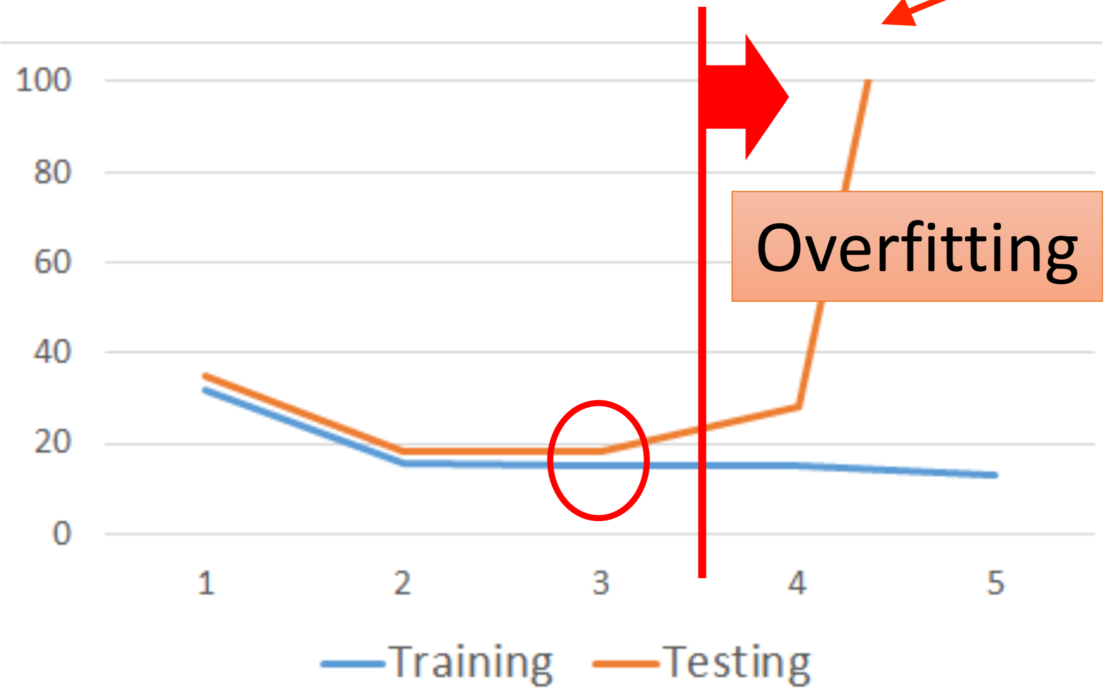
1. $y = b + w \cdot x_{cp}$
2. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$
3. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$
4. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$
5. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2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



A more complex model yields lower error on training data.

If we can truly find the best function

Model Selection



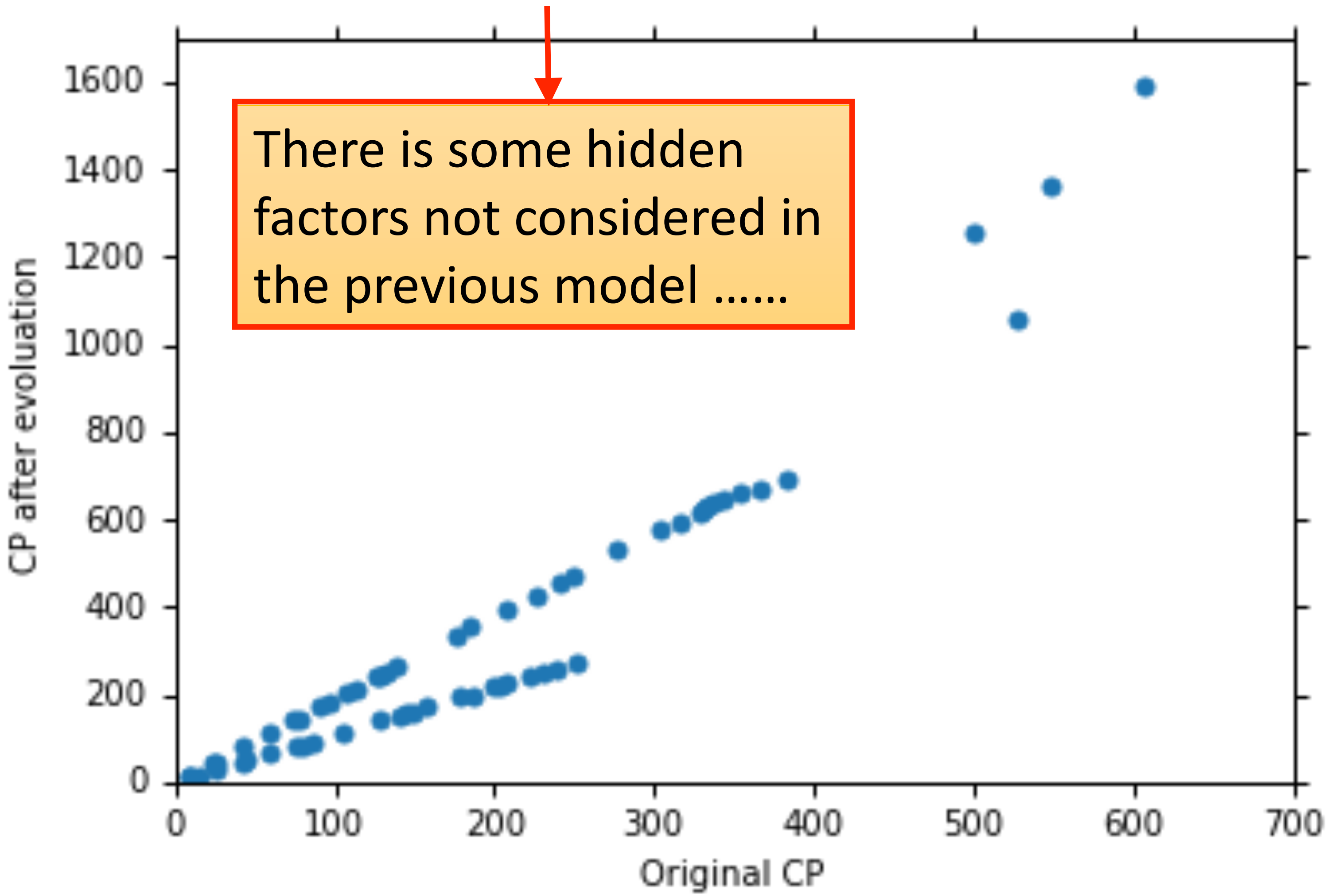
	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

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

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

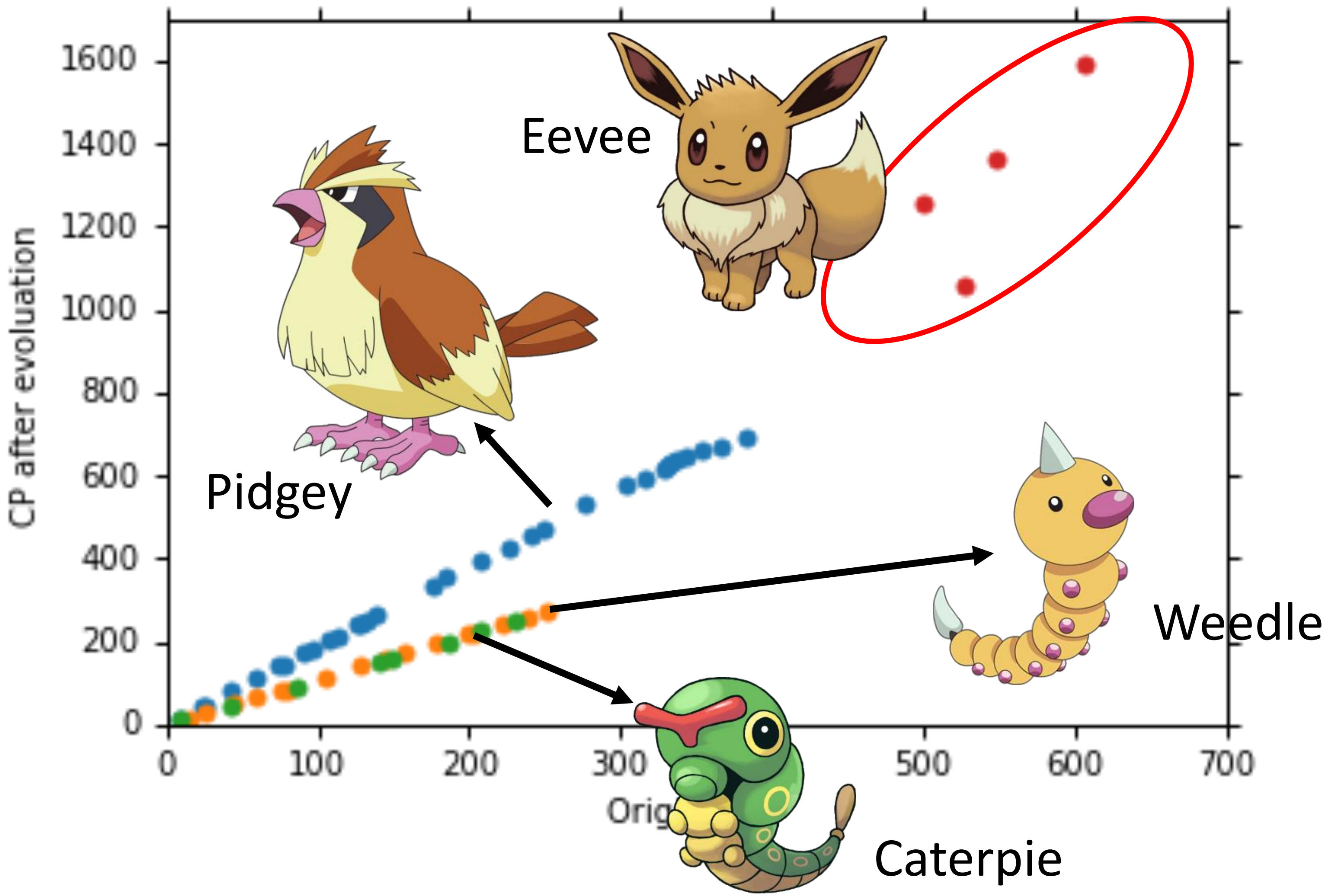
Let’s collect more data

收集更多 data 後發現：原來的 CP 與進化後的 CP 不是單單一條 Regression 的關係



將「物種」也考慮進來！

What are the hidden factors?



Back to step 1: Redesign the Model

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

Linear model?

x

x_s = species of 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: $y = b_4 + w_4 \cdot x_{cp}$

不同的物種，就會有不同的 weight 與 bias

y

Back to step 1: Redesign the Model

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

Linear model?

$$
\begin{aligned}
y = \; & b_1 \cdot \delta(x_s = \text{Pidgey}) \\
& + w_1 \cdot \delta(x_s = \text{Pidgey}) x_{cp} \\
& + b_2 \cdot \delta(x_s = \text{Weedle}) \\
& + w_2 \cdot \delta(x_s = \text{Weedle}) x_{cp} \\
& + b_3 \cdot \delta(x_s = \text{Caterpie}) \\
& + w_3 \cdot \delta(x_s = \text{Caterpie}) x_{cp} \\
& + b_4 \cdot \delta(x_s = \text{Eevee}) \\
& + w_4 \cdot \delta(x_s = \text{Eevee}) x_{cp}
\end{aligned}
$$

將上面的四條式子結合成一條

$$\delta(x_s = \text{Pidgey})$$

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

所以，新的 Model 仍屬於 Linear Model：「進化後 CP」同時考慮「原 CP」與「物種」

Back to step 1: Redesign the Model

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

Linear model?

$$
\begin{aligned}
y = b_1 \cdot\ & 1 \\
+w_1 \cdot\ & 1 \quad x_{cp} \\
+b_2 \cdot\ & 0 \\
+w_2 \cdot\ & 0 \\
+b_3 \cdot\ & 0 \\
+w_3 \cdot\ & 0 \\
+b_4 \cdot\ & 0 \\
+w_4 \cdot\ & 0
\end{aligned}
$$

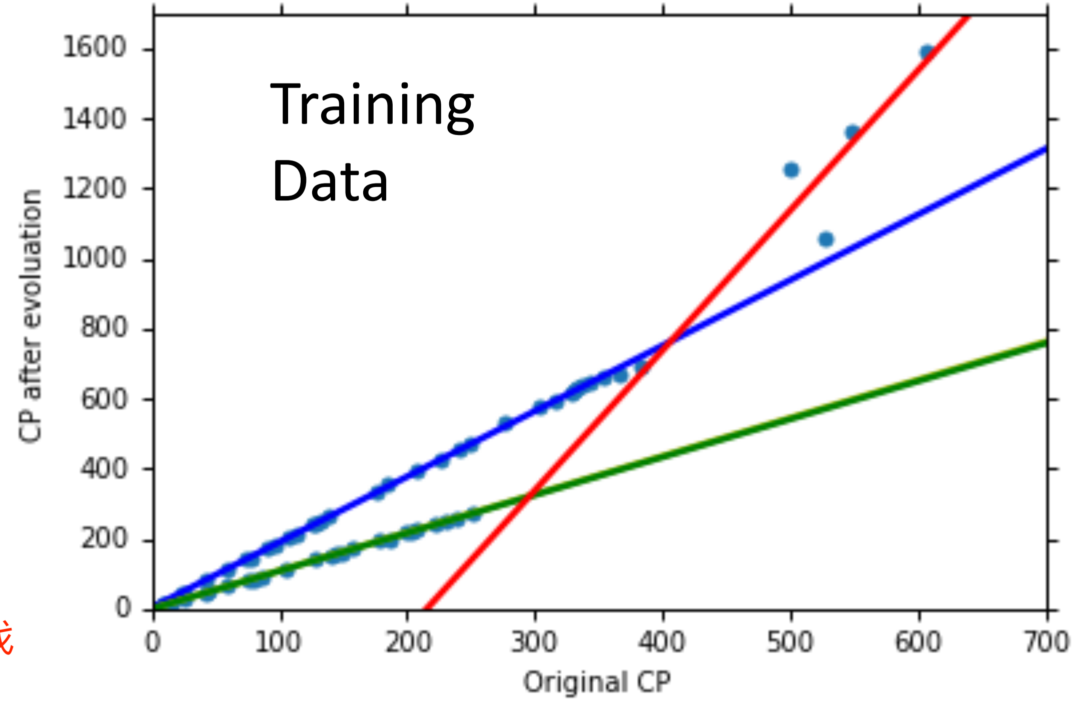
$\delta(x_s = \text{Pidgey})$

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

If $x_s = \text{Pidgey}$

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

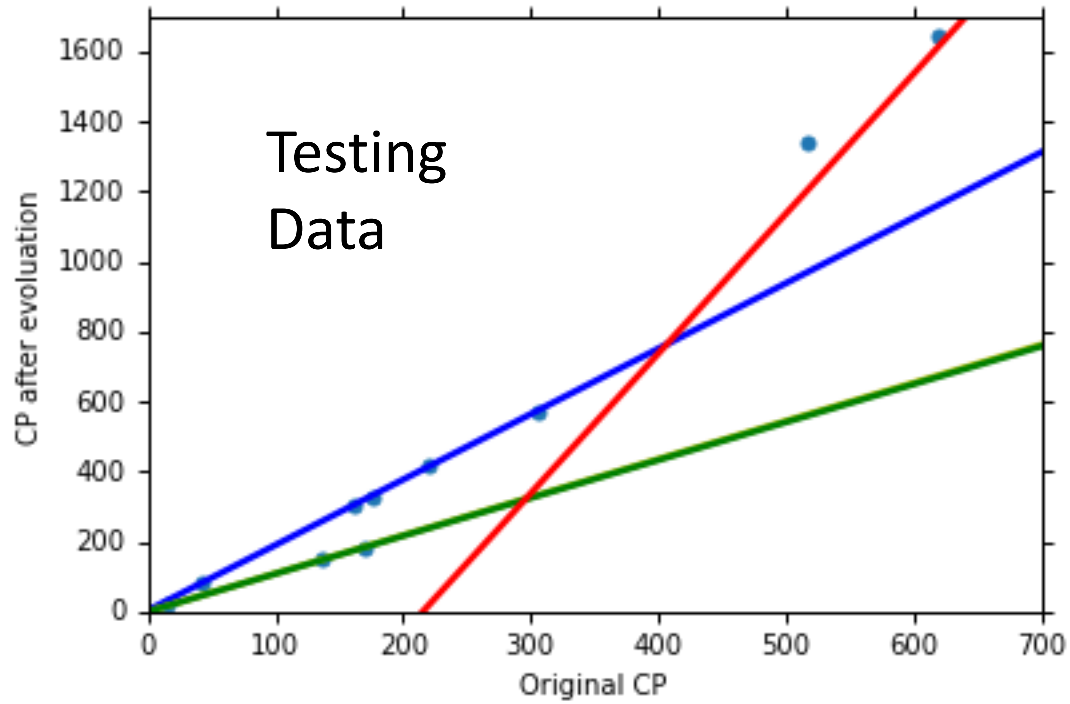
Average error = 3.8



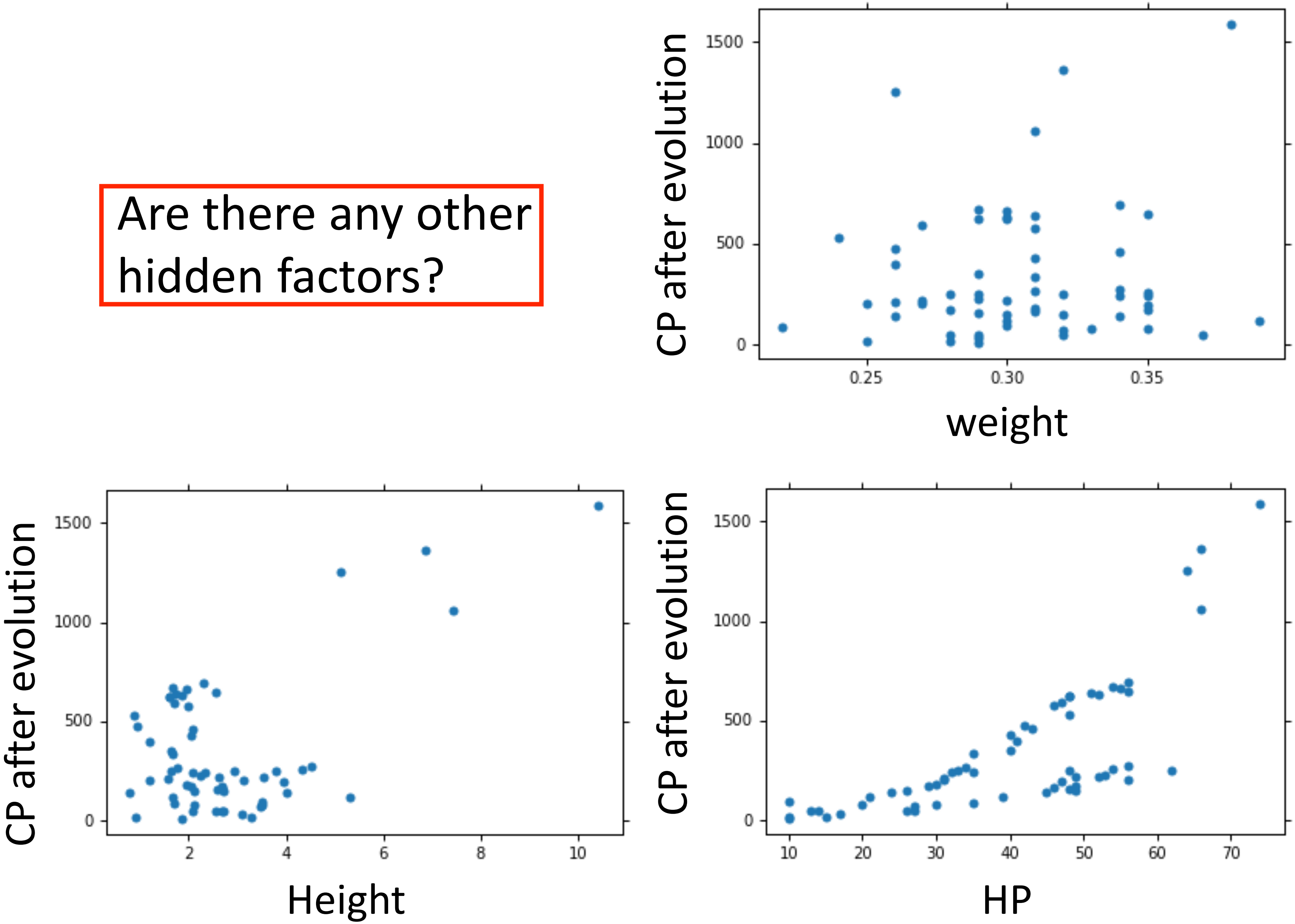
利用新的 Model (Function Set)，從中找到一個 Dest Function 後，確實在 Test Data 上得到更小的 Error。

但是，仍有 Error 代表可能有些「因素」還沒考慮進 Model 中！

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

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

- Smaller w_i means … smoother

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

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

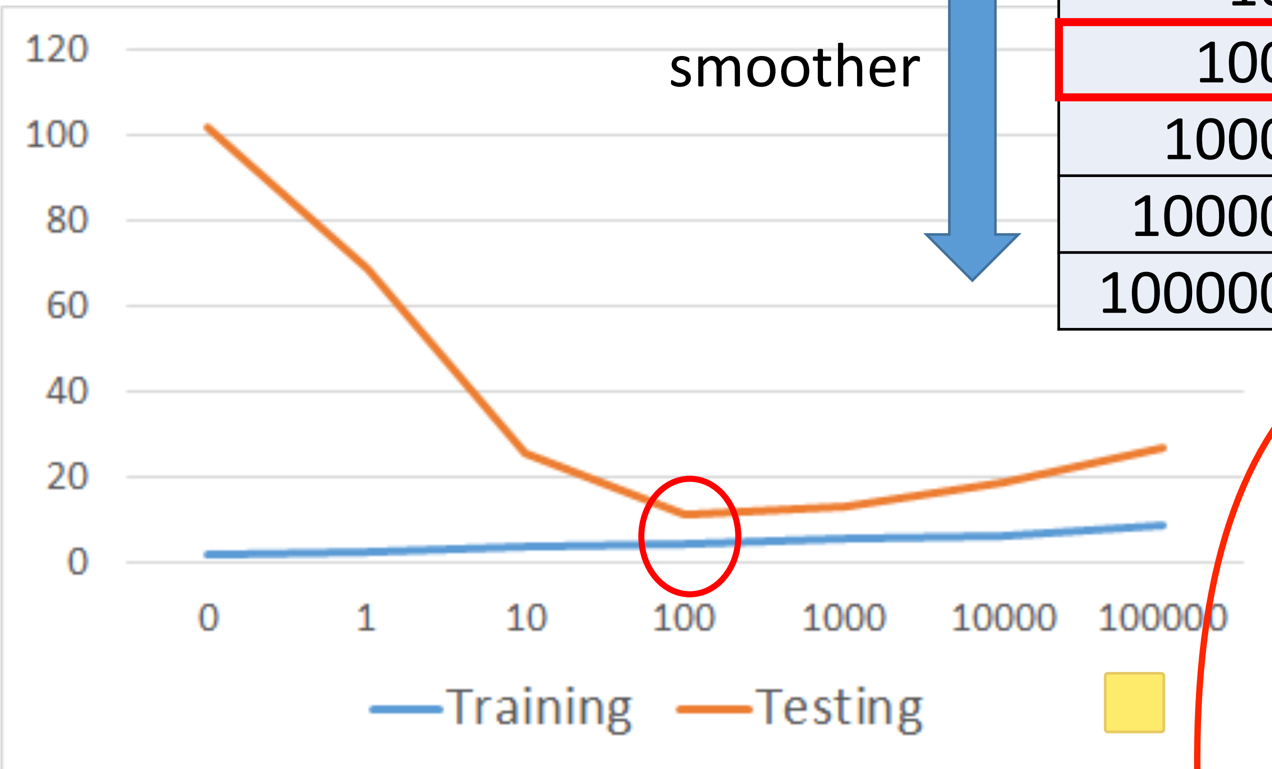
- We believe smoother function is more likely to be correct

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.

Conclusion

- Pokémon: Original CP and species almost decide the CP after evolution
  - There are probably other hidden factors
- Gradient descent
  - More theory and tips in the following lectures
- We finally get average error = 11.1 on the testing data
  - How about new data? Larger error? Lower error?
- Next lecture: Where does the error come from?
  - More theory about overfitting and regularization
  - The concept of validation