# Regression

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# Regression: Output a scalar

- Stock Market Forecast

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

- Self-driving Car

$f($  $) =$ 方向盤角度

- Recommendation

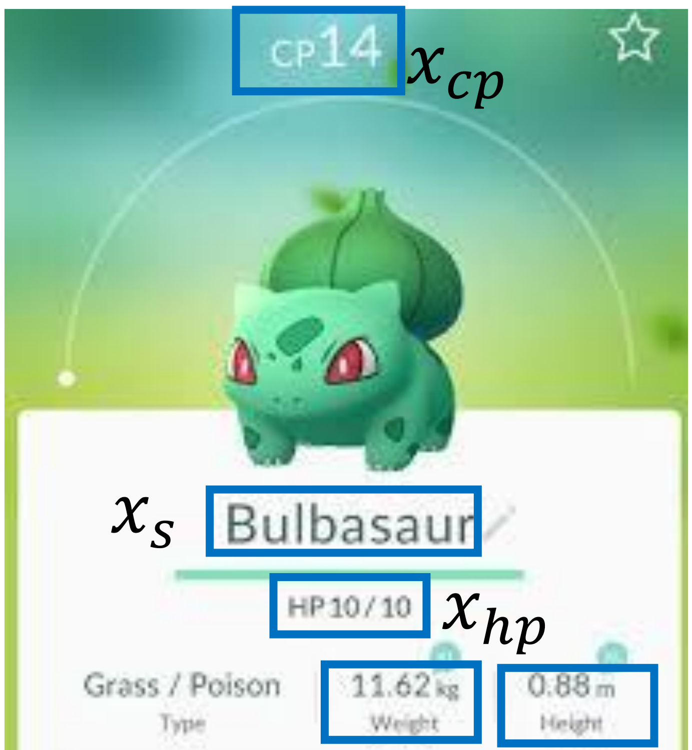
$f($ 使用者 A 商品 B $) =$ 購買可能性

# Example Application

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

$X = \{x_i, x_j \cdots\}$

$f($




$x_{cp}$ $x_s$ $x_{hp}$ $x_w$ $x_h$

$x$

$) =$ 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 $y$

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

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

feature

$w_i$: weight, b: bias

# Step 2: Goodness of Function

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

A set of function

Model

$f_1, f_2 \cdots$

shang

Training Data

function input:

function Output (scalar):

# Step 2: Goodness of Function

Training Data:
10 pokemons

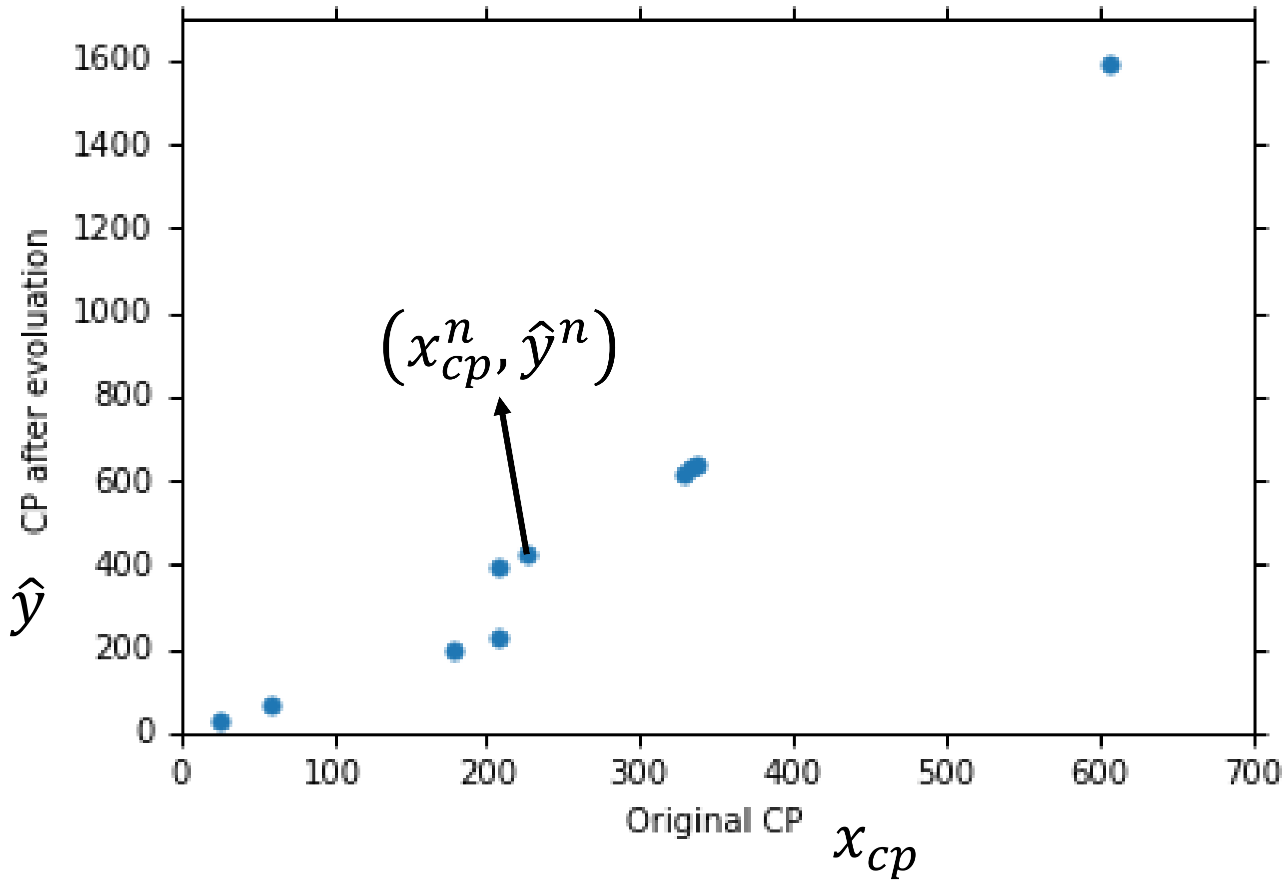
$(x^1, \hat{y}^1)$

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

⋮

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

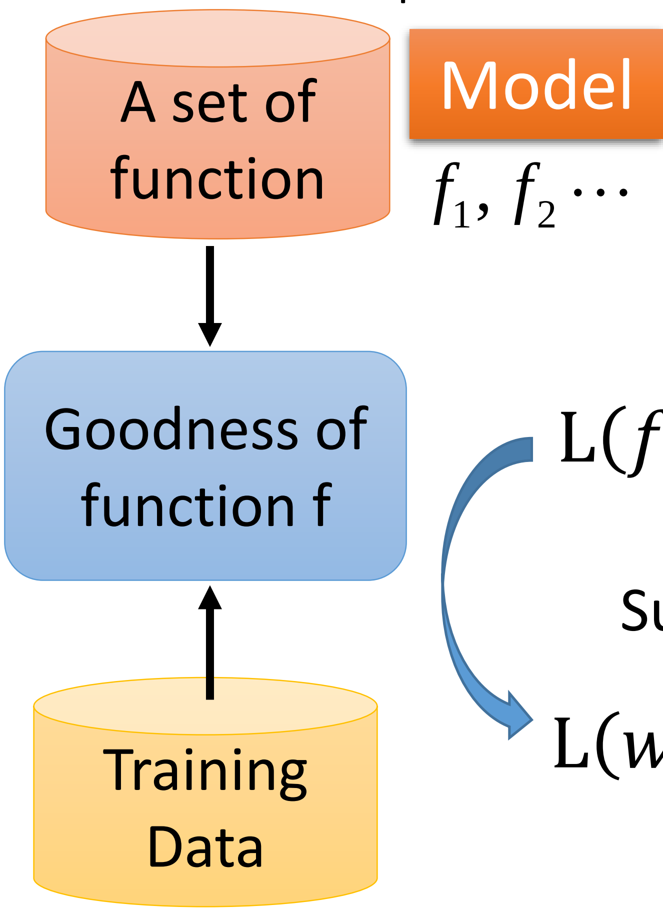
This is real data.




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

# 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

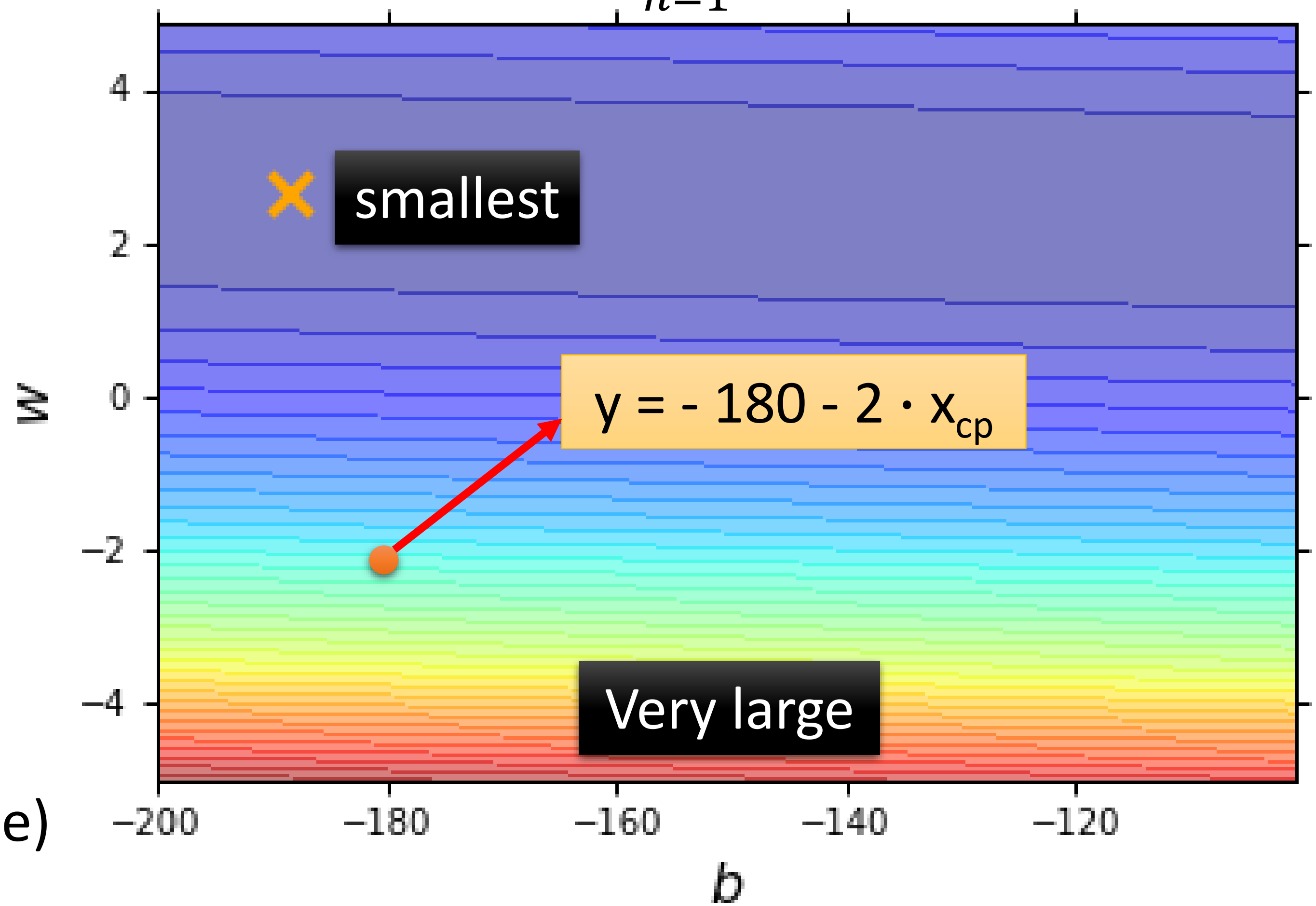
- Loss Function

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

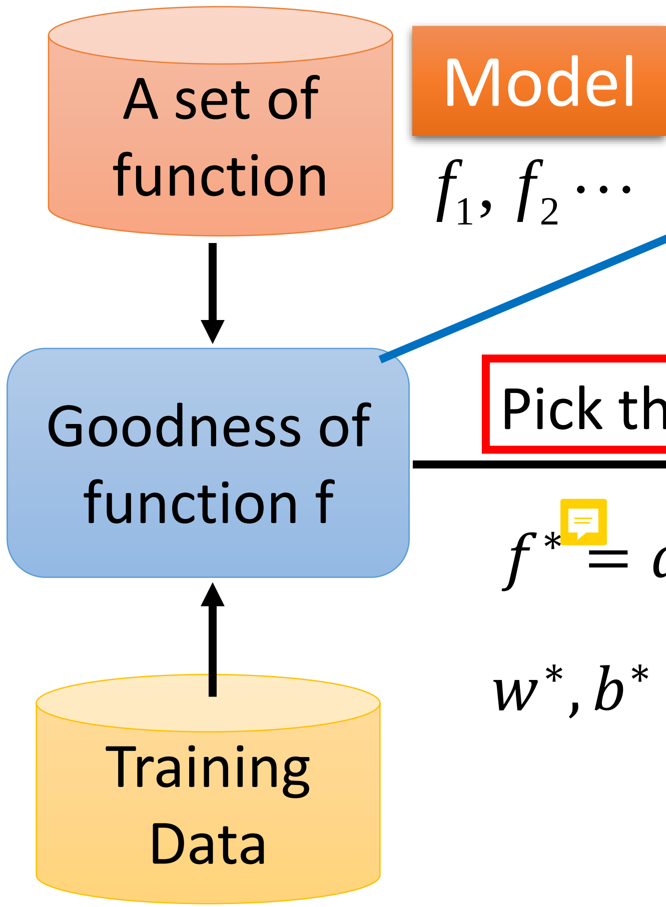
Each point in the figure is a function

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

(true example)



# Step 3: Best Function




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

Pick the "Best" Function

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

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

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

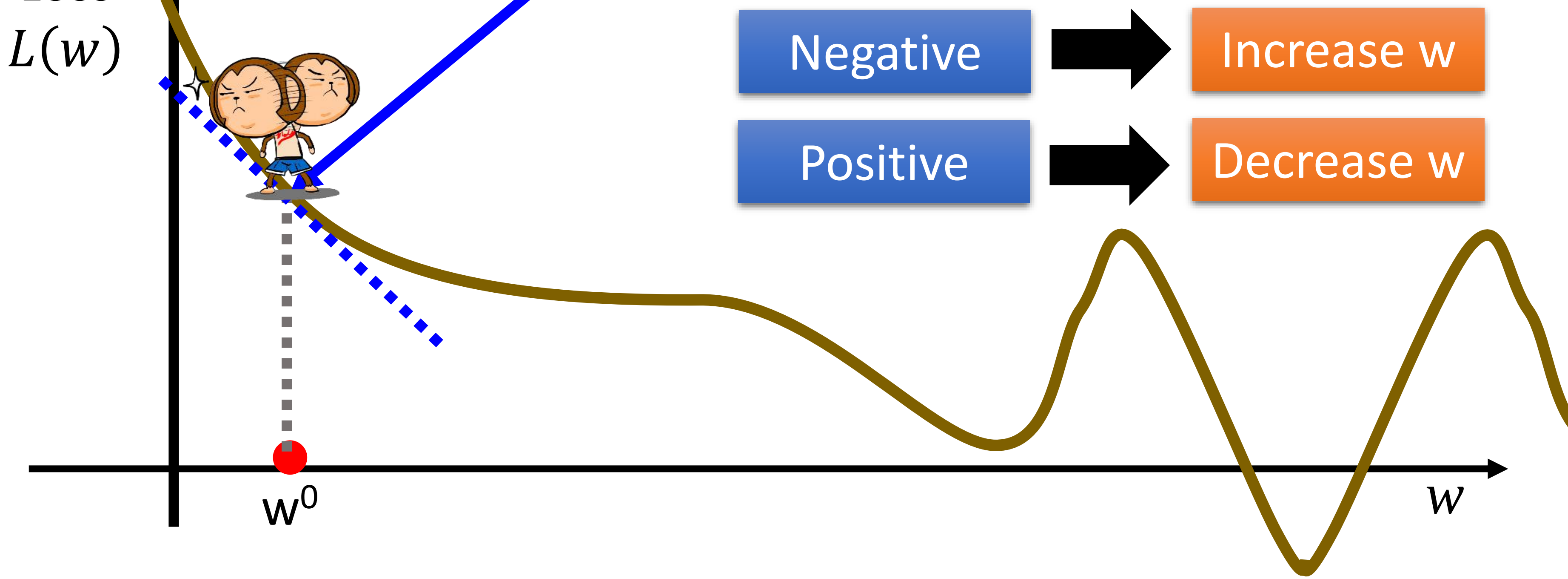
Gradient Descent

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



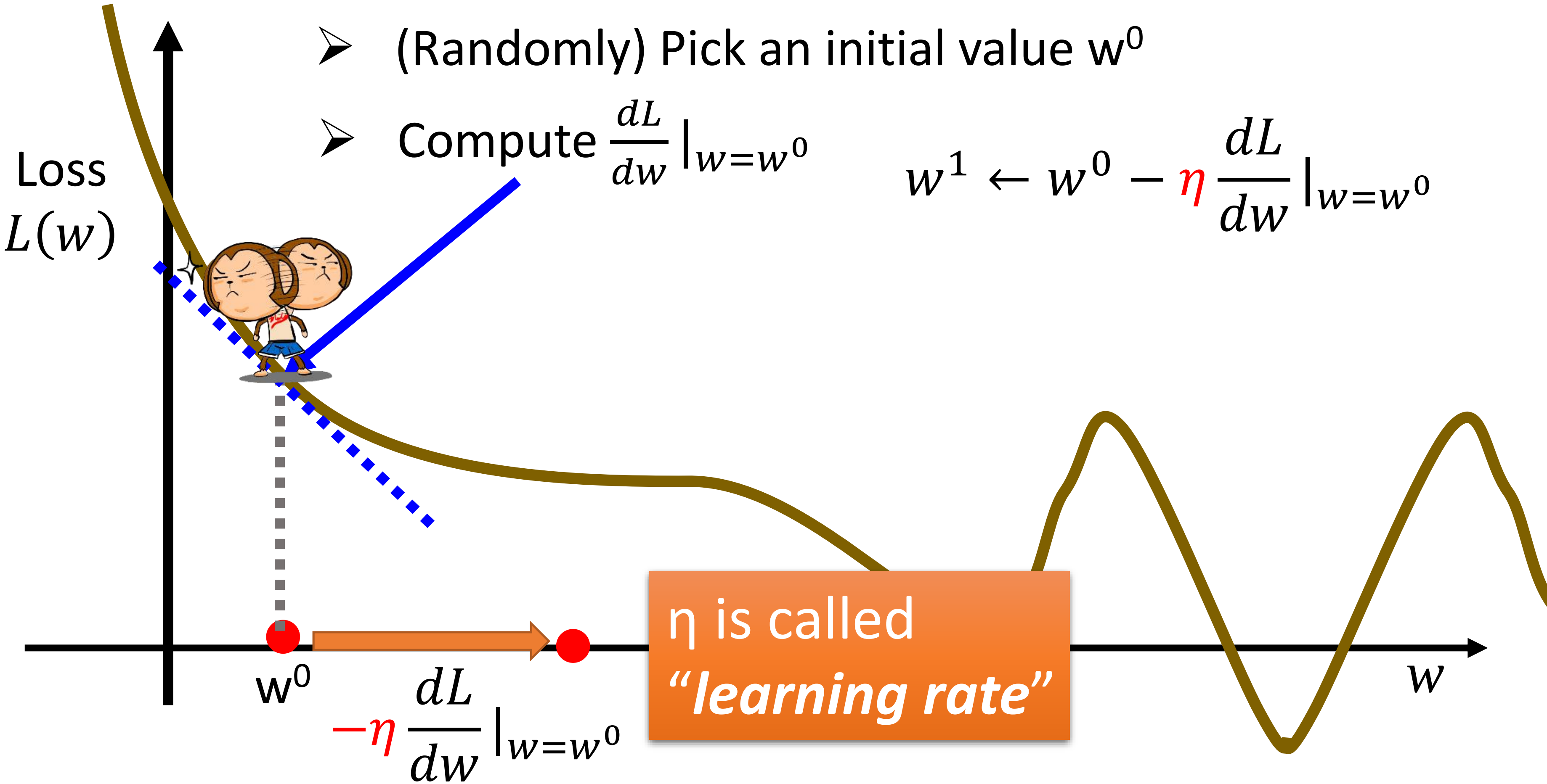
http://chico386.pixnet.net/album/photo/171572850

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

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



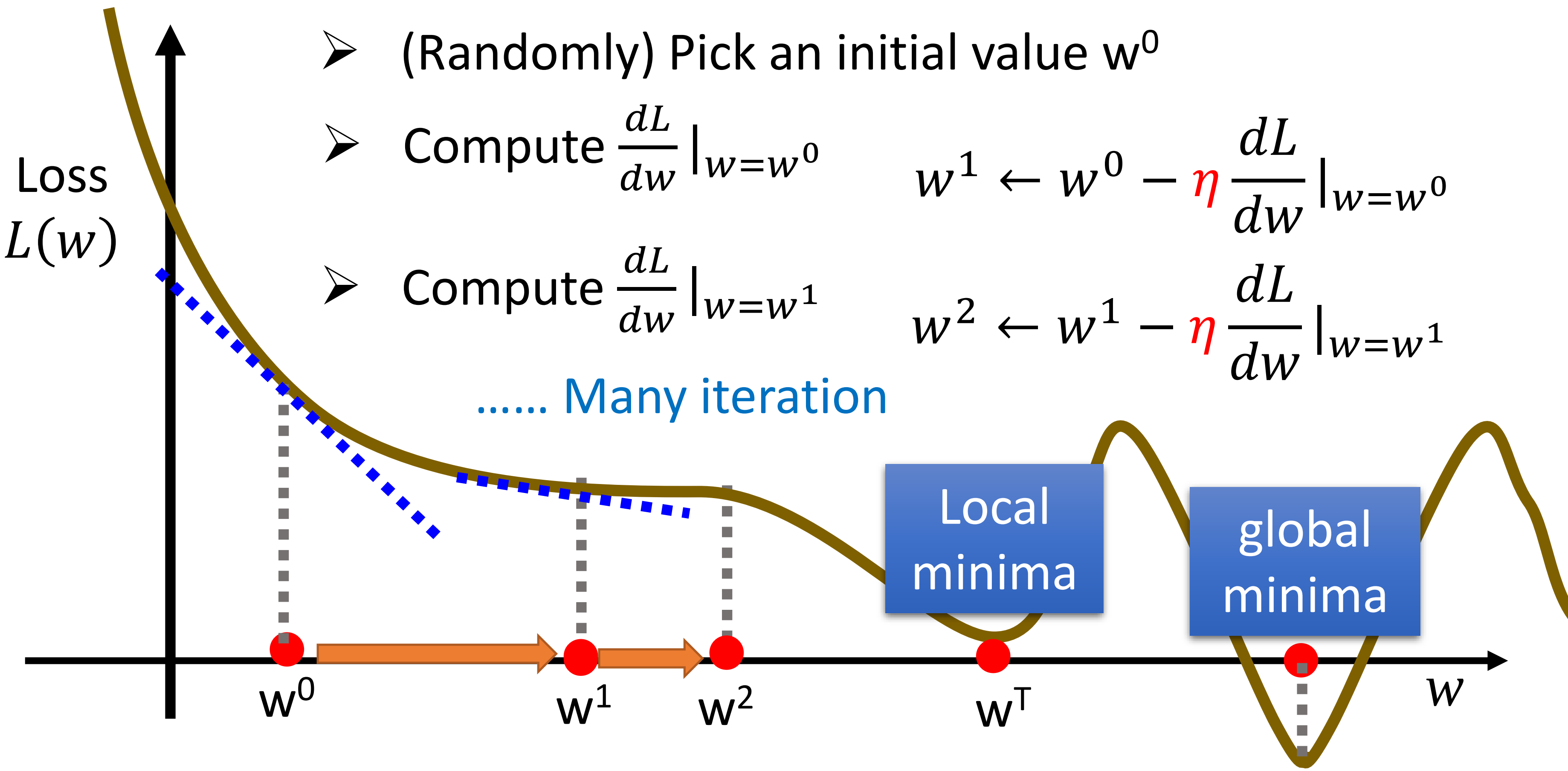
# Step 3: Gradient Descent

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

- 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

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

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

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

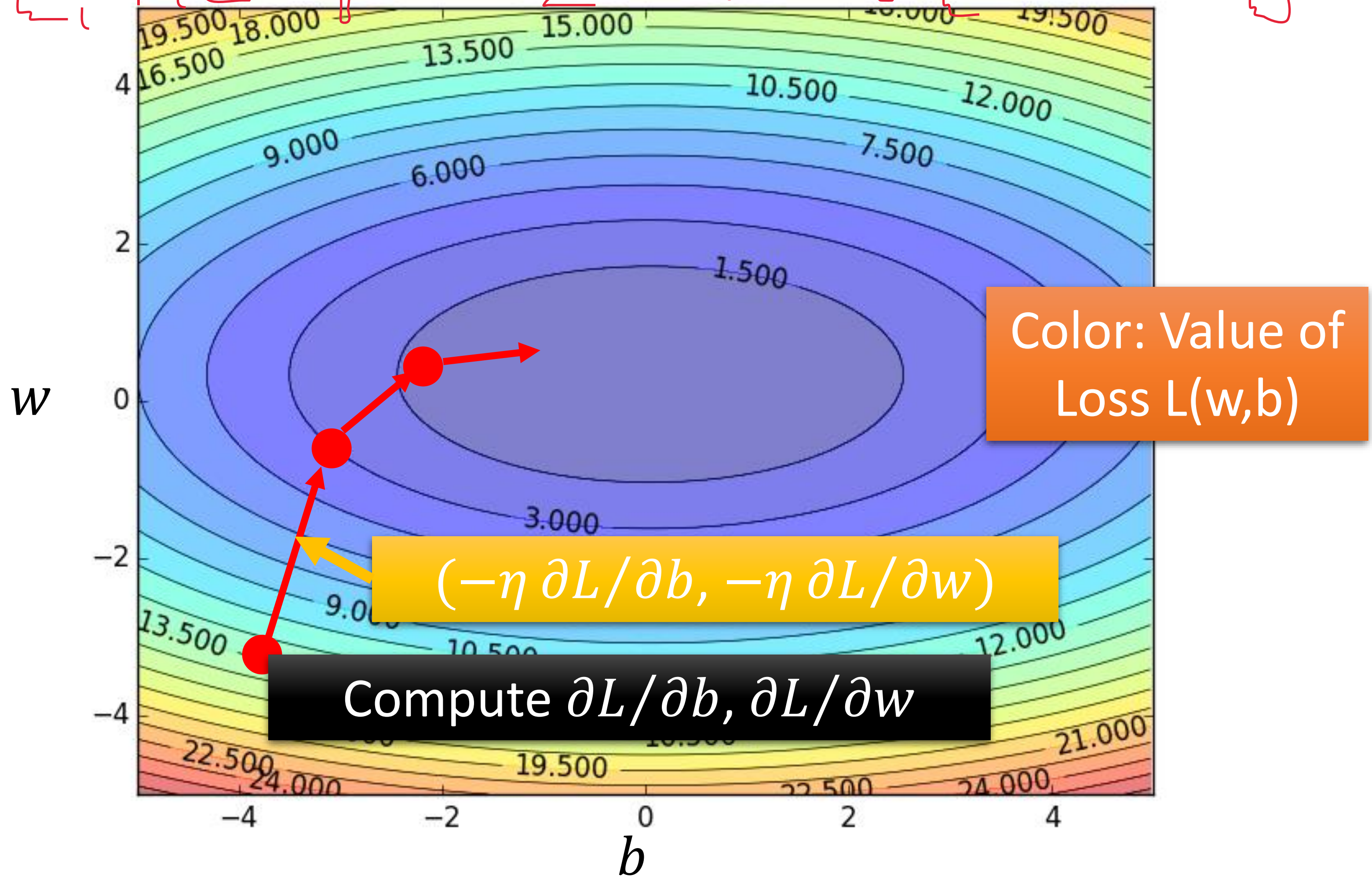
$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \qquad b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

  - 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

L: Linear 是 Convex 的



# Step 3: Gradient Descent

- When solving:

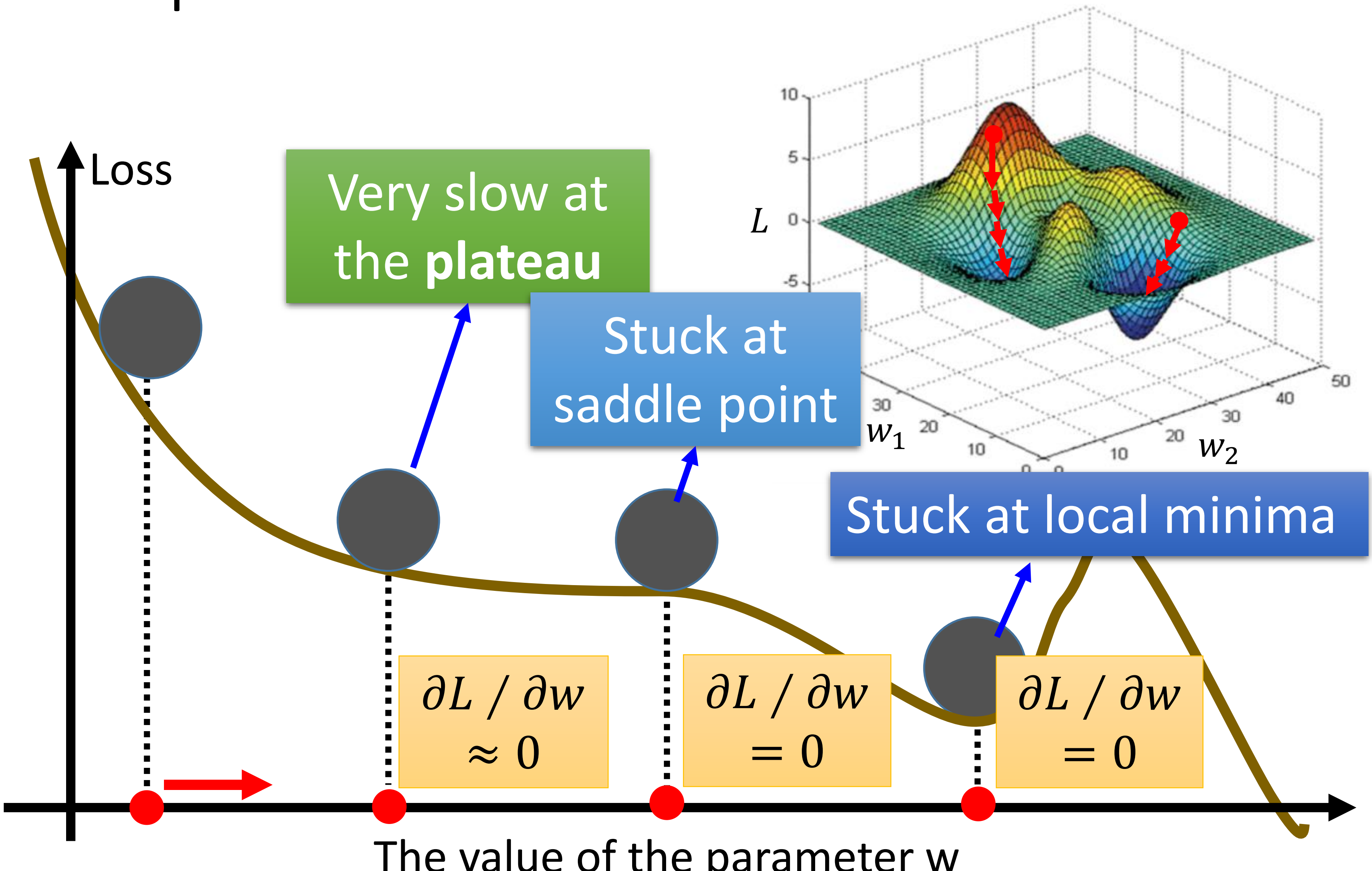
$$\theta^* = \arg\max_{\theta} L(\theta) \quad \text{by gradient descent}$$

- Each time we update the parameters, we obtain $\theta$ 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?

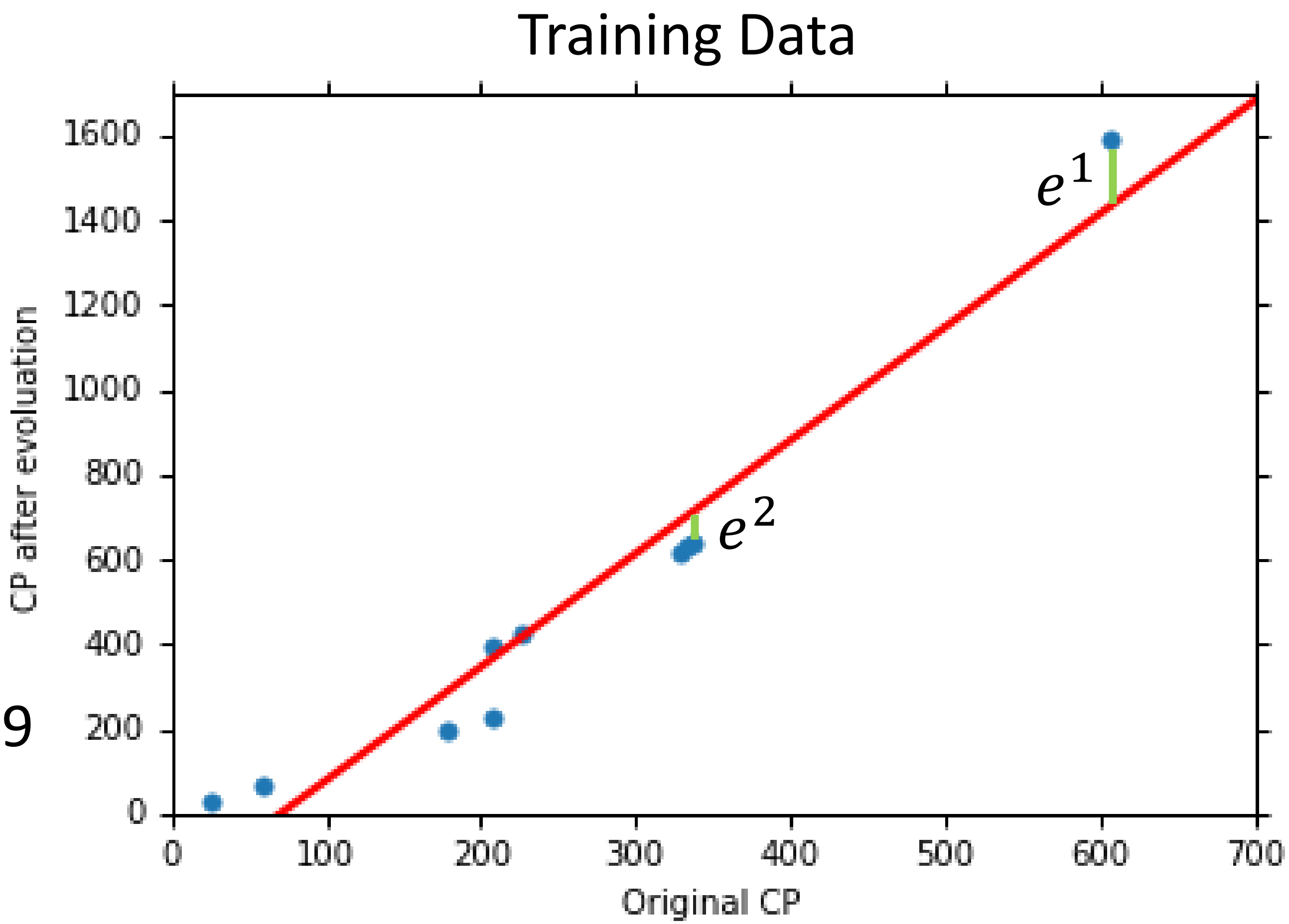
$y = b + w \cdot x_{cp}$

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

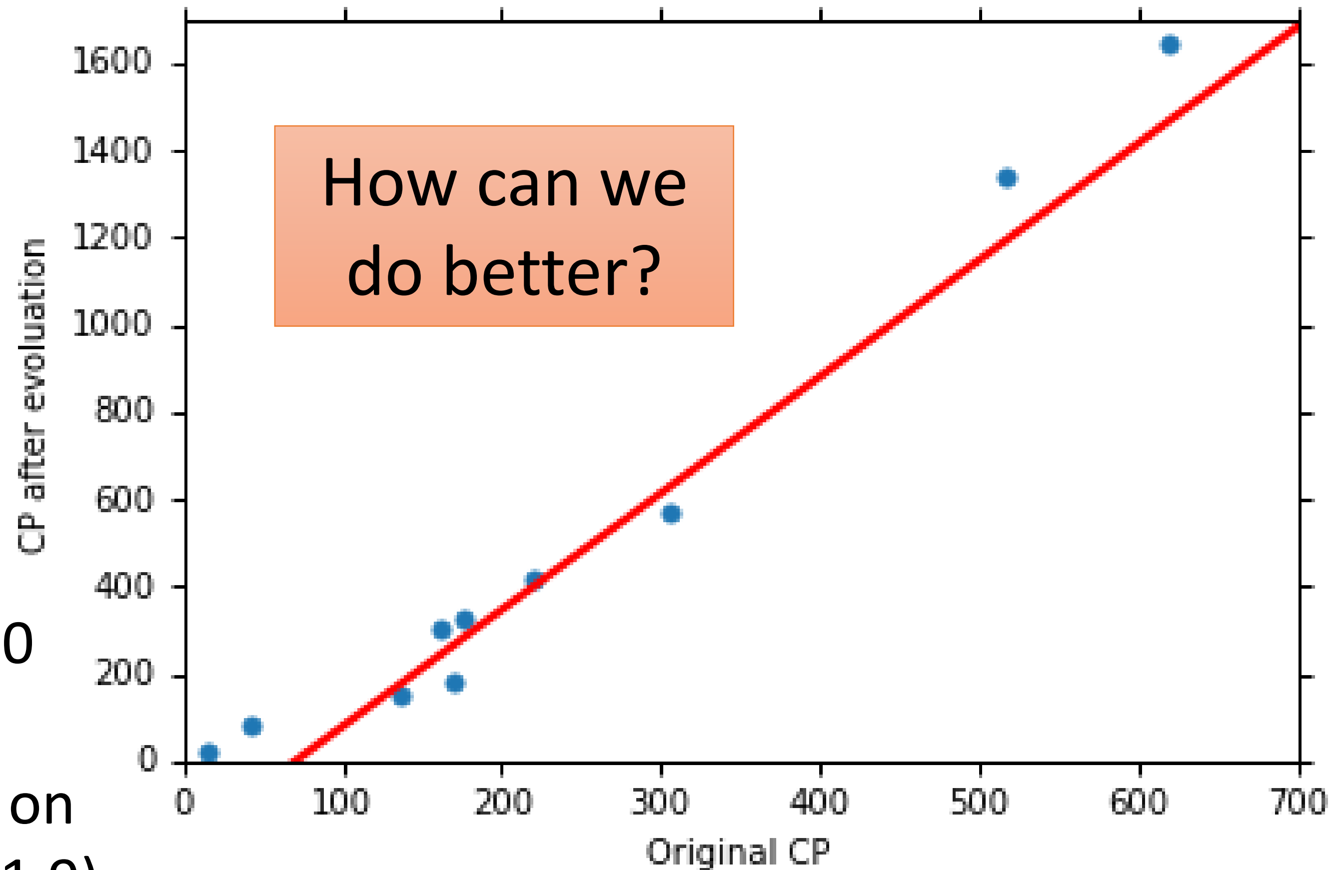
w = 2.7

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***

$b = -10.3$

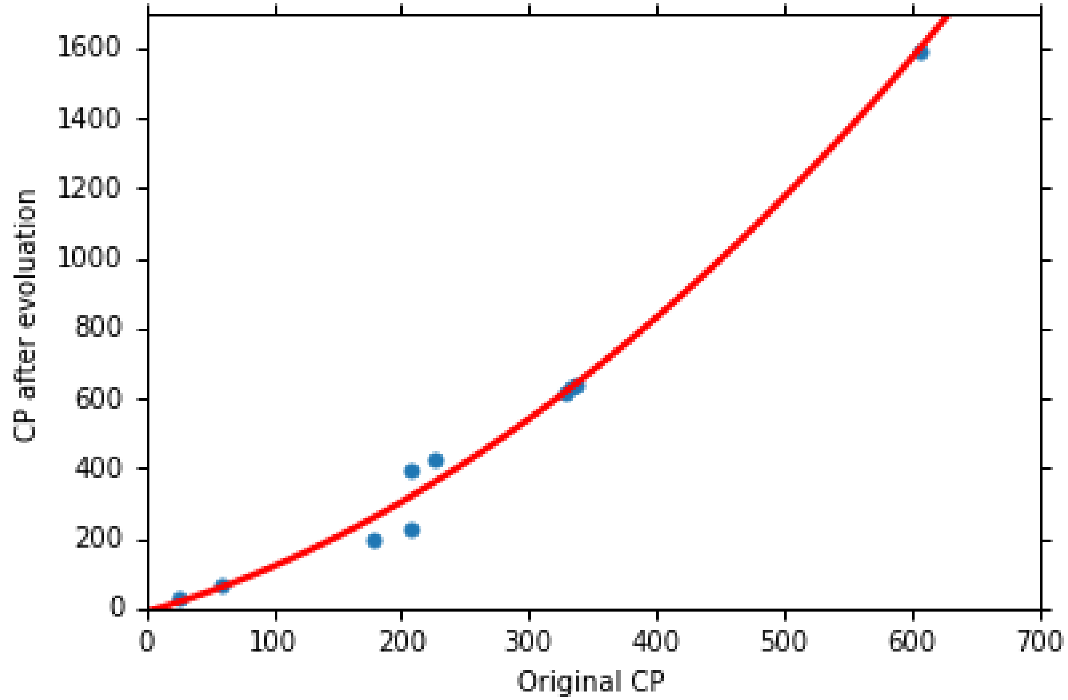
$w_1 = 1.0$, $w_2 = 2.7 \times 10^{-3}$

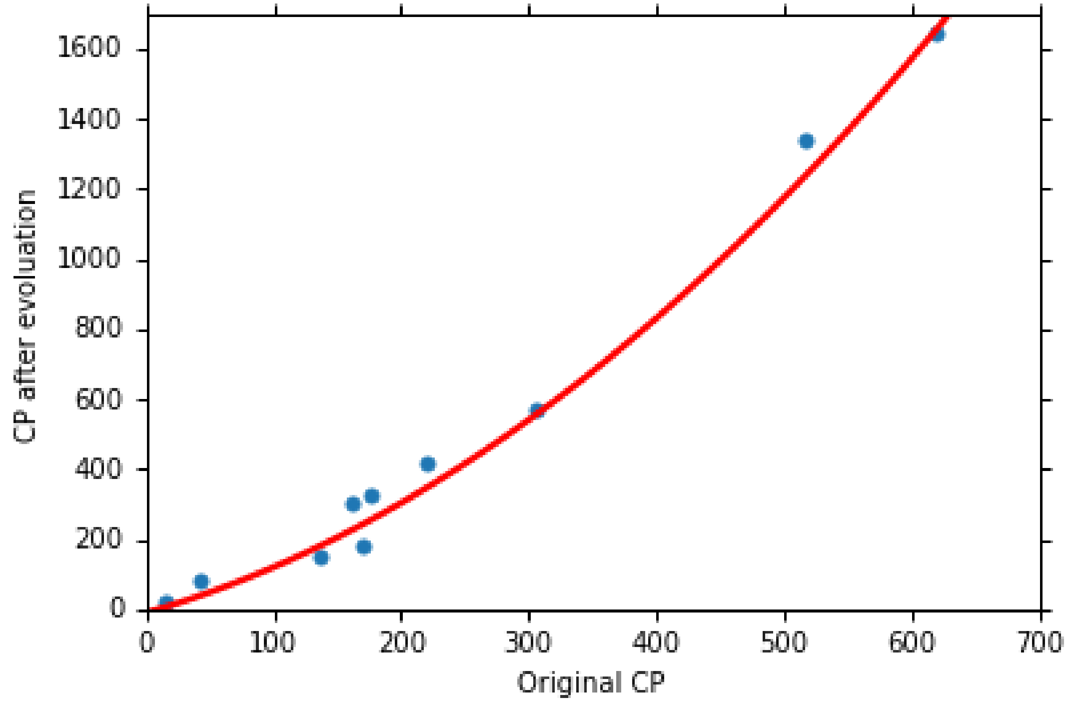
Average Error = 15.4

## ***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***

$b = 6.4$, $w_1 = 0.66$

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

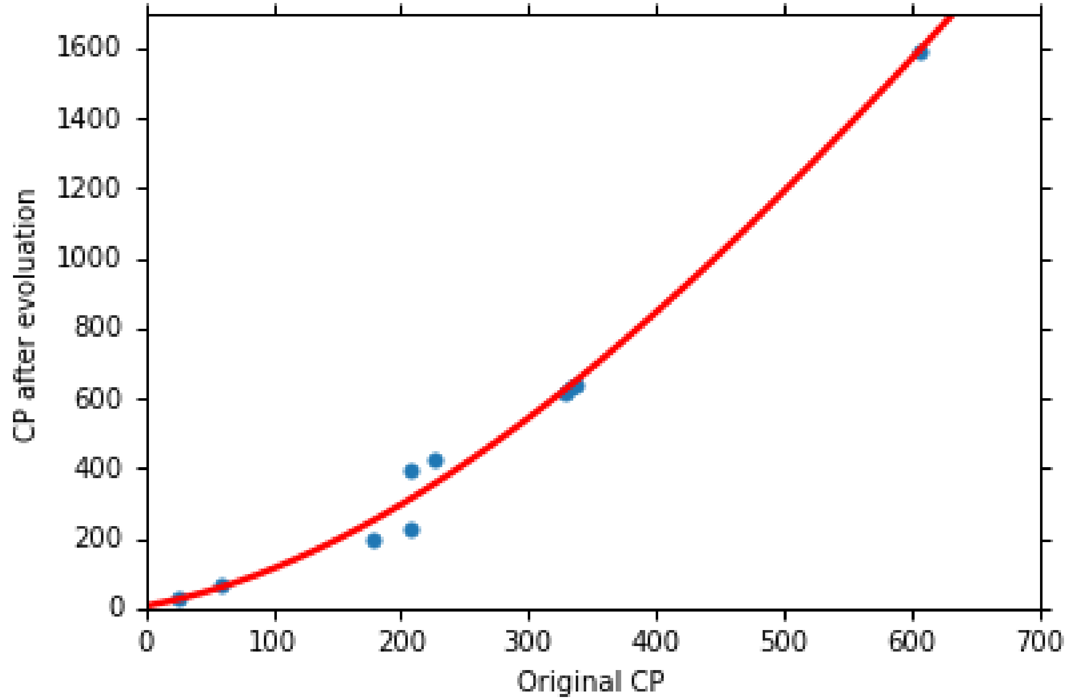
$w_3 = -1.8 \times 10^{-6}$

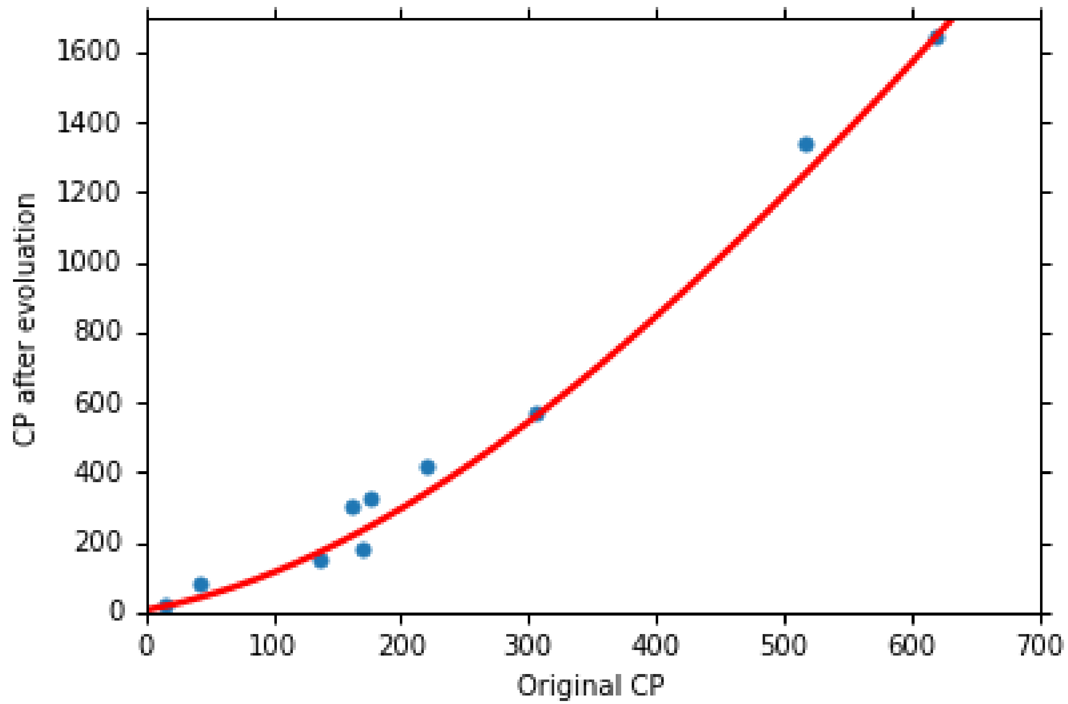
Average Error = 15.3

### ***Testing:***

Average Error = 18.1

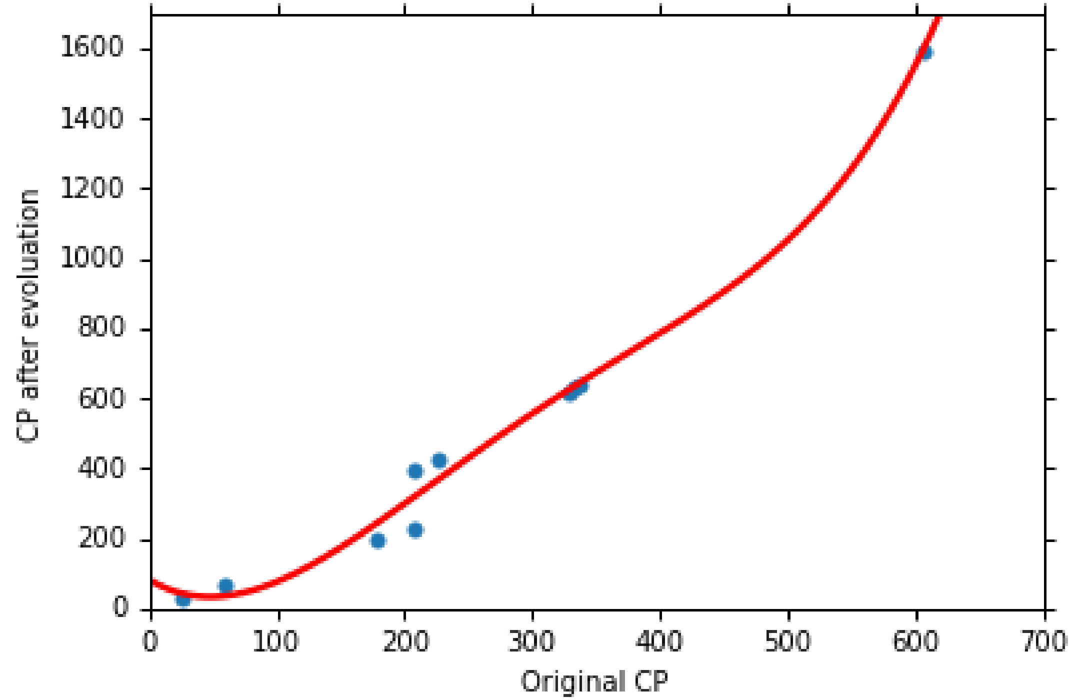
Slightly better.
How about more complex model?



# Selecting another Model

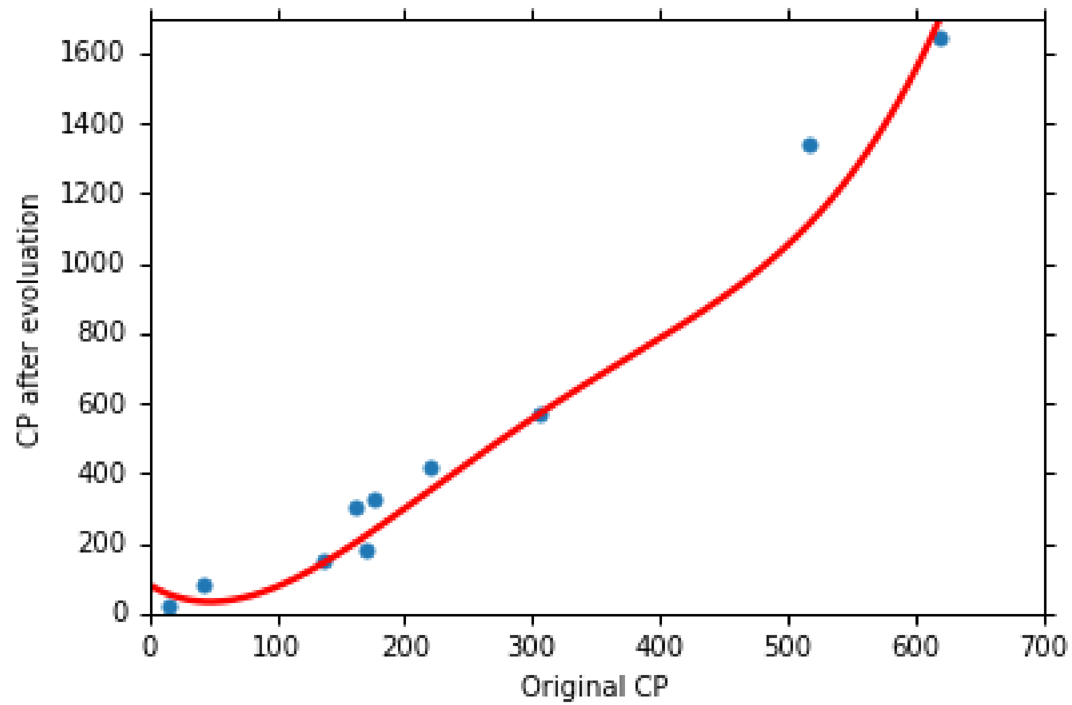
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$$




## Best Function

Average Error = 14.9

## Testing:

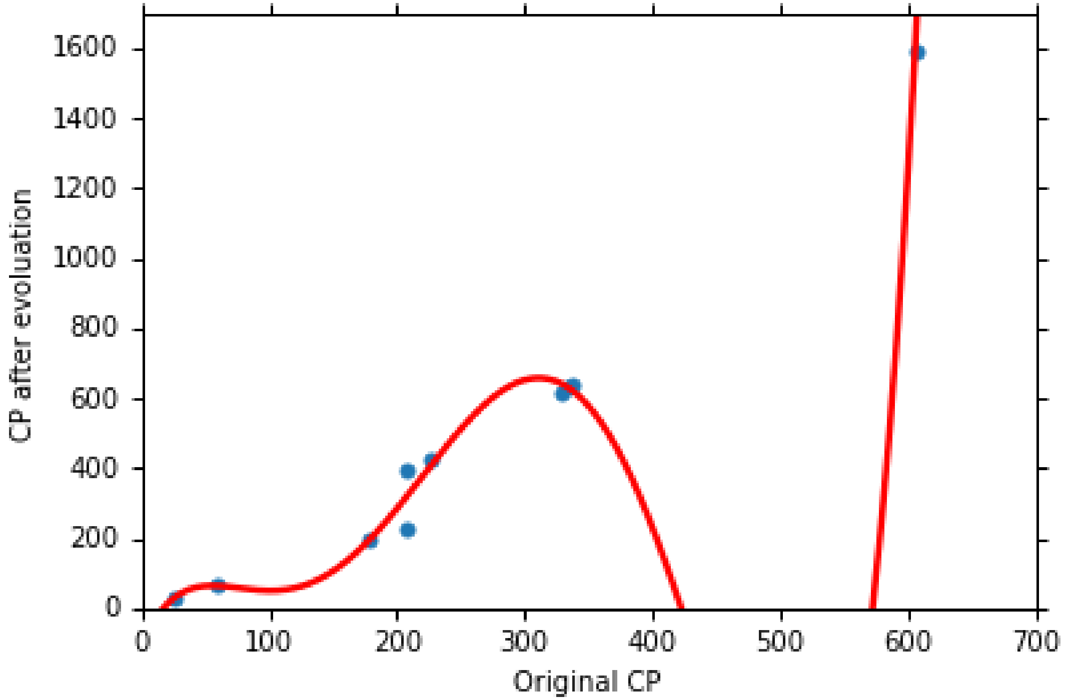



Average Error = 28.8

The results become worse ...

## ***Selecting another Model***

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

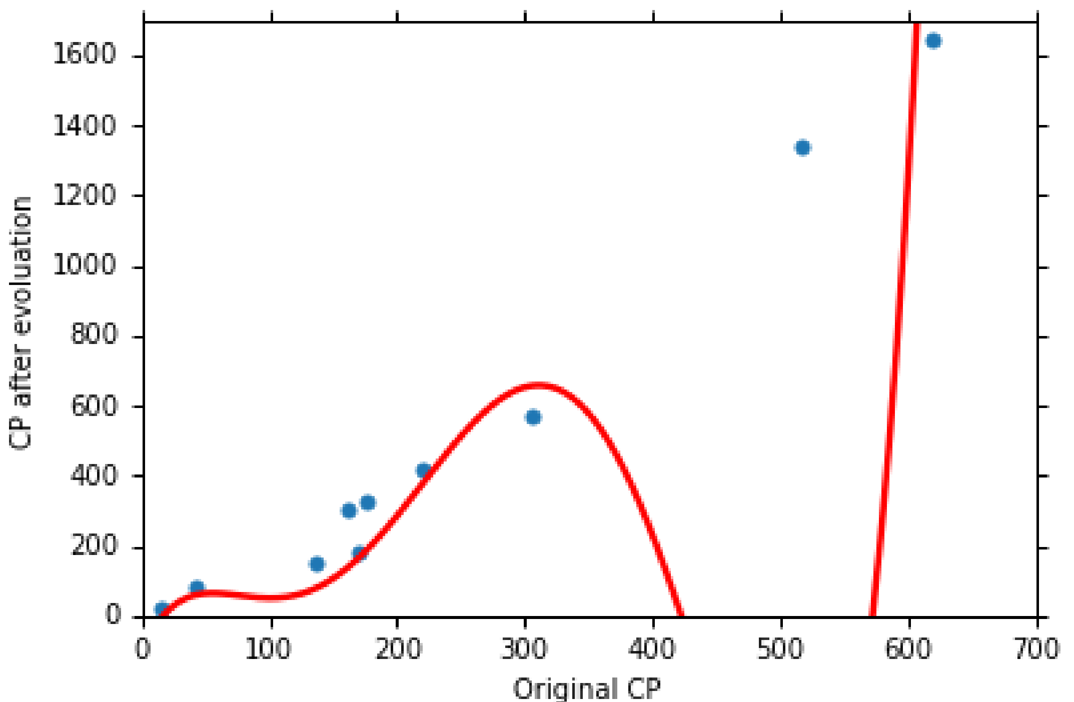



## ***Best Function***

Average Error = 12.8

## ***Testing:***

Average Error = 232.1




The results are so bad.

# Model Selection

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

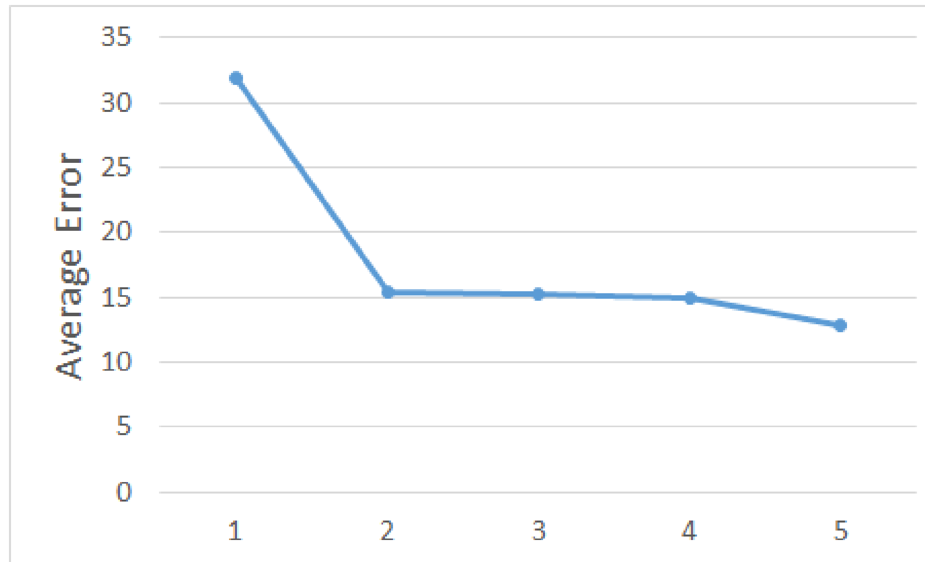
2. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$

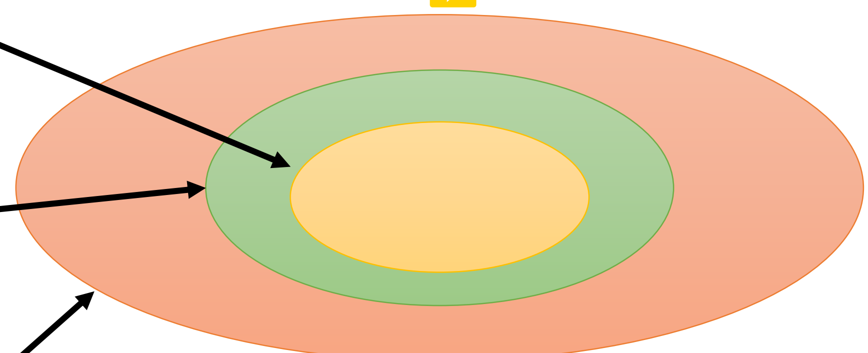
3. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$

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

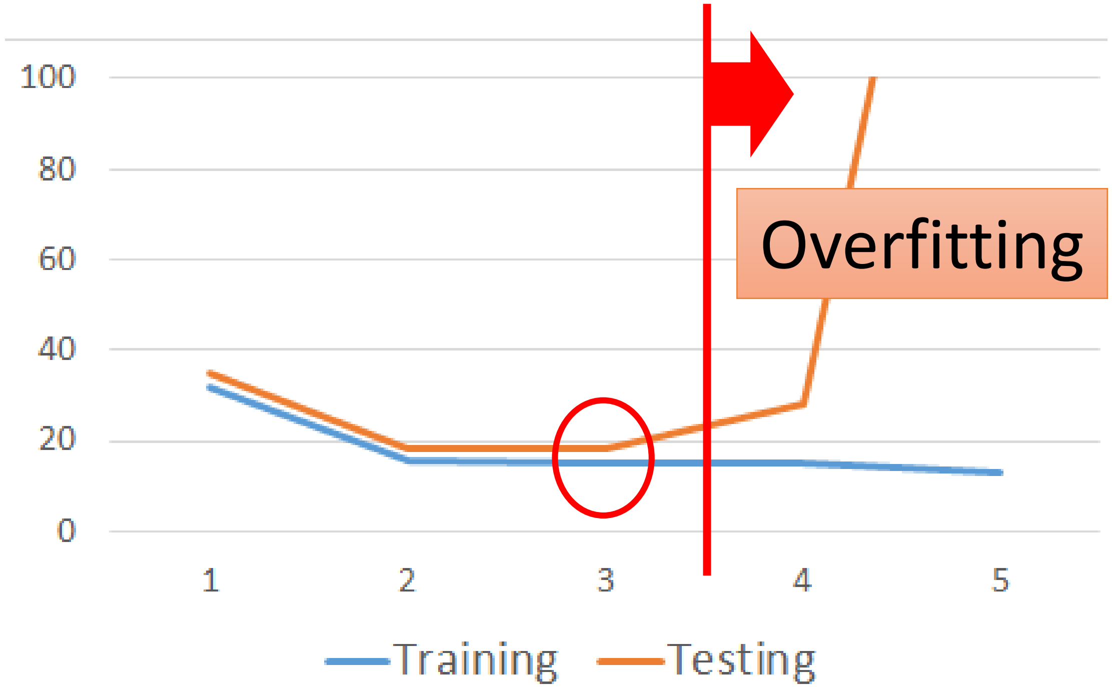


A more complex model yields lower error on training data.

If we can truly find the best function

# Model Selection

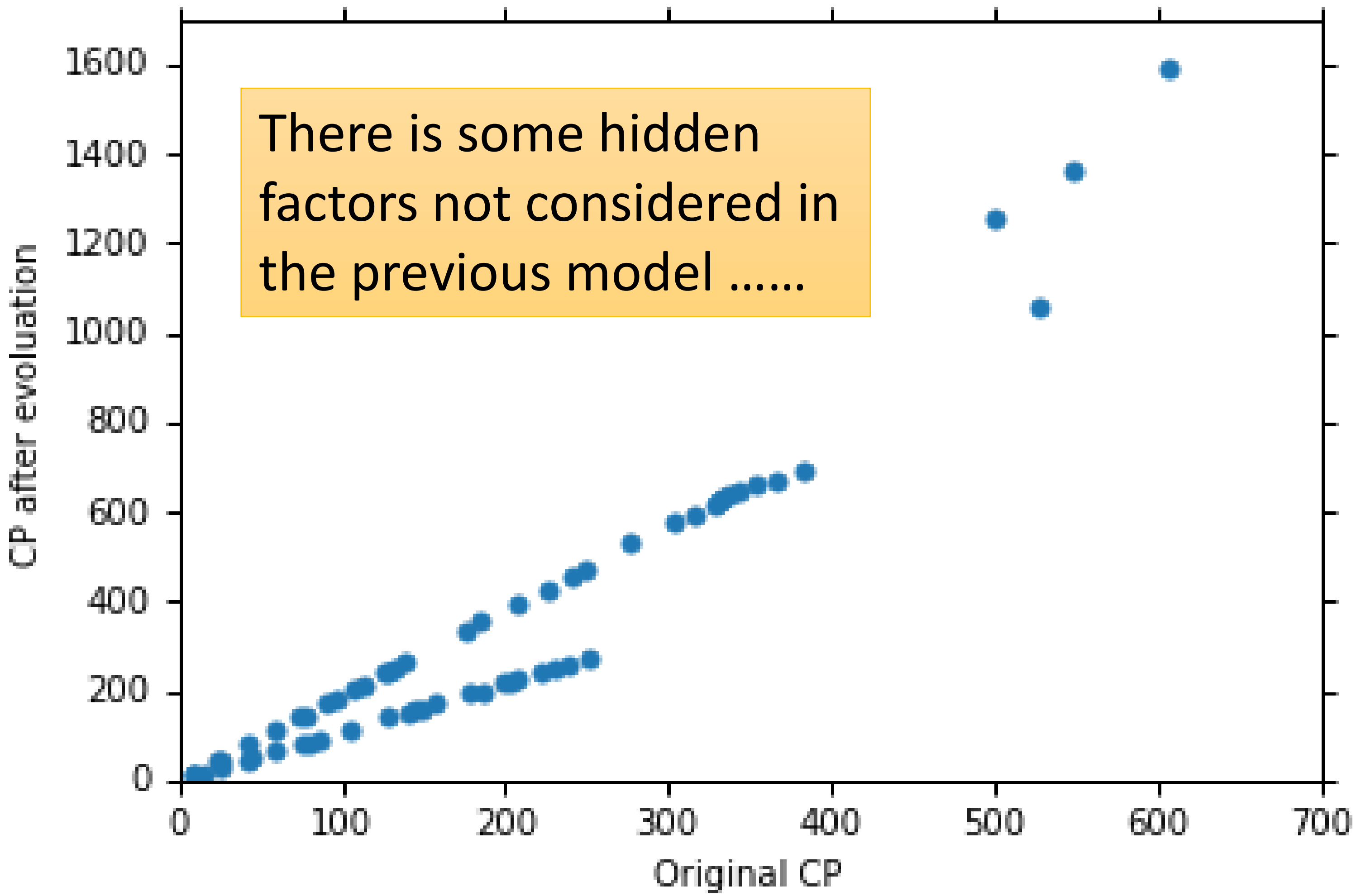



| | Training | Testing |
|---|---|---|
| 1 | 31.9 | 35.0 |
| 2 | 15.4 | 18.4 |
| 3 | 15.3 | 18.1 |
| 4 | 14.9 | 28.2 |
| 5 | 12.8 | 232.1 |

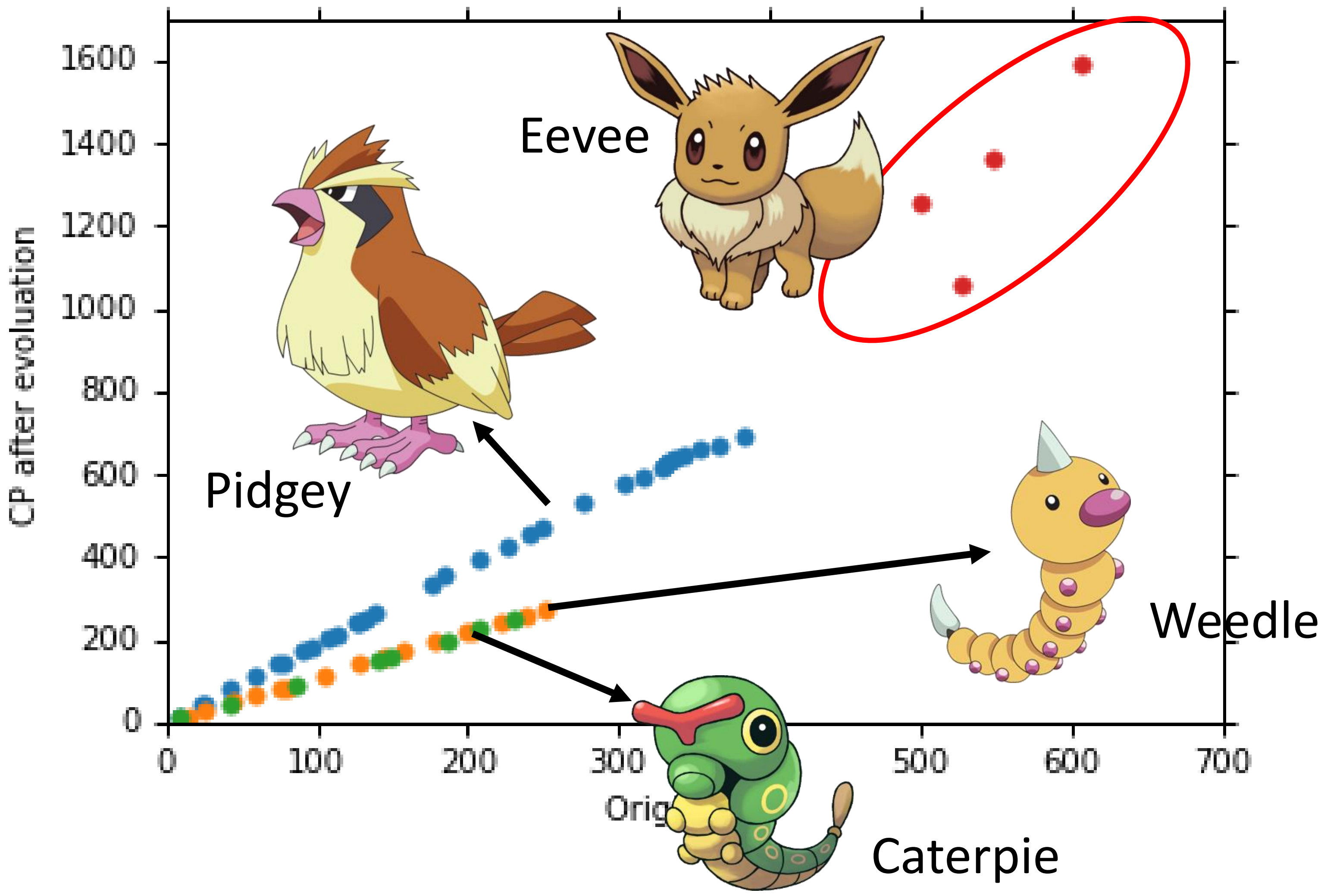
A more complex model does not always lead to better performance on ***testing data***.

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

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

Linear model?

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

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

/ 1:18:34

$w_i \boxed{x_i}$

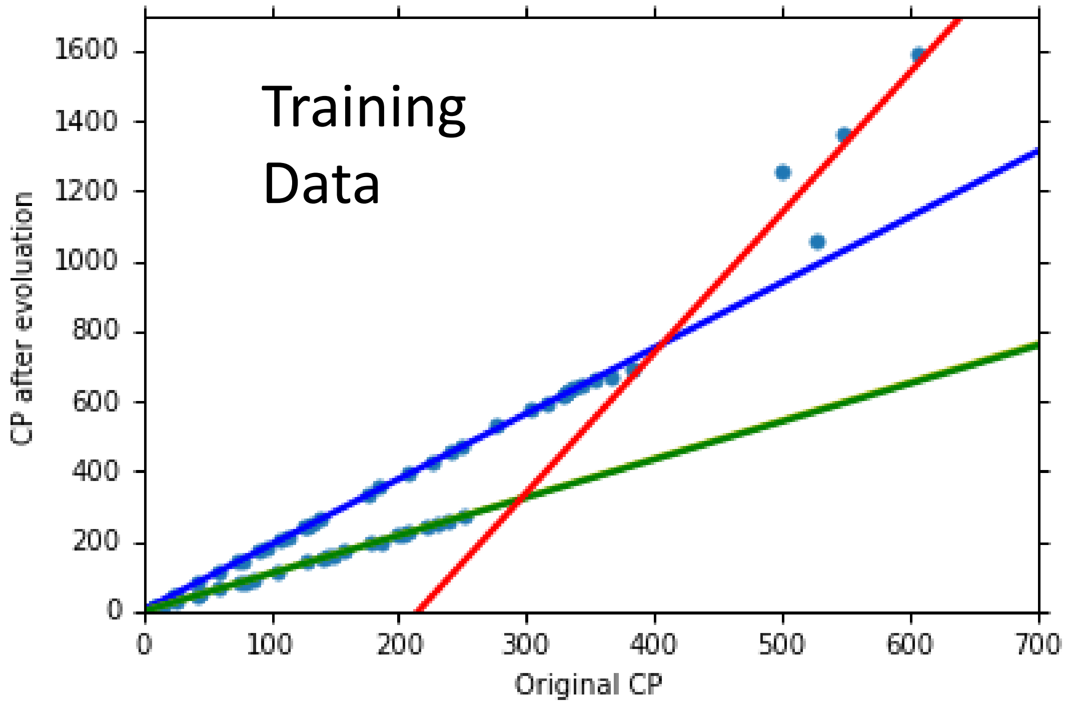
el?

ey

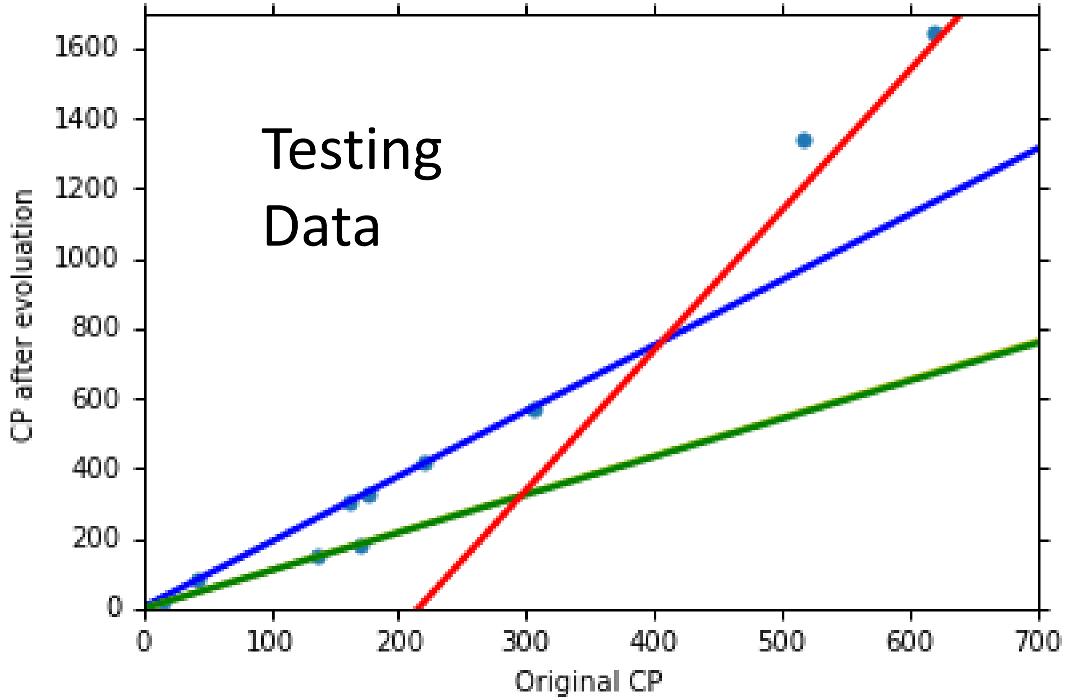
$x_{cp}$

$+w_4 \cdot$ 0

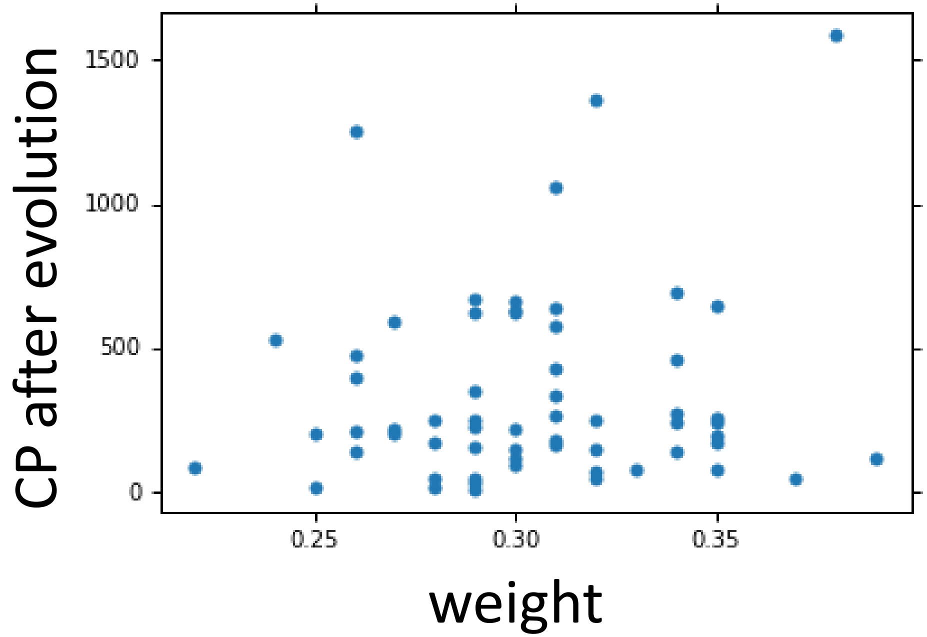
Average error = 3.8

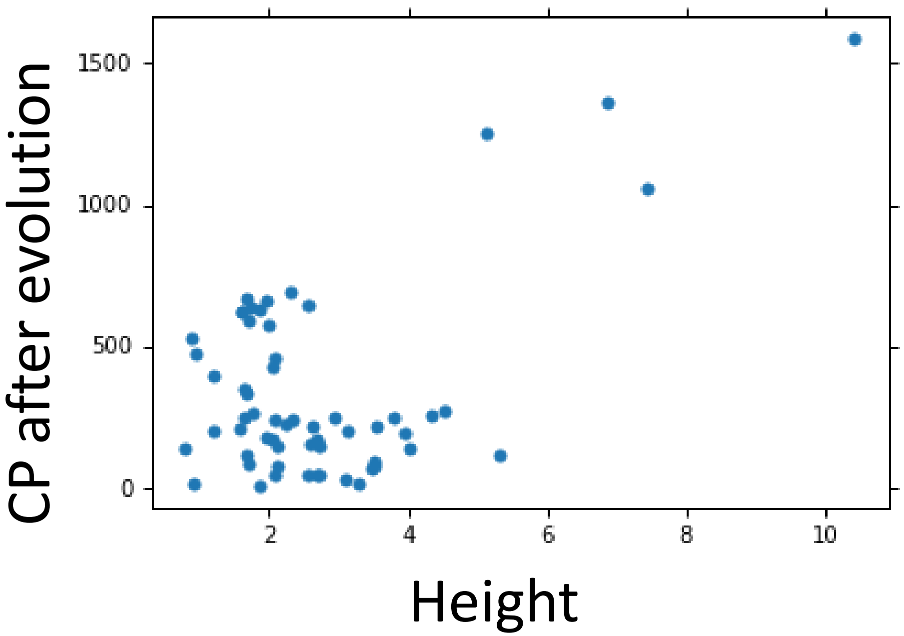


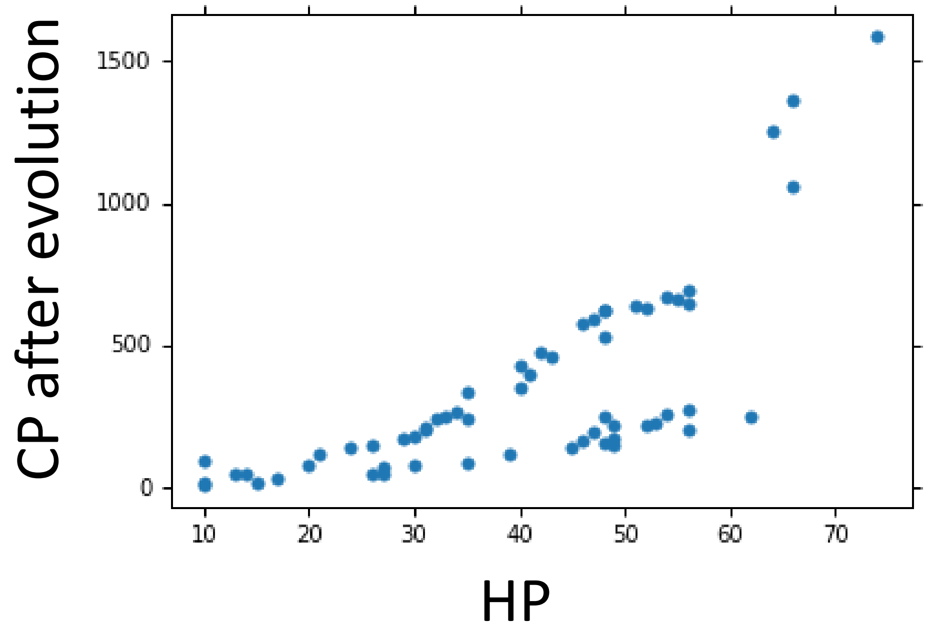

Average error = 14.3



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

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

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

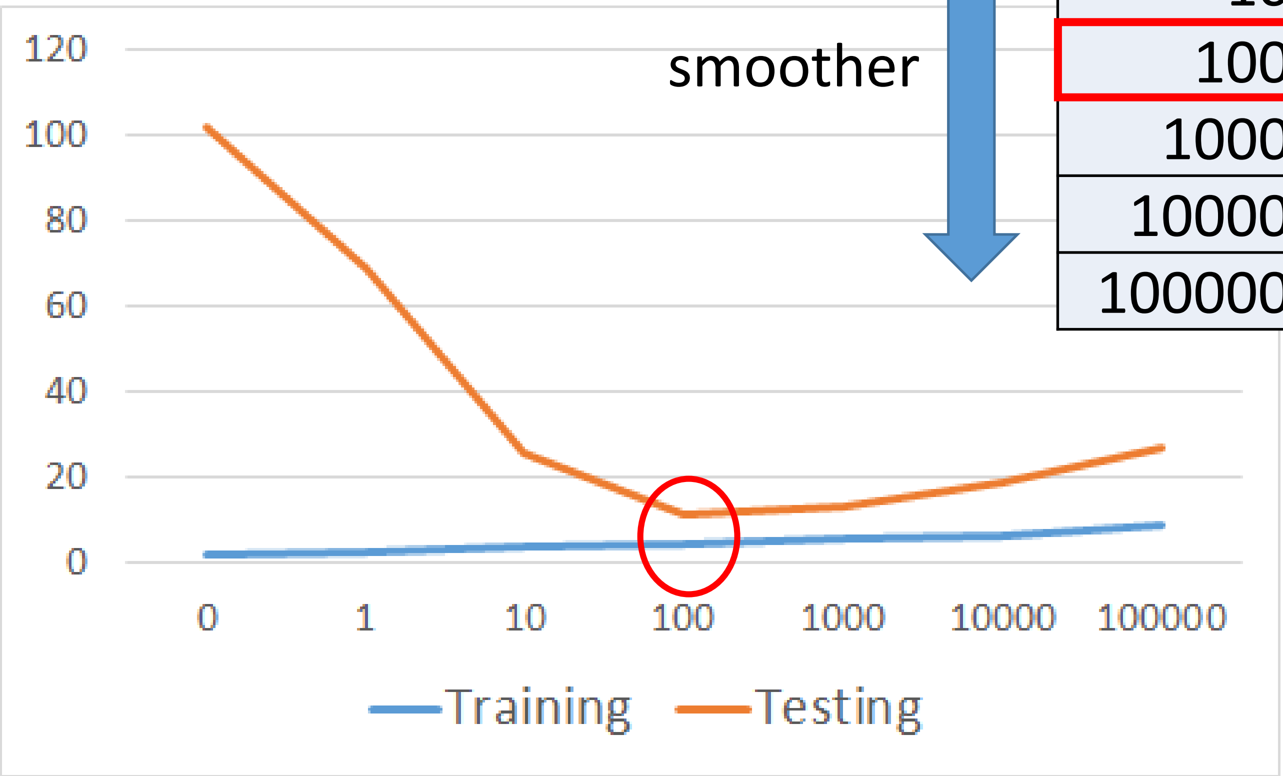
- We believe smoother function is more likely to be correct

Do you have to apply regularization on bias?

# Regularization

| $\lambda$ | 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 $\lambda$ obtaining the best model

- Training error: larger $\lambda$, 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

# Reference

- Bishop: Chapter 1.1

# Acknowledgment

- 感謝 鄭凱文 同學發現投影片 上的符號錯誤
- 感謝 童寬 同學發現投影片 上的符號錯誤
- 感謝 黃振綸 同學發現課程網頁上影片 連結錯誤的符號錯誤