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

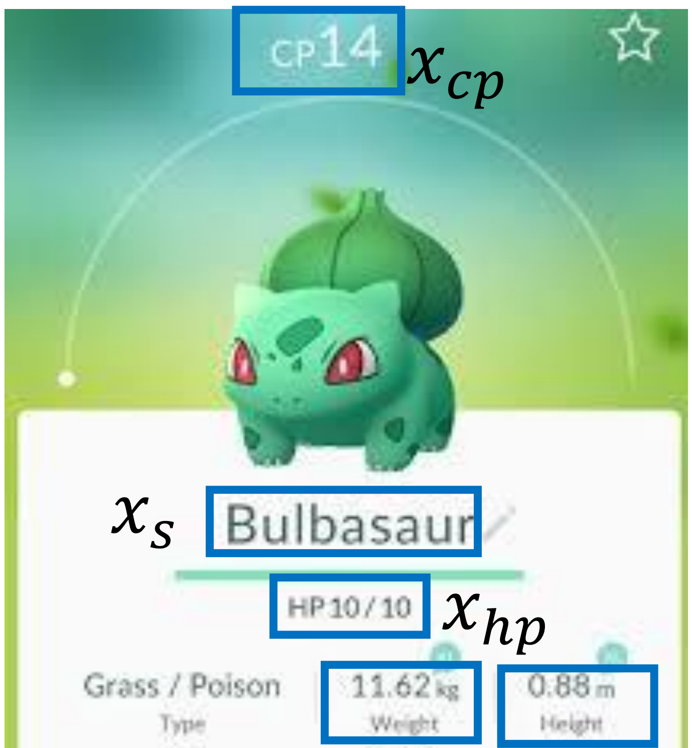
- Recommendation

$f($ 使用者 A 商品 B $) =$ 購買可能性

Example Application

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

$f($



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 …

feature

w_i: weight, b: bias

Step 2: Goodness of Function

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

A set of function

Model

$f_1, f_2 \cdots$

function input:

function Output (scalar):

Training Data

Step 2: Goodness of Function

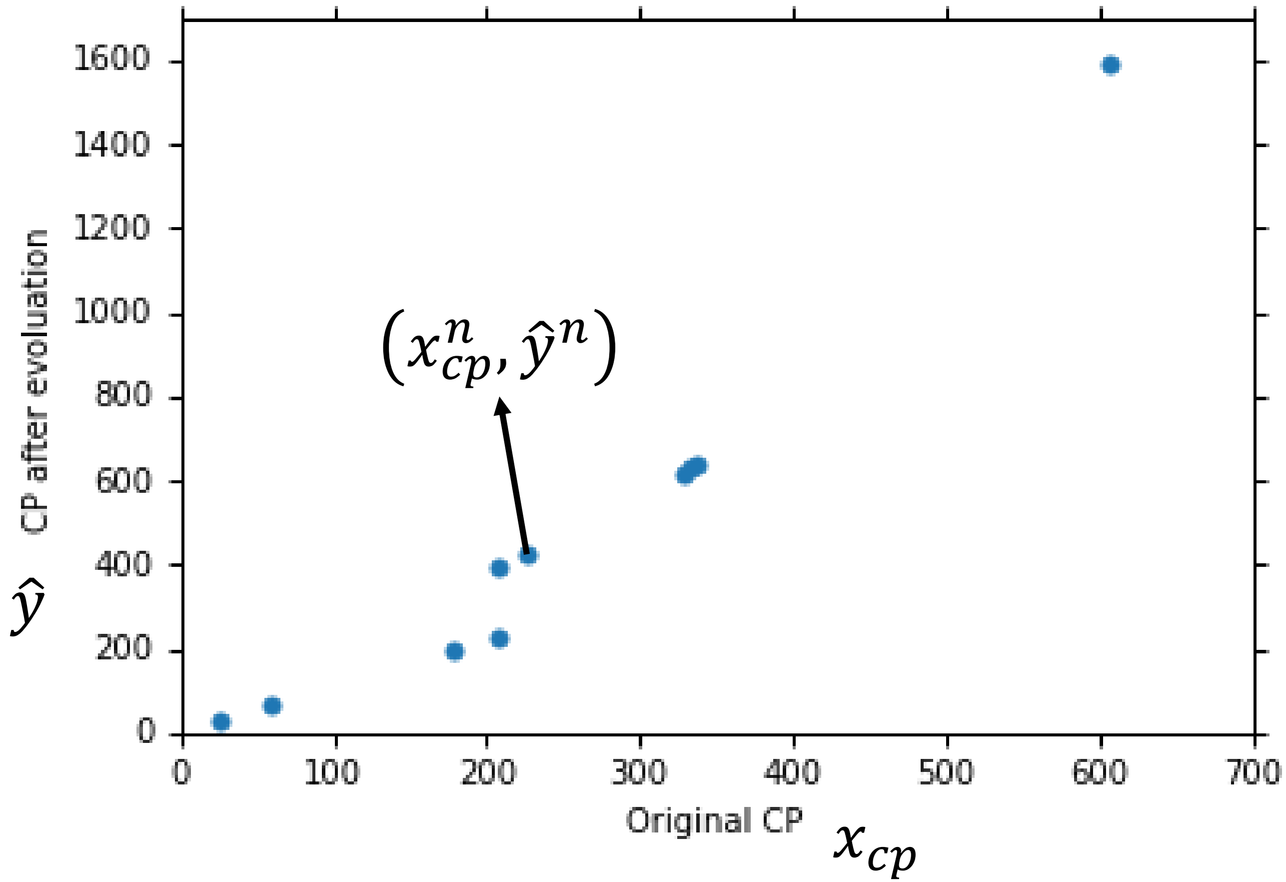
Training Data:
10 pokemons

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

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

$$\vdots$$

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

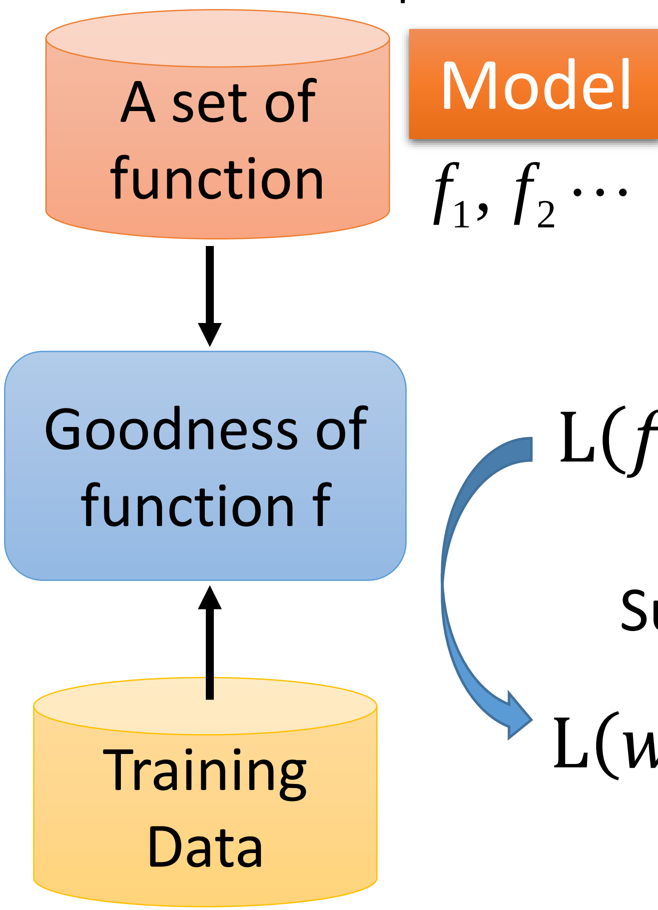


This is real data.

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

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

Sum over examples

Estimated y based on input function

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

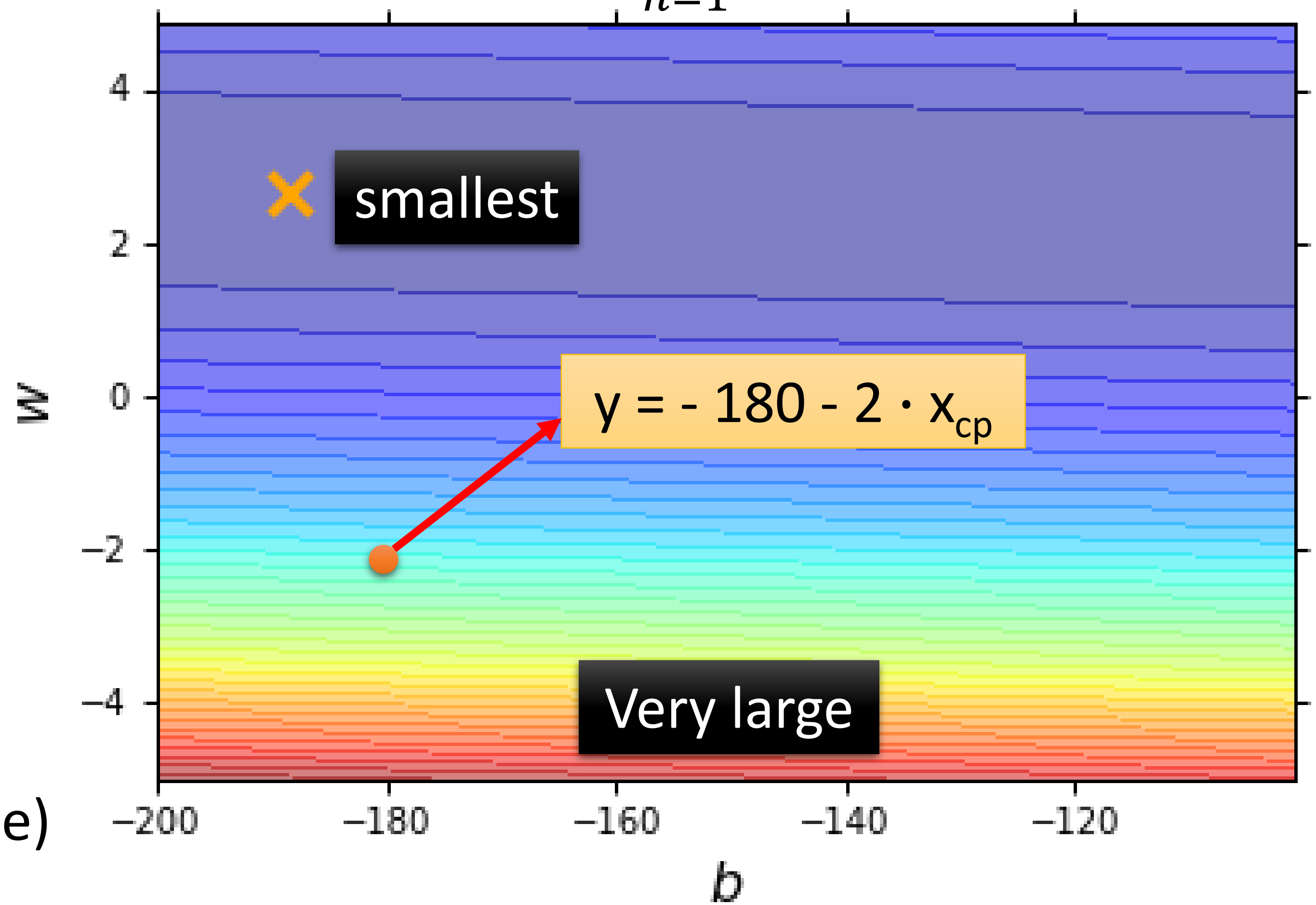
Step 2: Goodness of Function

- Loss Function

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

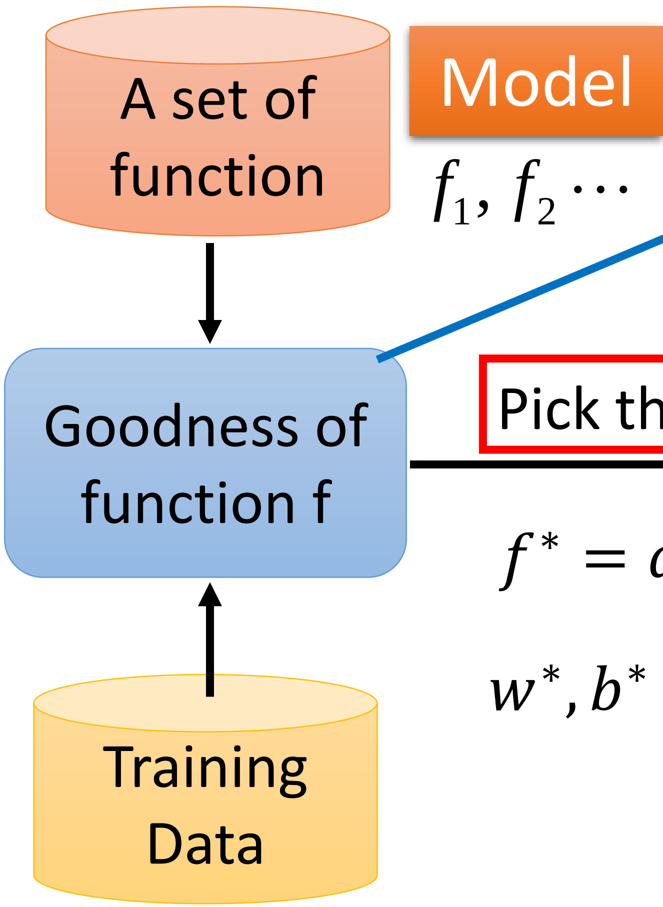
Each point in the figure is a function

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

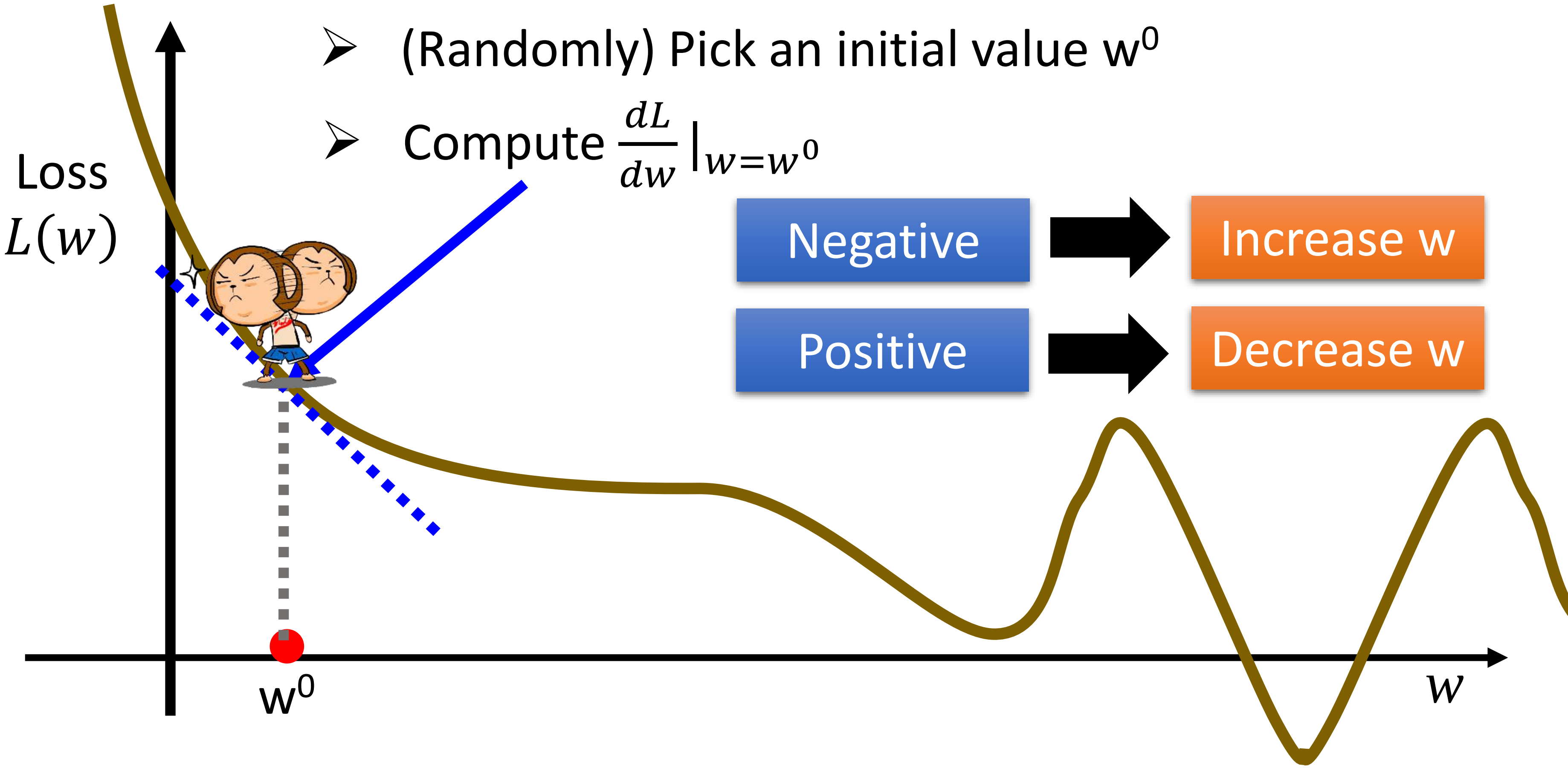
Step 3: Gradient Descent

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

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

Negative → Increase w

Positive → Decrease w



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Step 3: Gradient Descent

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

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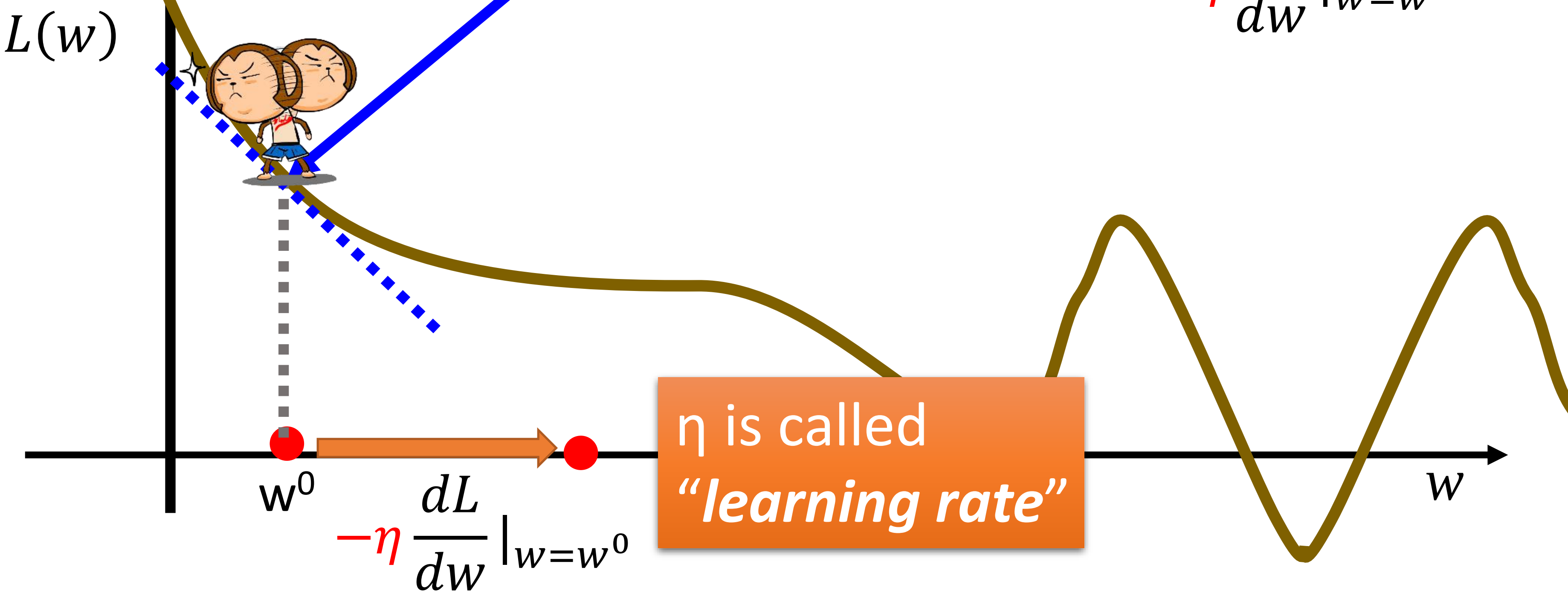
  - Compute $\frac{dL}{dw}|_{w=w^0}$

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



Step 3: Gradient Descent

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

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

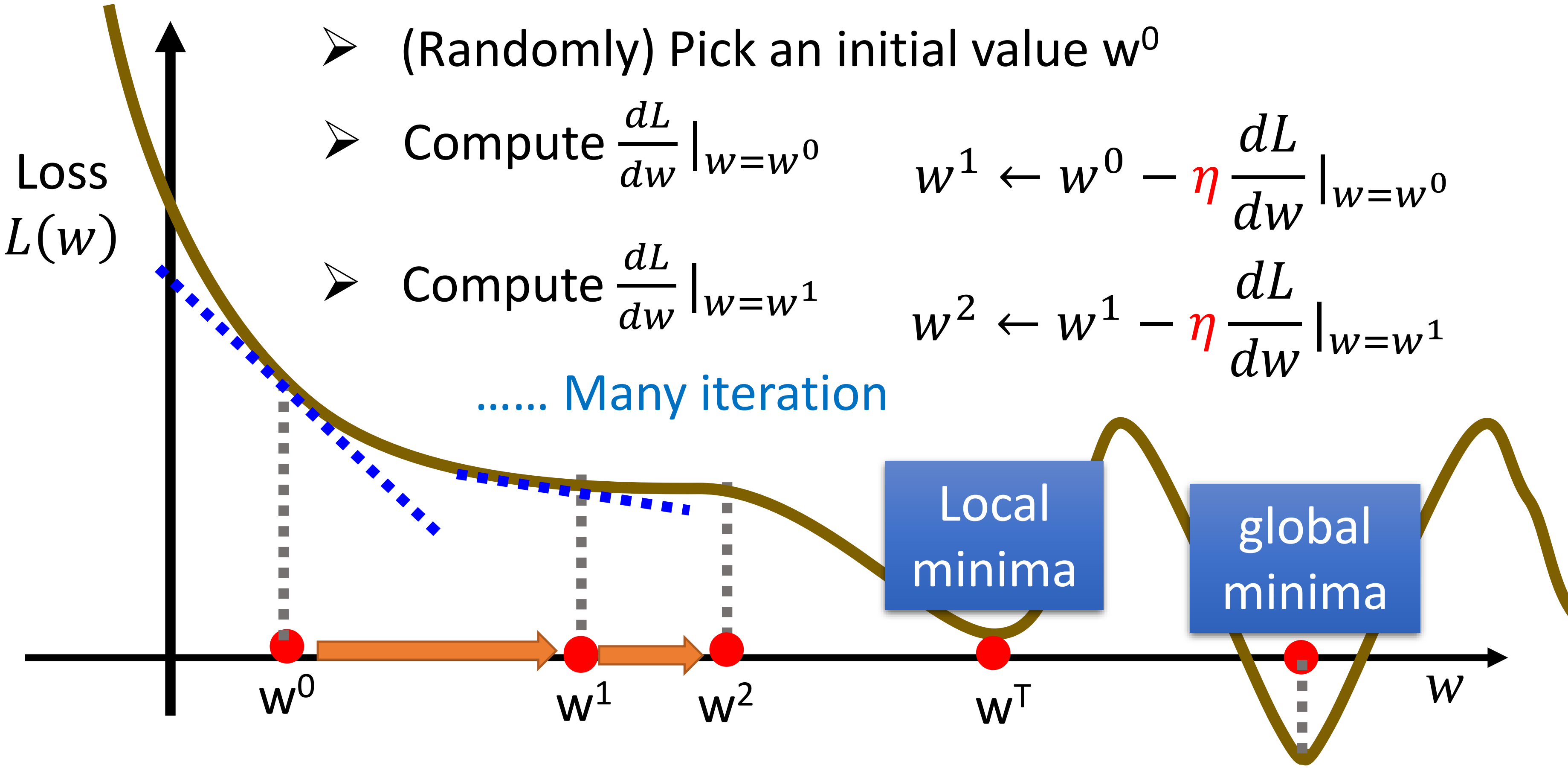
  - ➢ (Randomly) Pick an initial value w^0
  - ➢ Compute $\frac{dL}{dw}|_{w=w^0}$

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

  - ➢ Compute $\frac{dL}{dw}|_{w=w^1}$

$$w^2 \leftarrow w^1 - \eta \frac{dL}{dw}|_{w=w^1}$$

…… Many iteration



Step 3: Gradient Descent

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

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

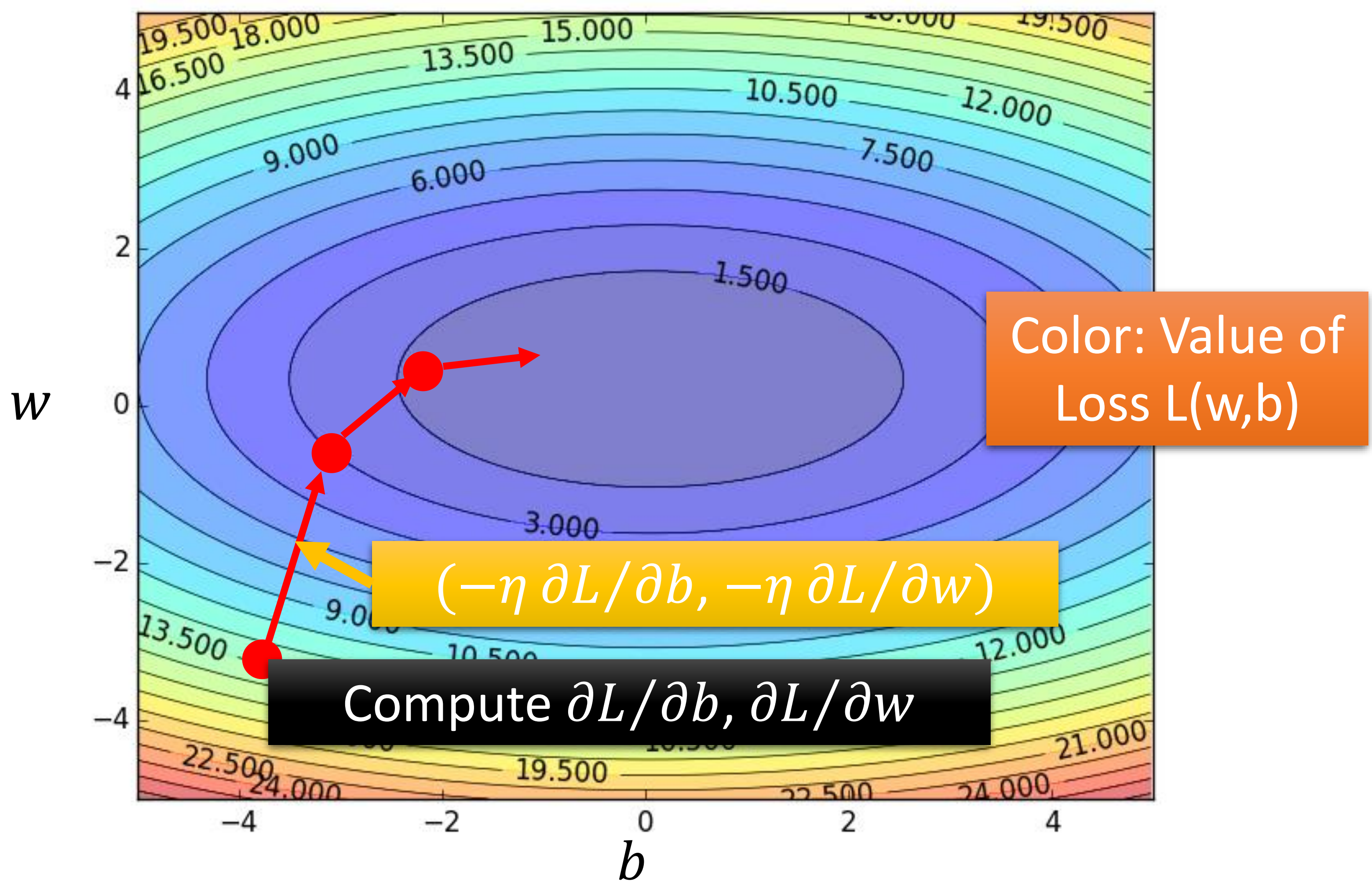
  - (Randomly) Pick an initial value w^0, b^0
  - Compute $\frac{\partial L}{\partial w}|_{w=w^0,b=b^0}$, $\frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$

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

  - 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:

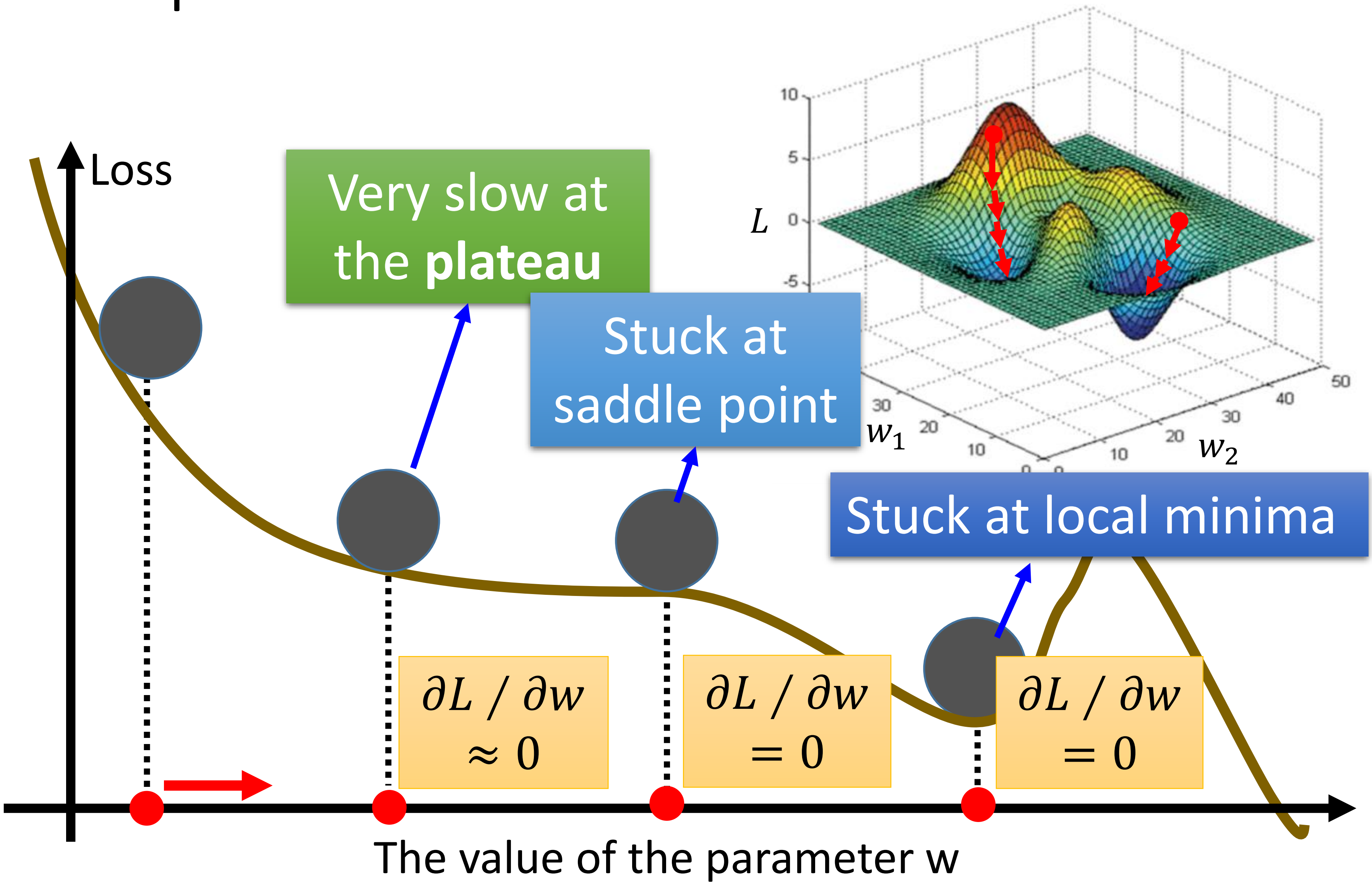
$$\theta^* = \arg\max_{\theta} L(\theta) \quad \text{by gradient descent}$$

- 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 $\partial L / \partial b$

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

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

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

Step 3: Gradient Descent

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

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

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

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

How’s the results?

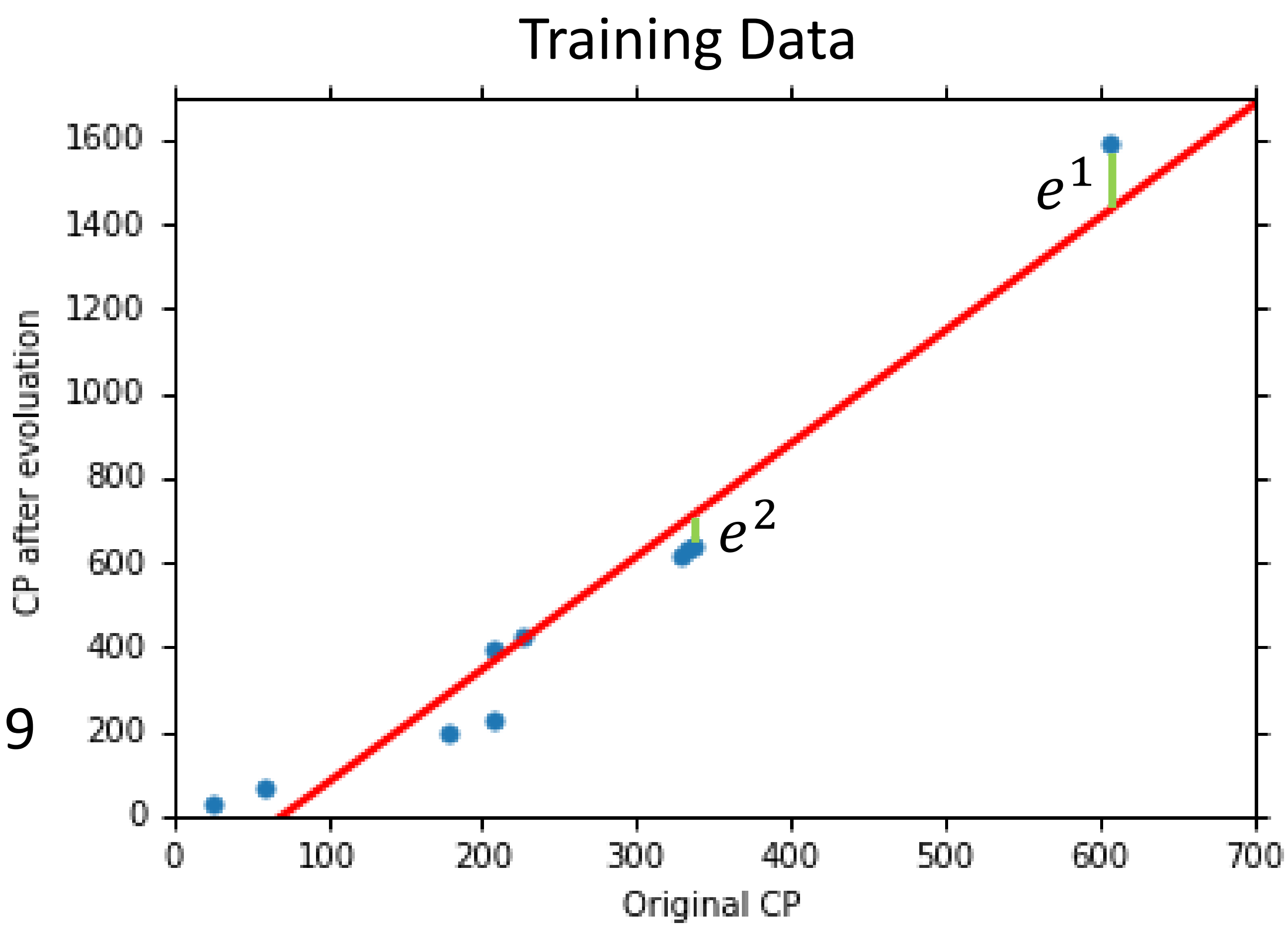
$y = b + w \cdot x_{cp}$

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

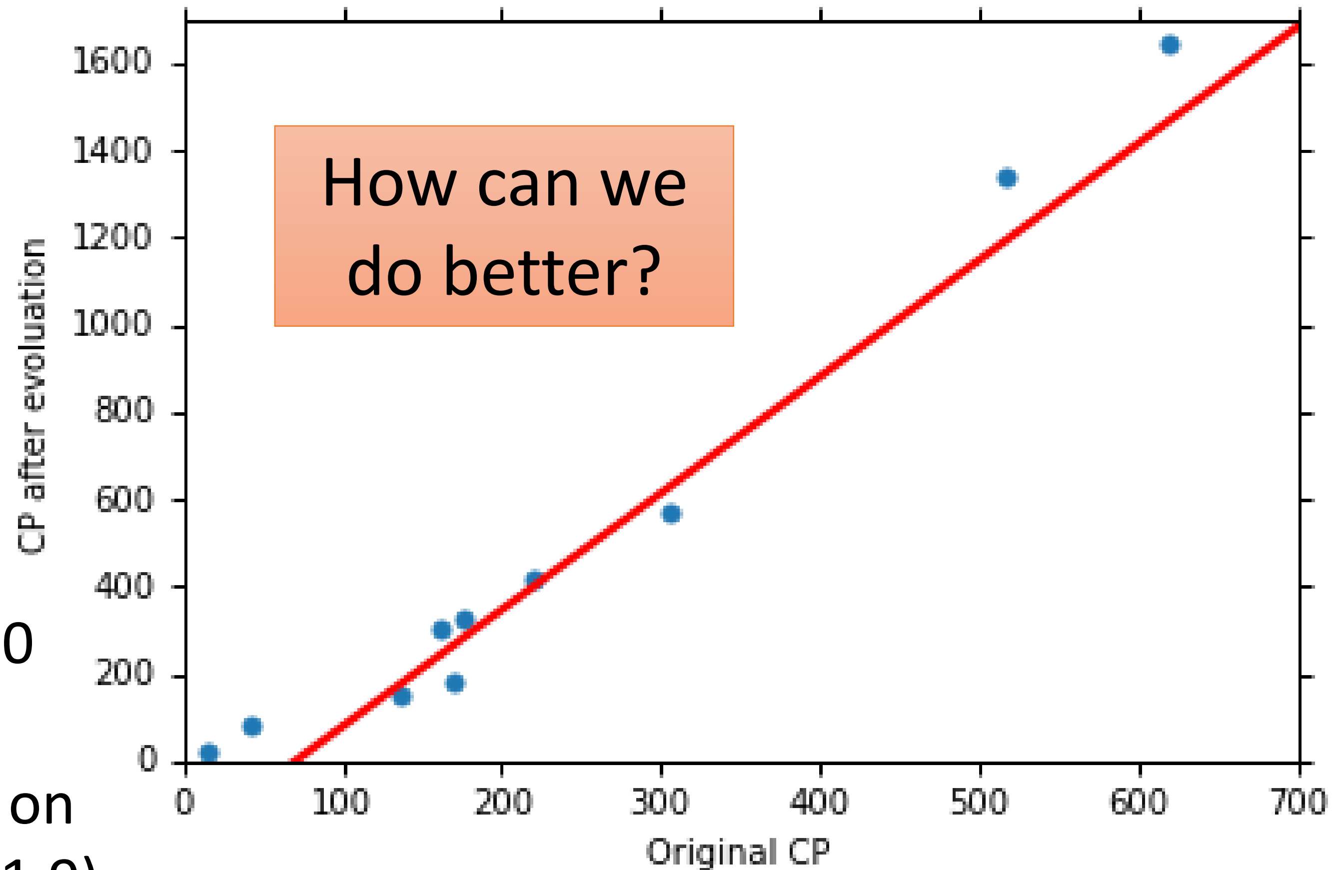
w = 2.7

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

$b = -10.3$

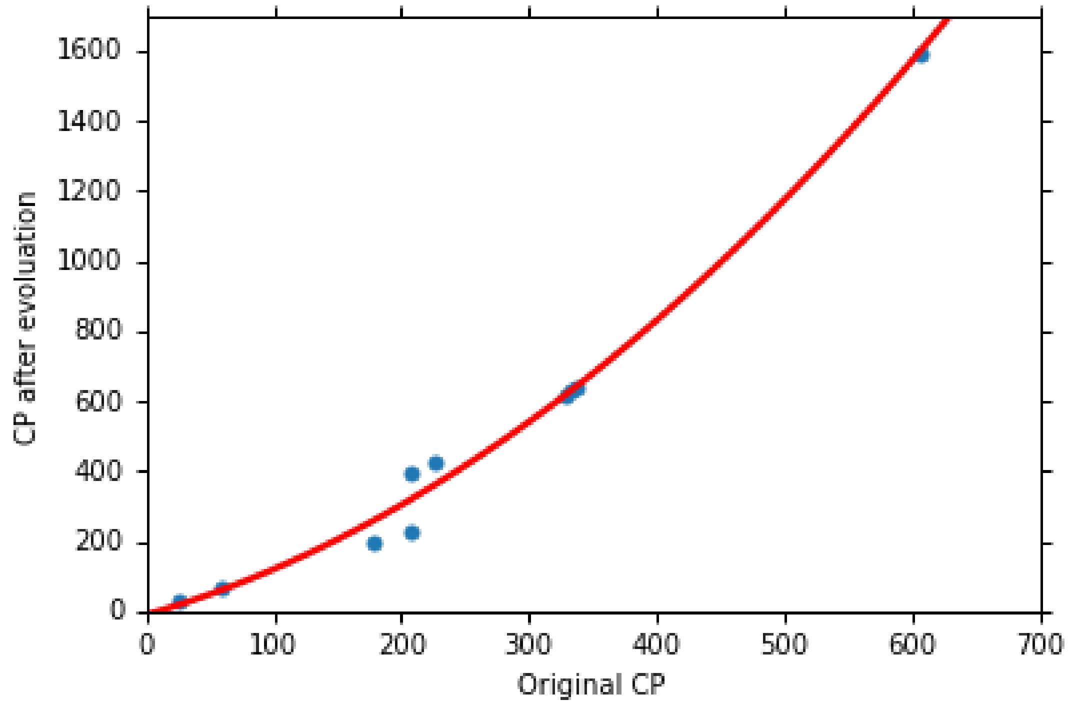
$w_1 = 1.0$, $w_2 = 2.7 \times 10^{-3}$

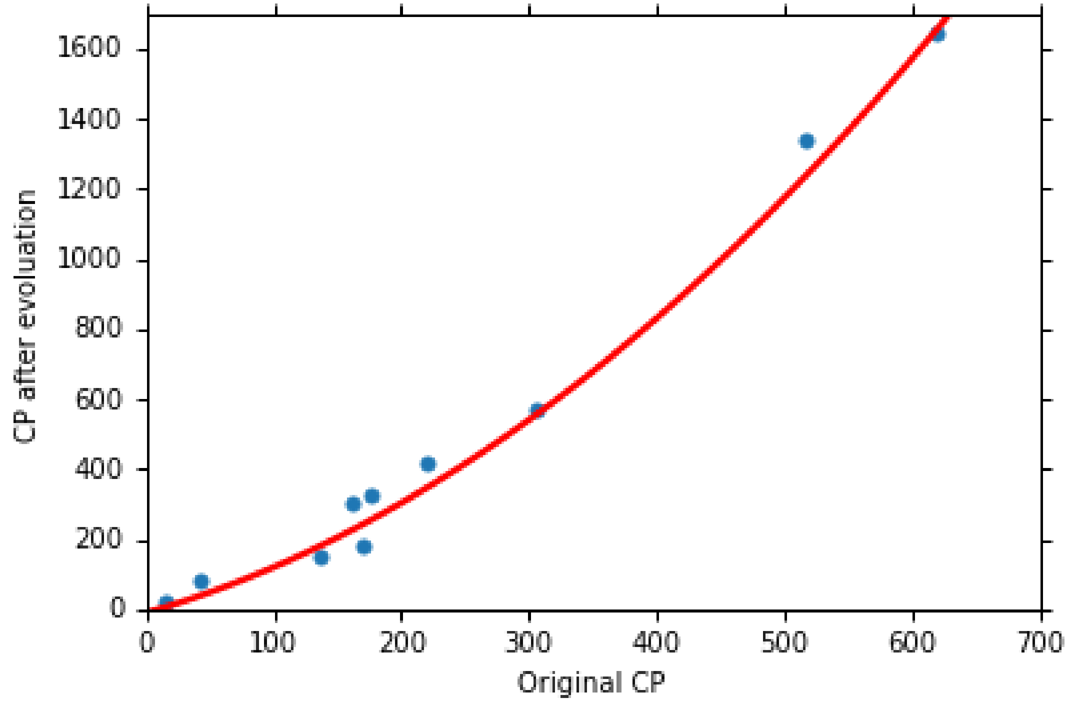
Average Error = 15.4

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

$b = 6.4$, $w_1 = 0.66$

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

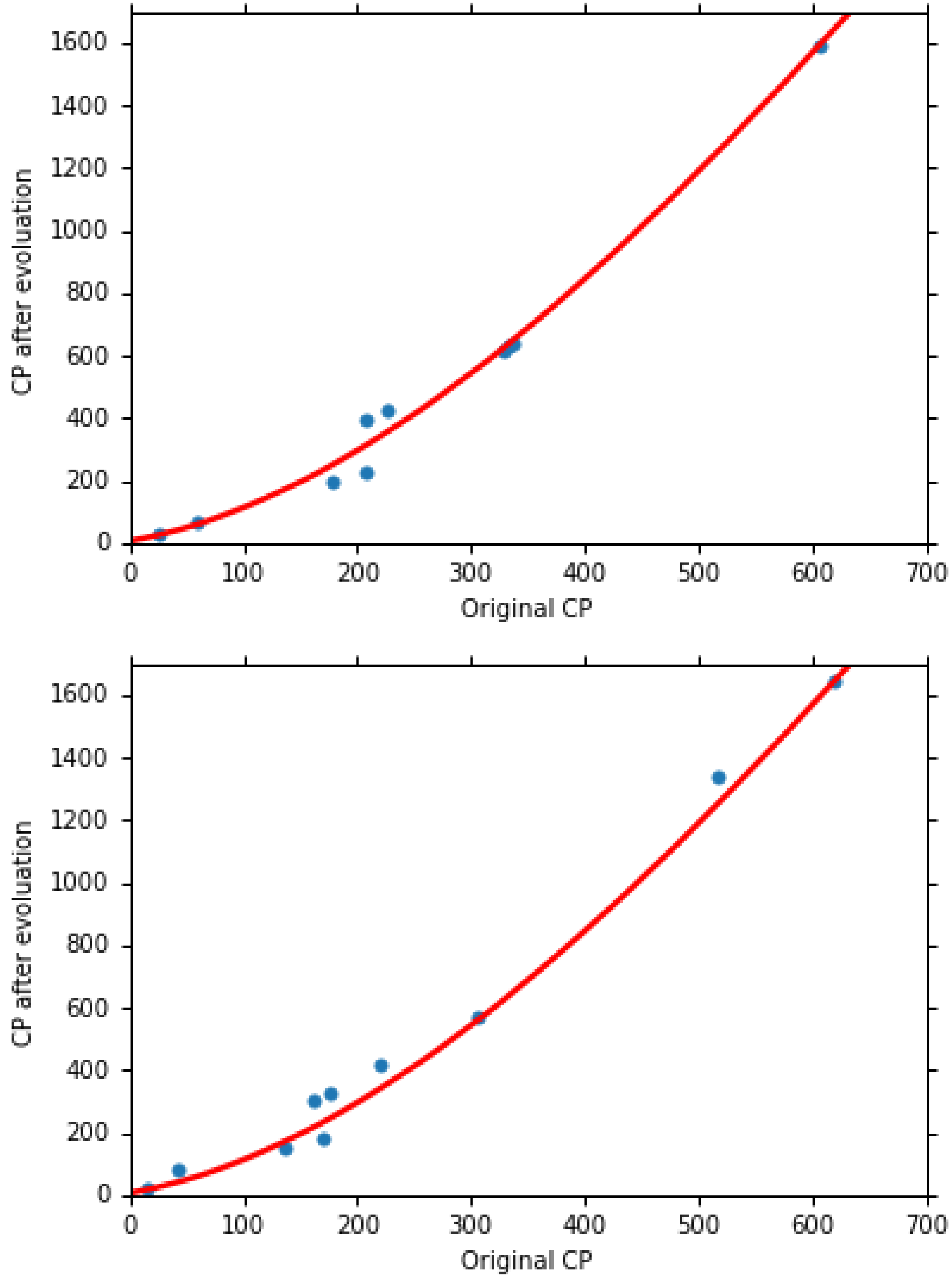
$w_3 = -1.8 \times 10^{-6}$

Average Error = 15.3

Testing:

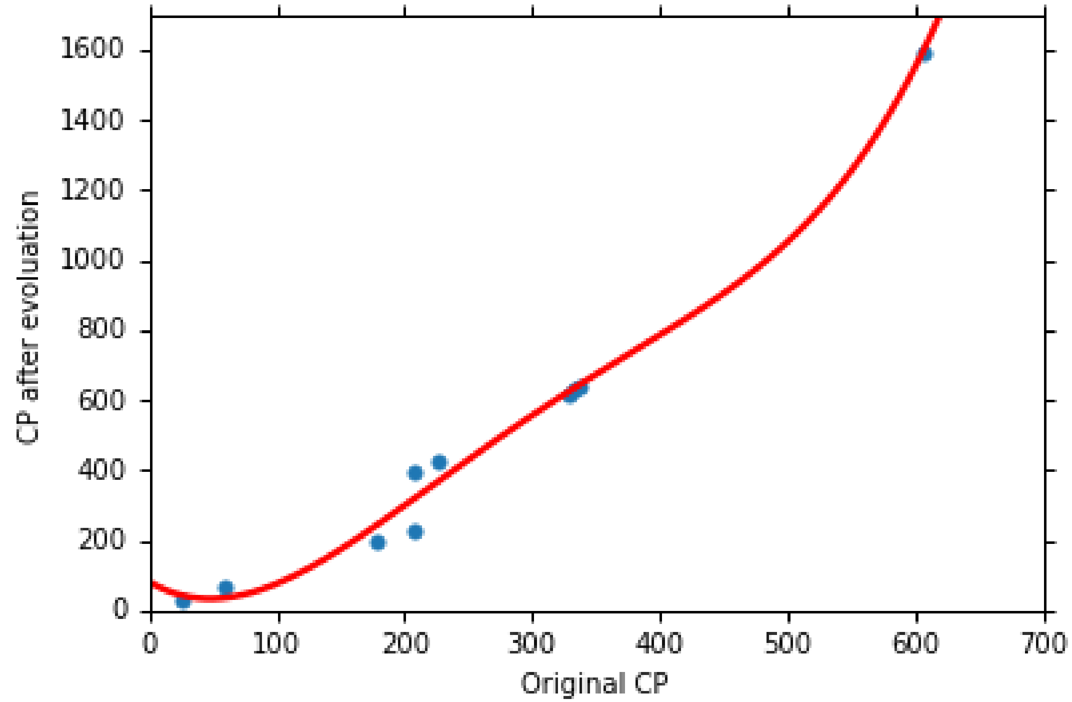
Average Error = 18.1

Slightly better.
How about more complex model?



Selecting another Model

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



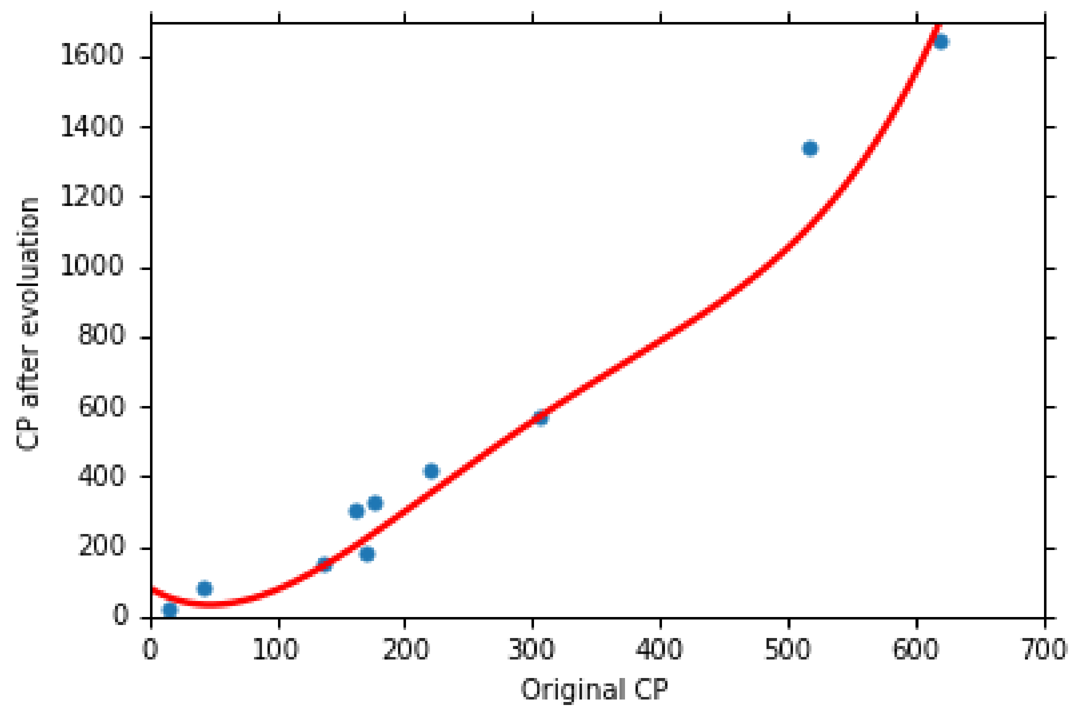
Best Function

Average Error = 14.9

Testing:

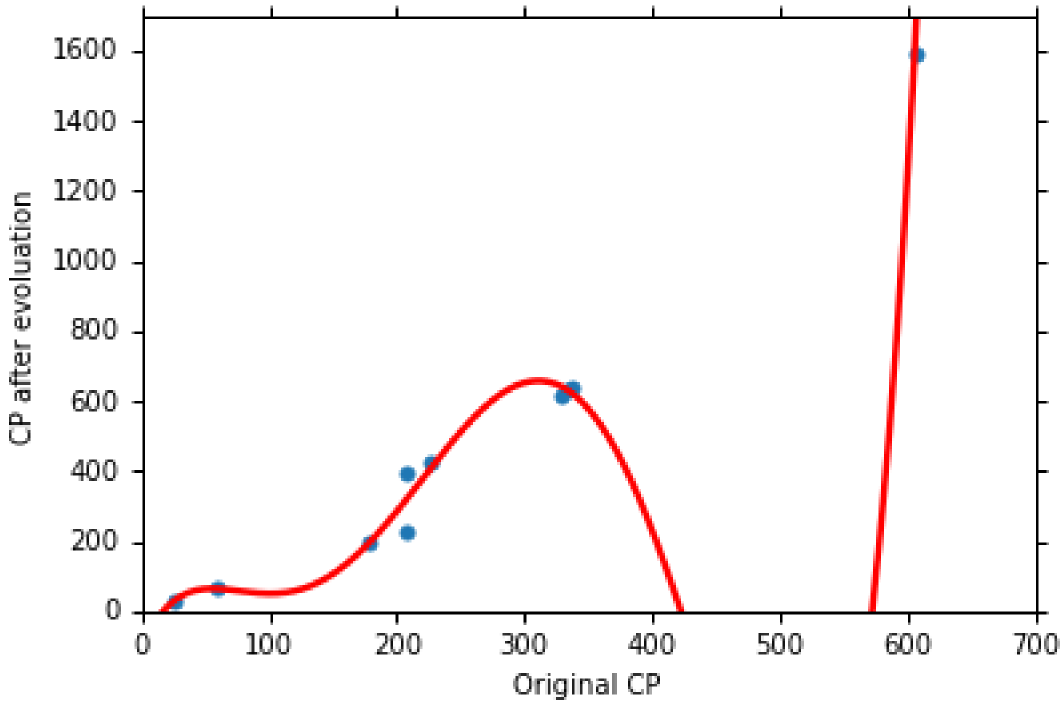
Average Error = 28.8

The results become worse ...



Selecting another Model

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



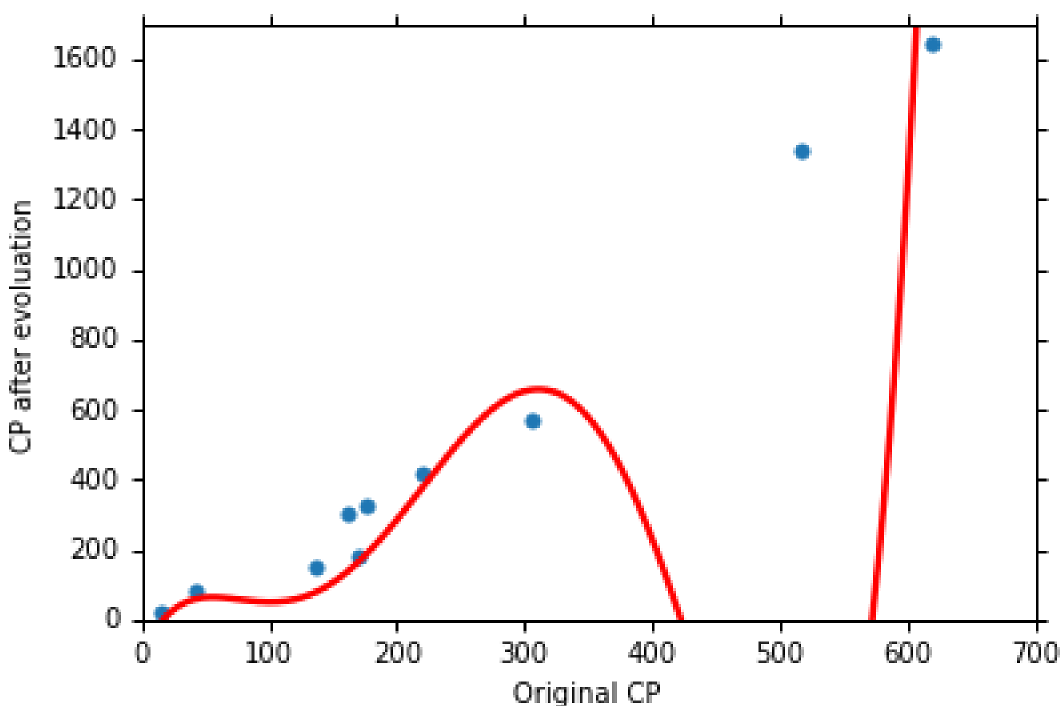
Best Function

Average Error = 12.8

Testing:

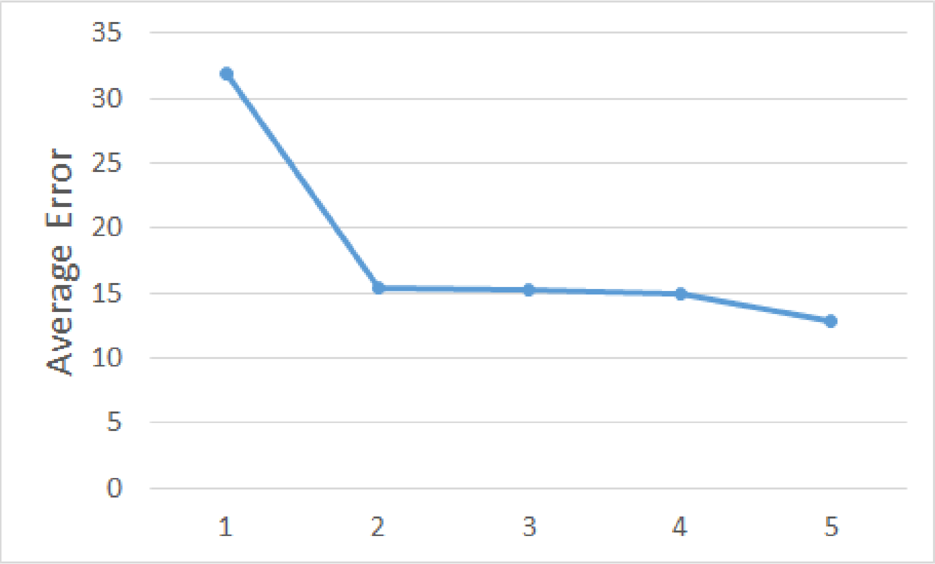
Average Error = 232.1

The results are so bad.

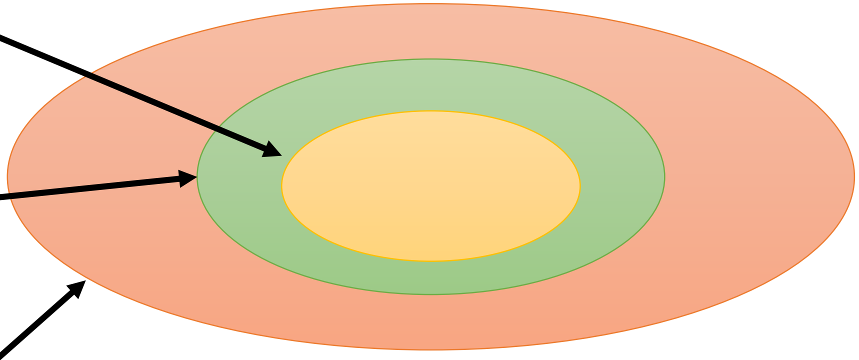


Model Selection

Training Data



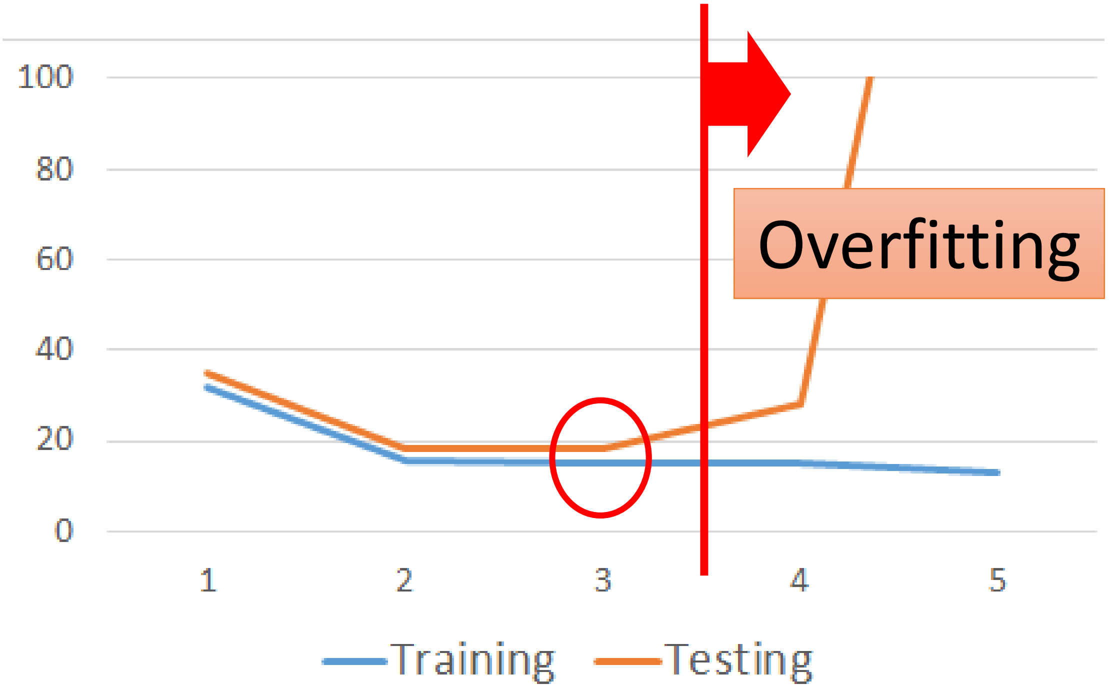
1. $y = b + w \cdot x_{cp}$
2. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2$
3. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3$
4. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4$
5. $y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2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



A more complex model yields lower error on training data.

If we can truly find the best function

Model Selection

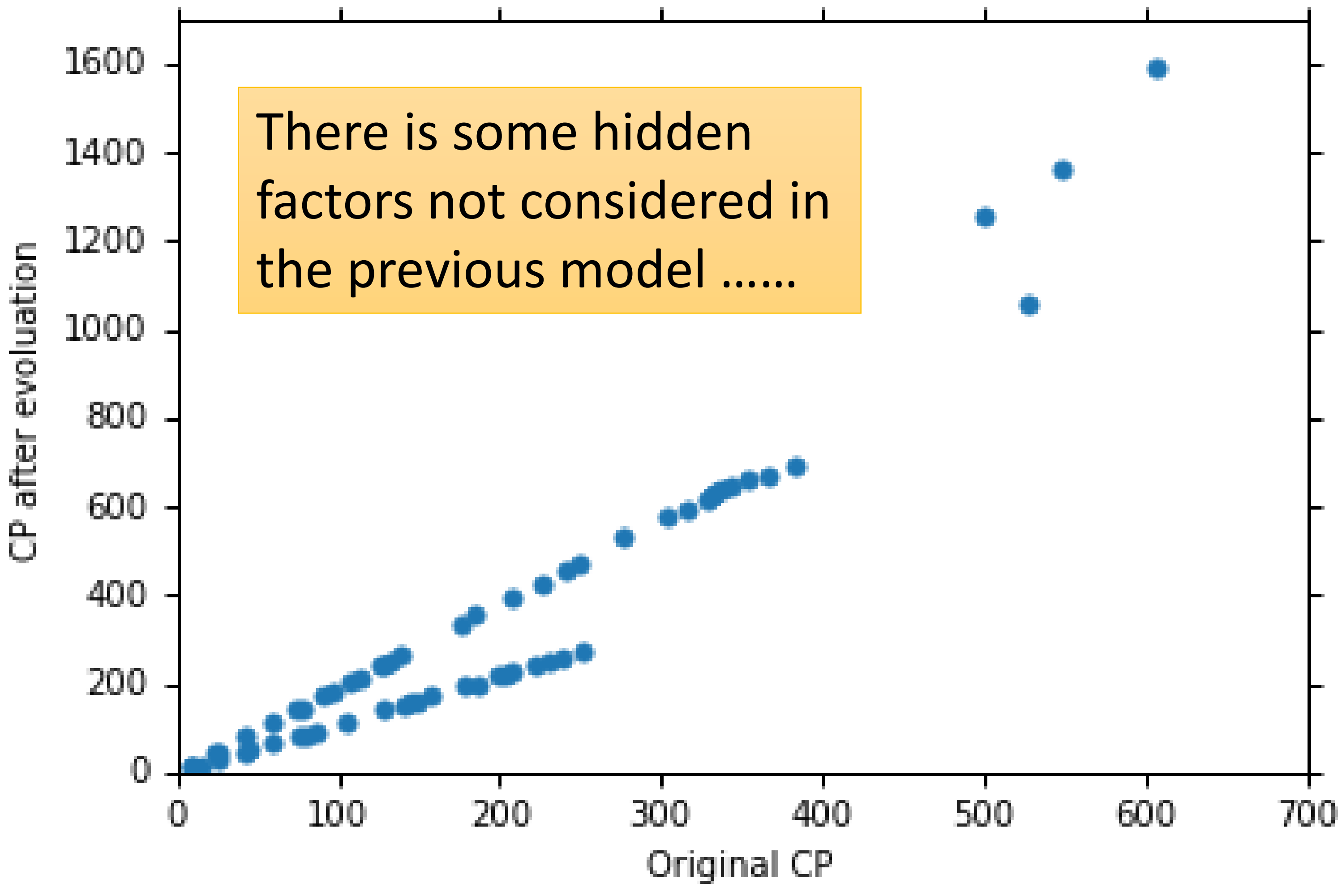


	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

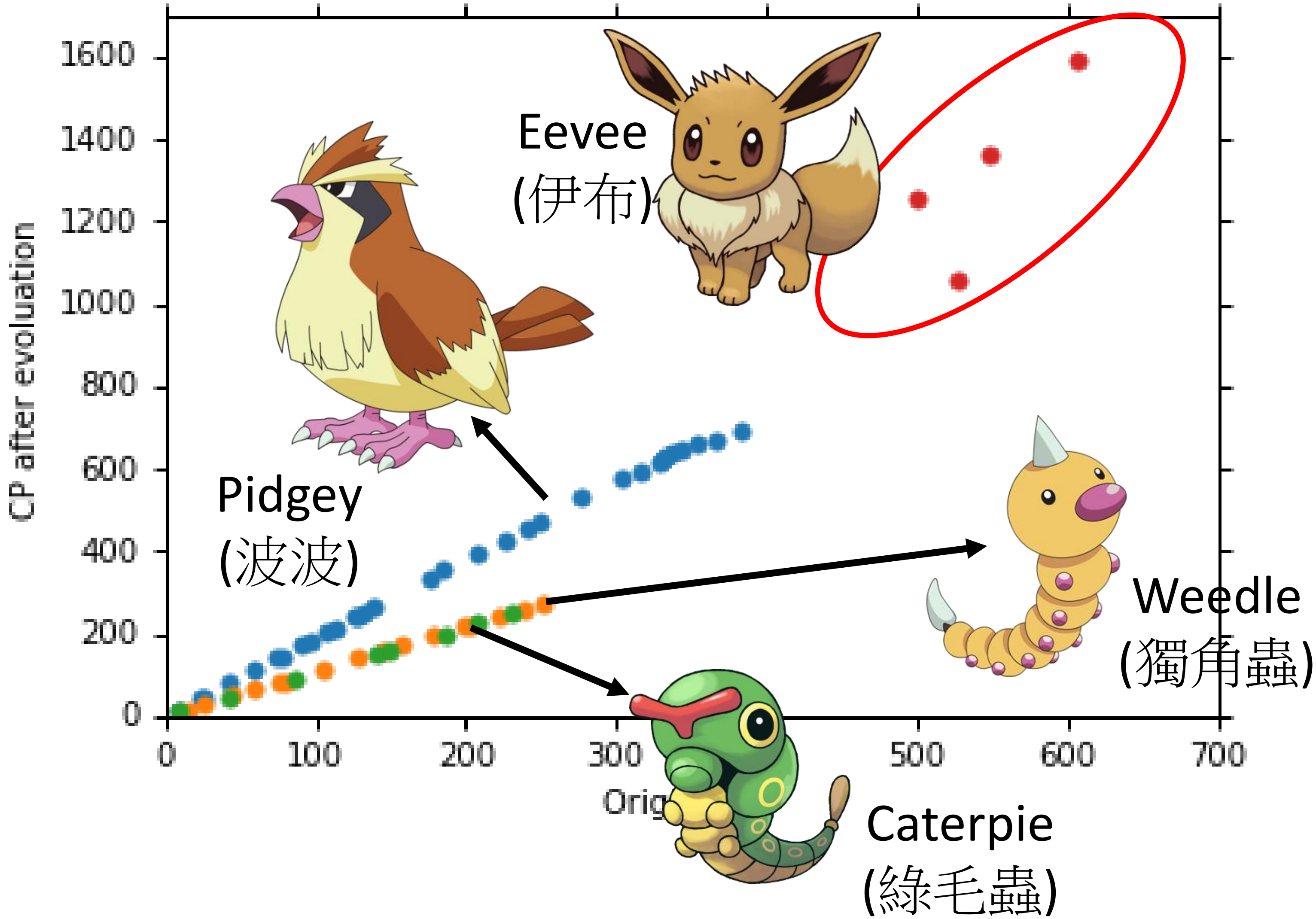
A more complex model does not always lead to better performance on ***testing data***.

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

Let’s collect more data



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?

$y = b_1 \cdot$ 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

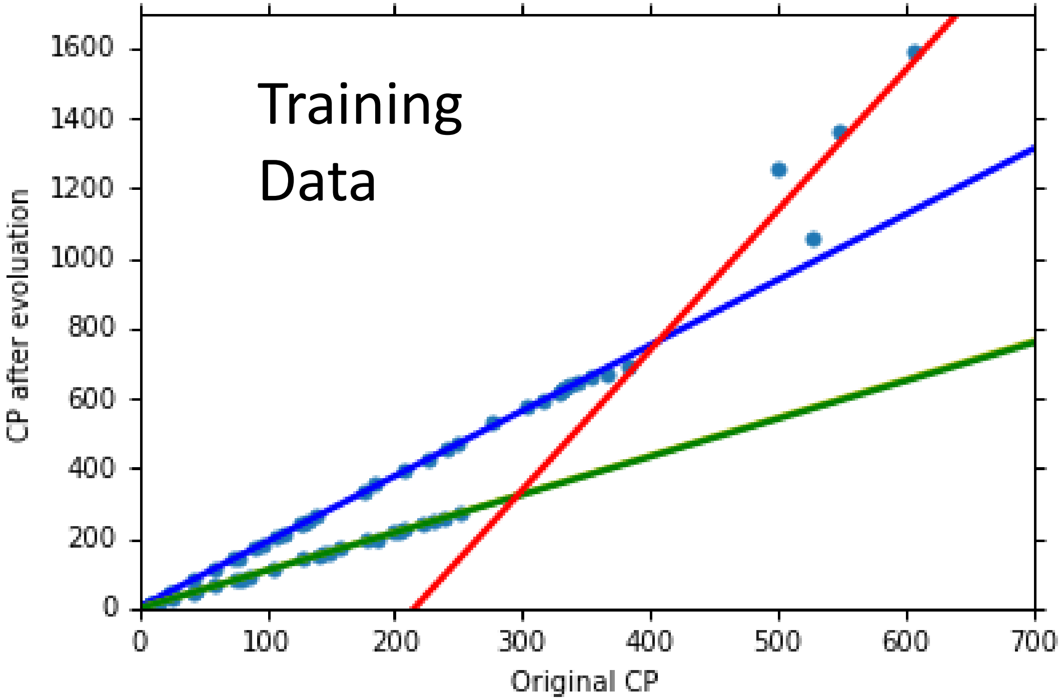
$\delta(x_s =$ Pidgey$)$

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

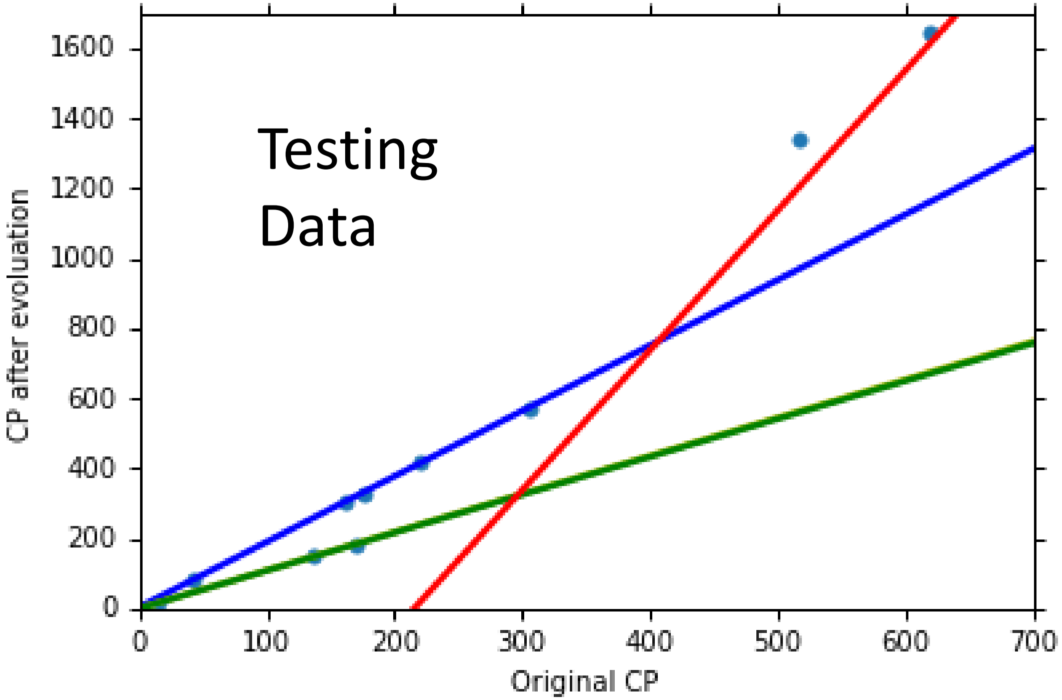
If $x_s =$ Pidgey

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

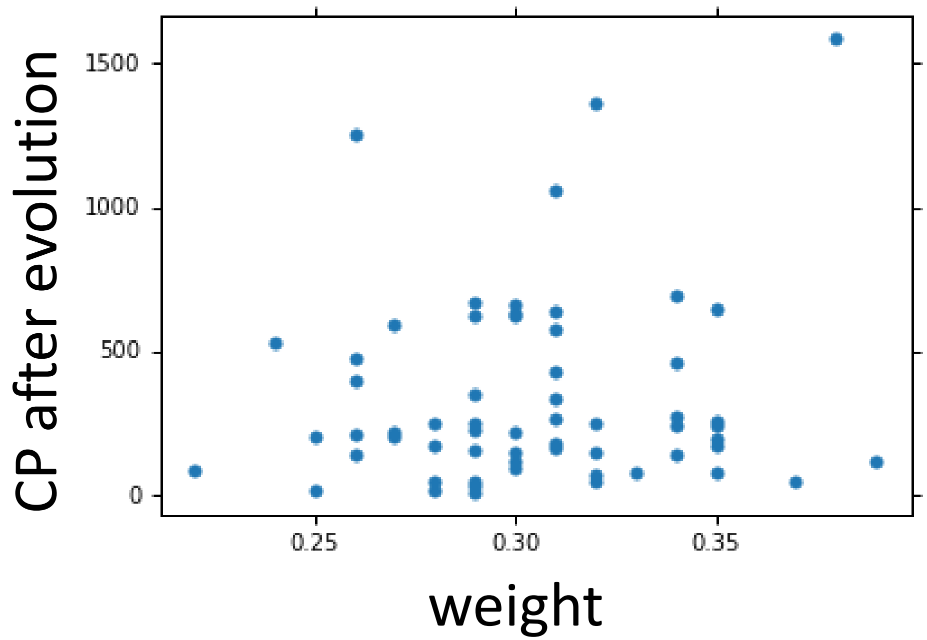
Average error = 3.8

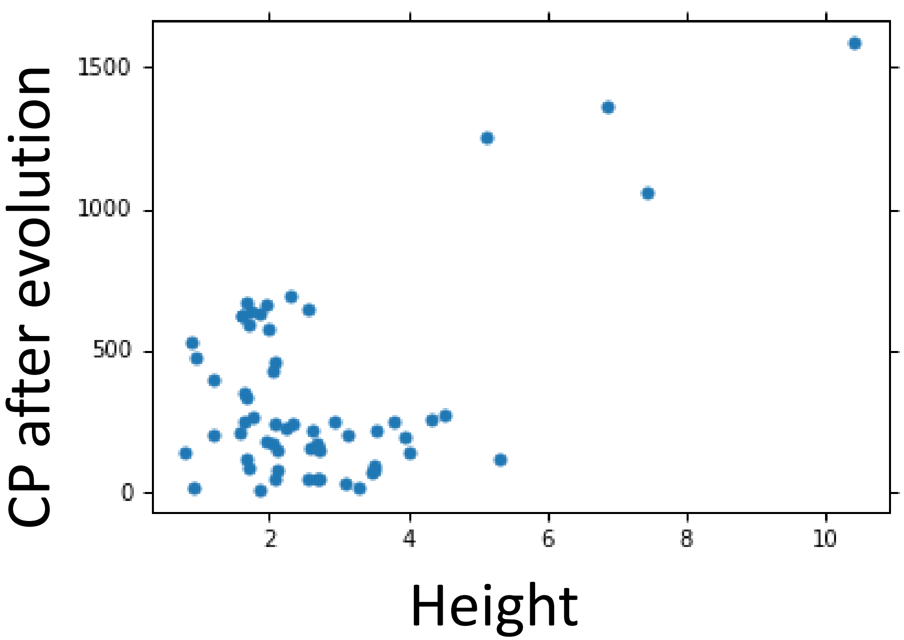


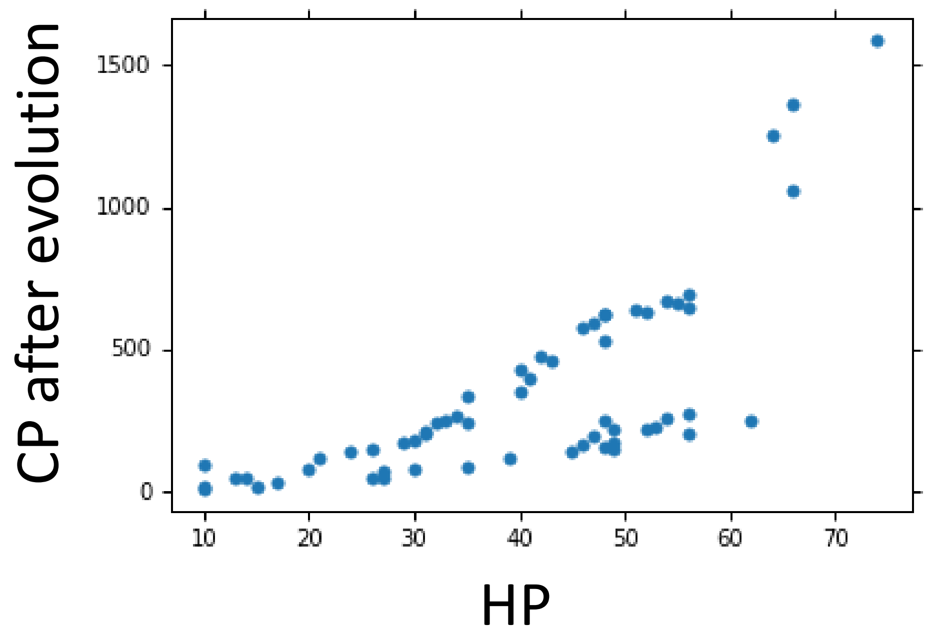
Average error = 14.3



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

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

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

$$+\lambda \sum (w_i)^2$$

The functions with smaller w_i are better

- Smaller w_i means … smoother

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

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

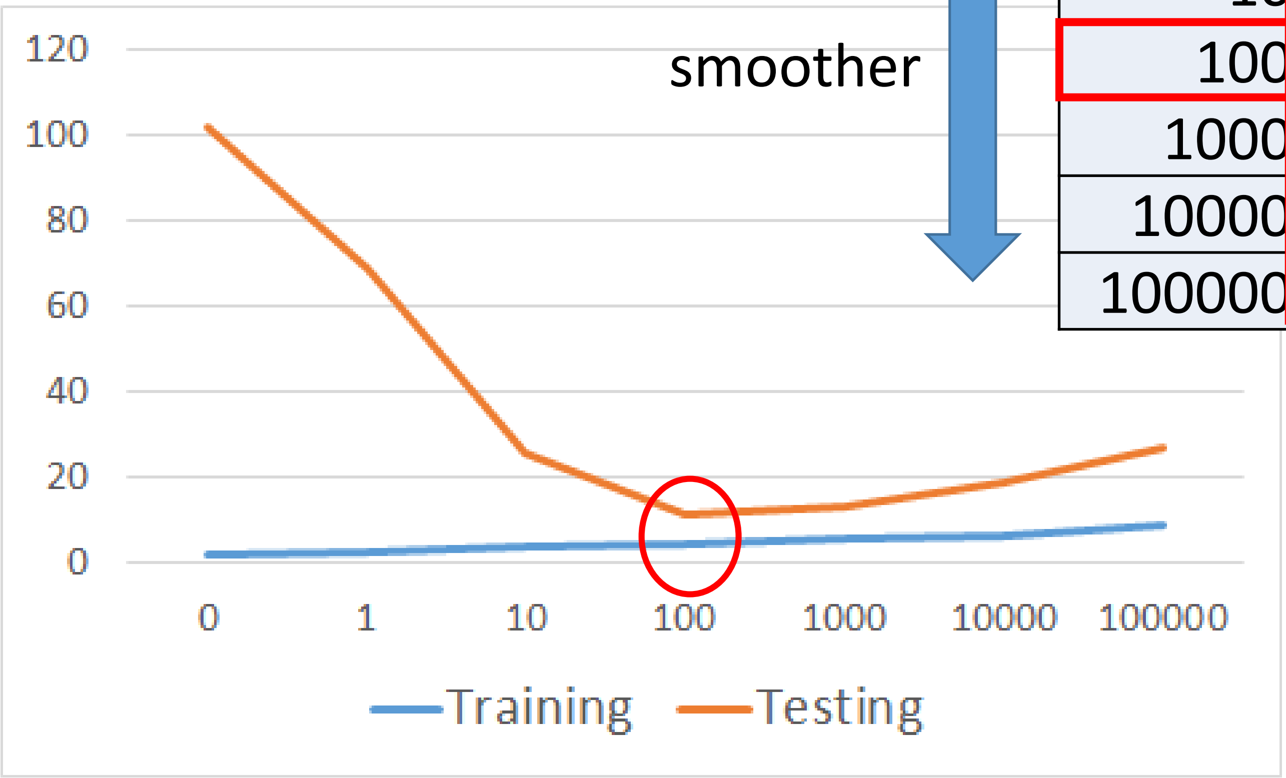
- We believe smoother function is more likely to be correct

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

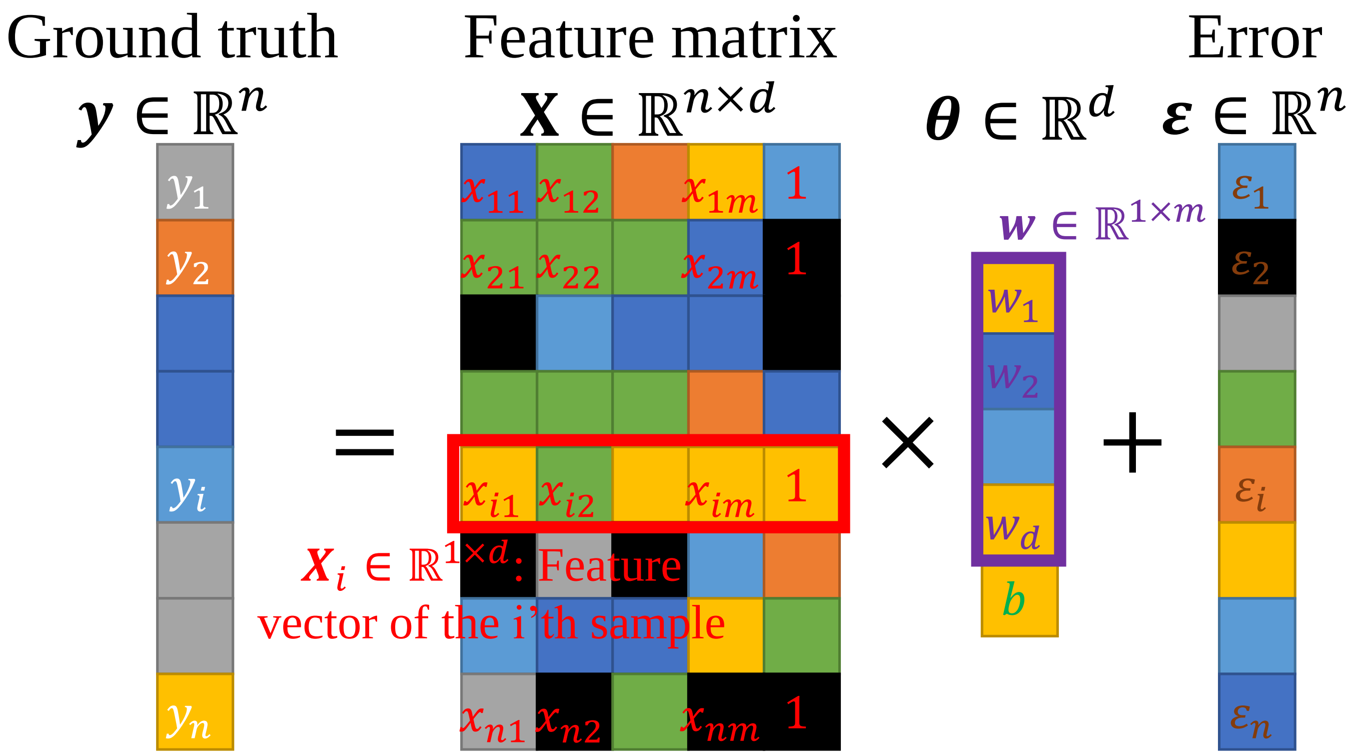


How smooth?

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.

Matrix Form $\boldsymbol{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\varepsilon}$



With bias term: $d = m + 1$ (denote $x_{i\,m+1} = 1$)
No bias term: $d = m$

Sum of Squared Error:
$$\varepsilon_1^2 + \cdots + \varepsilon_n^2 = \|\boldsymbol{\varepsilon}\|_2^2$$

Sum of Absolute Error:
$$|\varepsilon_1| + \cdots + |\varepsilon_n| = \|\boldsymbol{\varepsilon}\|_1$$

Famous Regression Methods

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\varepsilon} \Rightarrow \boldsymbol{\varepsilon} = \boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}$$

$$\boldsymbol{\Omega} = diag(\omega_1, \ldots, \omega_n) = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & \omega_n \end{bmatrix}$$

Regression methods	$L(\boldsymbol{\theta})$	Matrix form
Least-squares linear regr.	$\sum_i (y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})^2$	$\lVert\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\rVert_2^2$
Weighted least squares	$\sum_i \omega_i (y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})^2$	$(y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})^T \boldsymbol{\Omega} (y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})$
Ridge regr.	$\sum_i (y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})^2 + \lambda \sum_i w_i^2$	$\lVert\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\rVert_2^2 + \lambda \lVert\boldsymbol{w}\rVert_2^2$
LASSO	$\sum_i (y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta})^2 + \lambda \sum_i \lvert w_i \rvert$	$\lVert\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\rVert_2^2 + \lambda \lVert\boldsymbol{w}\rVert_1$
Least absolute deviations	$\sum_i \lvert y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta}\rvert$	$\lVert\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\rVert_1$
Chebyshev criterion	$\max_i \lvert y_i - \boldsymbol{X}_\mathrm{i}\boldsymbol{\theta}\rvert$	$\lVert\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\rVert_\infty$

Quadratic cost; minimize w/calculus

Quadratic programming

Linear programming

We usually do not pose regularization on the bias term b
(a larger bias does not make the model more "non-smooth")

Minimize Quadratic Cost with Calculus

- For least-squares linear regr., write
$$L(\boldsymbol{\theta}) = \|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 = (\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta})^T(\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta})$$
$$= \boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{\theta}^T\boldsymbol{X}^T\boldsymbol{y} - \boldsymbol{y}^T\mathbf{X}\boldsymbol{\theta} + \boldsymbol{\theta}^T\boldsymbol{X}^T\mathbf{X}\boldsymbol{\theta}$$
- Taking gradient
$$\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) = 2\boldsymbol{X}^T\mathbf{X}\boldsymbol{\theta} - 2\boldsymbol{X}^T\boldsymbol{y}$$
- Optimal solution occurs when gradient vanishes, namely
$$\boldsymbol{\theta}^* = (\boldsymbol{X}^T\mathbf{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

For students obsessed with rigorous math:

Q: Does gradient equals zero implies minimal solution?

A: Counter-examples exist (think of functions like θ^3).
A more rigorous proof is to write
$$L(\boldsymbol{\theta}) = (\boldsymbol{\theta} - \boldsymbol{\theta}^*)^T(\boldsymbol{X}^T\mathbf{X})(\boldsymbol{\theta} - \boldsymbol{\theta}^*) + (\boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{y}^T\mathbf{X}(\boldsymbol{X}^T\mathbf{X})^{-1}\boldsymbol{X}^T\boldsymbol{y})$$
and recognize the fact that $\boldsymbol{X}^T\mathbf{X}$ is positive semi-definite.

Q: What if $\boldsymbol{X}^T\mathbf{X}$ is not invertible?

A: The optimal solution is not unique. The optimal solution with the minimum 2-norm is given by $\boldsymbol{\theta}^* = \boldsymbol{X}^\dagger\boldsymbol{y}$, where $\boldsymbol{X}^\dagger$ is the pseudo-inverse of $\boldsymbol{X}$. (Rather technically involved)

Minimize Quadratic Cost with Calculus

Regression methods	$L(\boldsymbol{\theta})$	Matrix form	Optimal solution (For simplicity assume no bias, namely $\theta = w$)
Least-squares linear regr.	$\sum_i (y_i - \boldsymbol{X}_i\boldsymbol{\theta})^2$	$\|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2$	$\boldsymbol{\theta}^* = (\boldsymbol{X}^T\mathbf{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$ (assume $\boldsymbol{X}^T\mathbf{X}$ is invertible)
Weighted least squares	$\sum_i \omega_i(y_i - \boldsymbol{X}_i\boldsymbol{\theta})^2$	$(y_i - \boldsymbol{X}_i\boldsymbol{\theta})^T\boldsymbol{\Omega}(y_i - \boldsymbol{X}_i\boldsymbol{\theta})$	$\boldsymbol{\theta}^* = (\boldsymbol{X}^T\boldsymbol{\Omega}\mathbf{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{y}$ (assume $\boldsymbol{X}^T\boldsymbol{\Omega}\mathbf{X}$ is invertible)
Ridge regr.	$\sum_i (y_i - \boldsymbol{X}_i\boldsymbol{\theta})^2 + \lambda \sum_i w_i^2$	$\|\boldsymbol{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2$	$\boldsymbol{\theta}^* = (\boldsymbol{X}^T\mathbf{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y}$

Homework questions ☺

$$\boldsymbol{\Omega} = diag(\omega_1, \ldots, \omega_n) = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 \\ 0 & \omega_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & \omega_n \end{bmatrix}$$

Besides intuitive "proof" (like setting derivatives to zero), you may challenge yourself to give rigorous proofs that really convince you, and/or cover the more general cases (say when $\boldsymbol{X}^T\boldsymbol{\Omega}\mathbf{X}$ is not invertible, considering the bias term b, etc.).