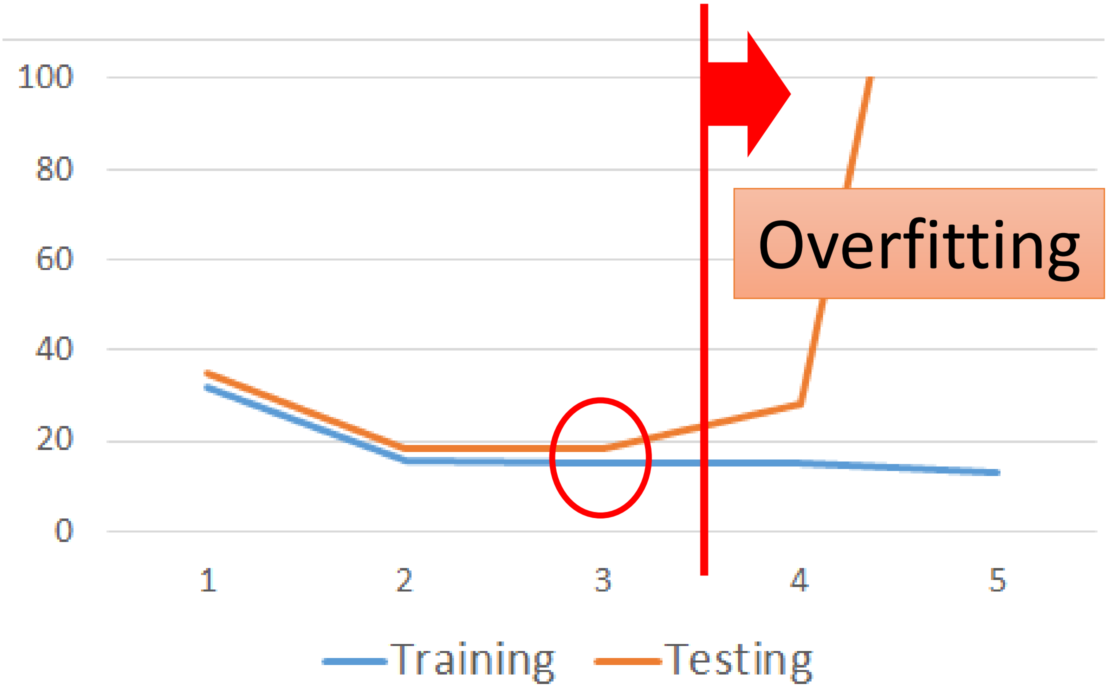
人工智能技术及应用

Artificial Intelligence and Application

Model Selection



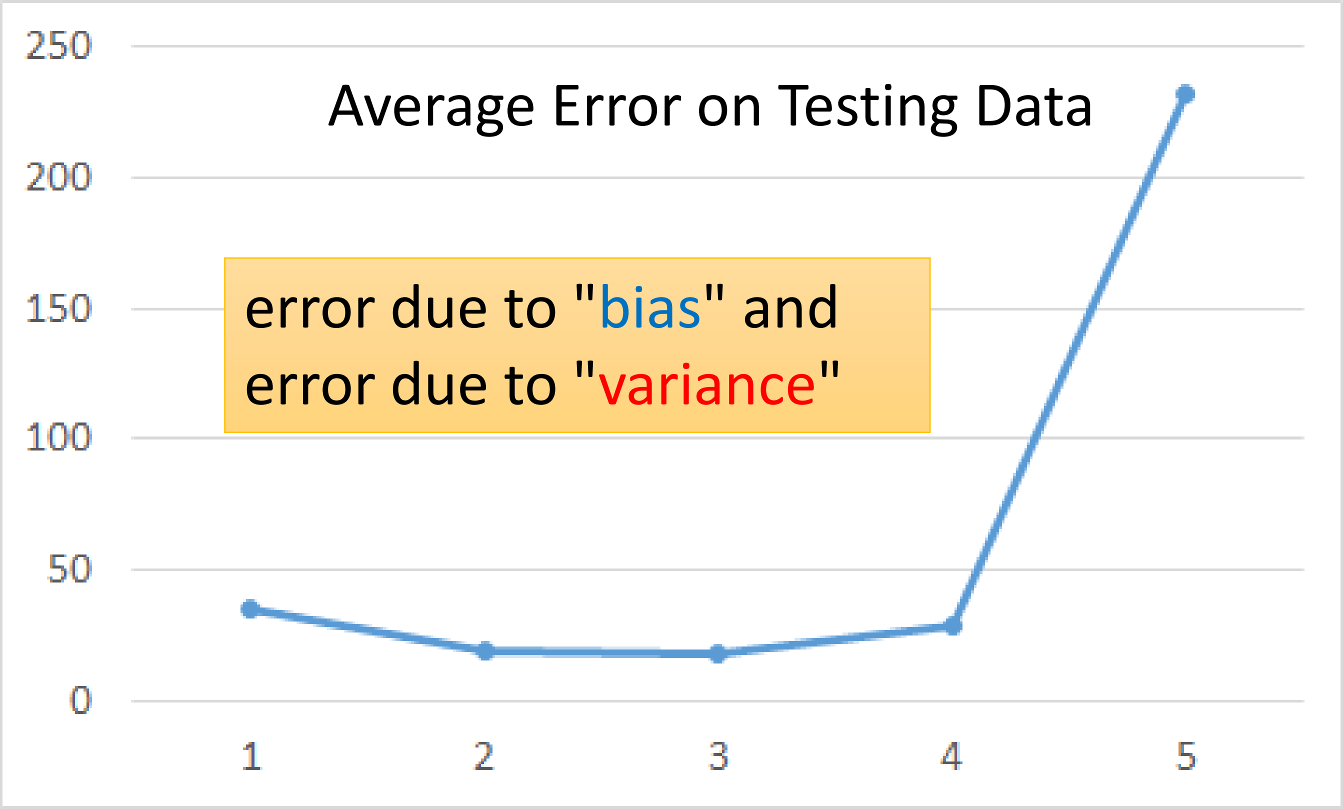
	Training	Testing
1	31.9	35.0
2	15.4	18.4
3	15.3	18.1
4	14.9	28.2
5	12.8	232.1

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

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

误差的来源

Review



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

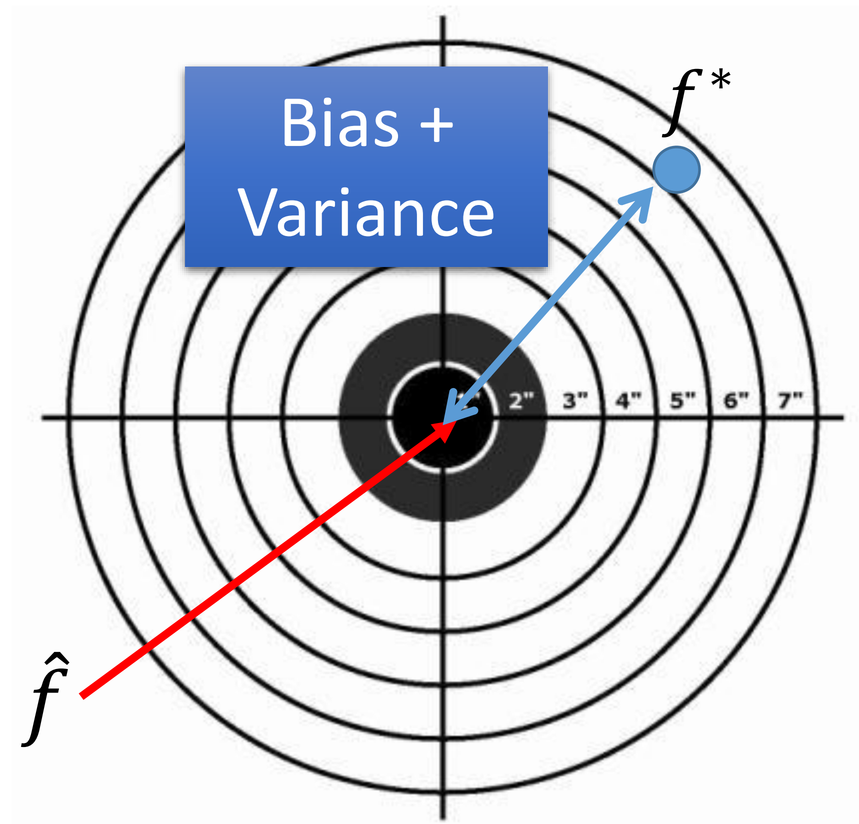
Estimator

$\hat{y} = \hat{f}($  $)$

Only Niantic knows $\hat{f}$

From training data, we find f^*

f^* is an estimator of $\hat{f}$



Bias and Variance of Estimator

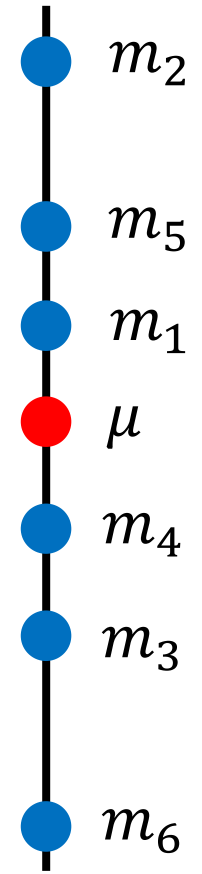
unbiased

- Estimate the mean of a variable x
  - assume the mean of x is μ
  - assume the variance of x is σ^2
- Estimator of mean μ
  - Sample N points: $\{x^1, x^2, \dots, x^N\}$

$$m = \frac{1}{N}\sum_n x^n \neq \mu$$

中心极限定理

$$E[m] = E\left[\frac{1}{N}\sum_n x^n\right] = \frac{1}{N}\sum_n E[x^n] = \mu$$



Bias and Variance of Estimator

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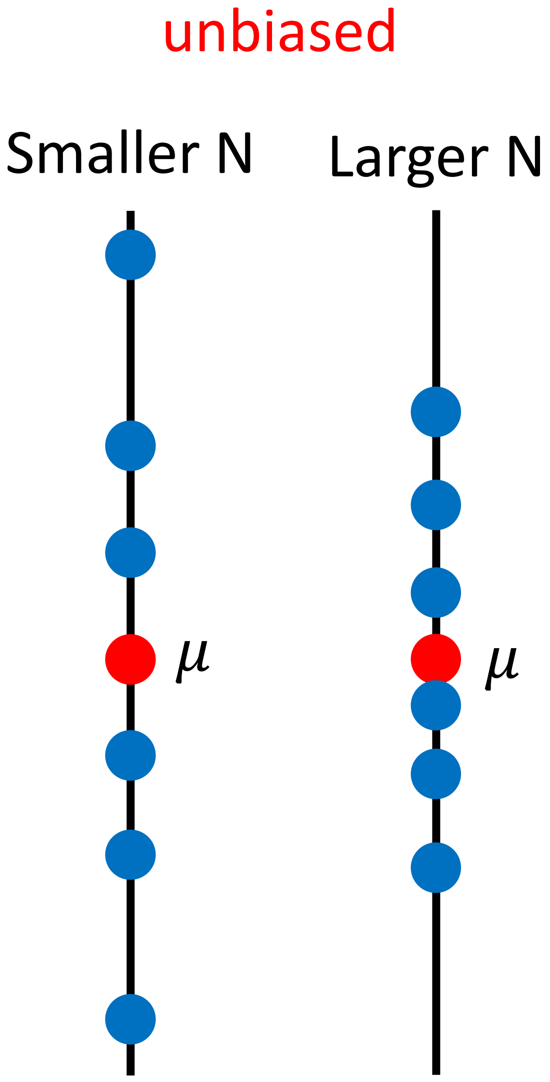
  - Sample N points: $\{x^1, x^2, \ldots, x^N\}$

$$m = \frac{1}{N}\sum_n x^n \neq \mu$$

$$Var[m] = \frac{\sigma^2}{N}$$

Variance depends on the number of samples



Bias and Variance of Estimator

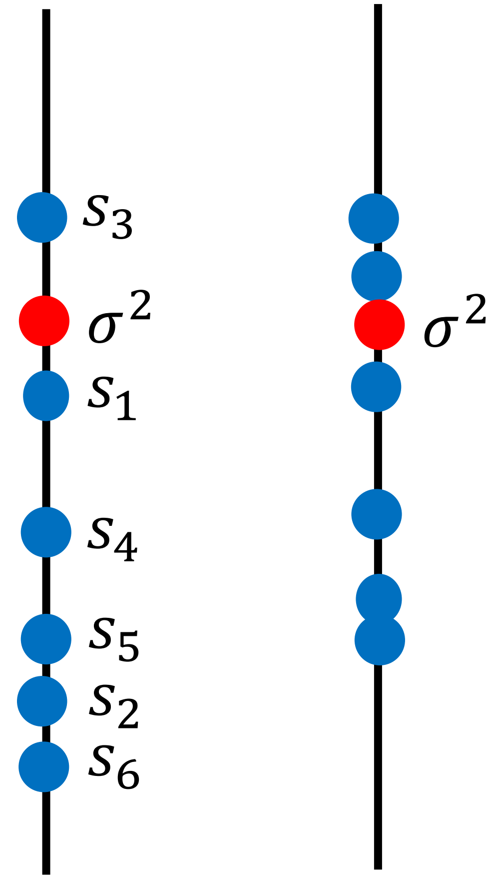
- Estimate the mean of a variable x
  - assume the mean of x is μ
  - assume the variance of x is σ^2
- Estimator of variance σ^2
  - Sample N points: $\{x^1, x^2, \dots, x^N\}$

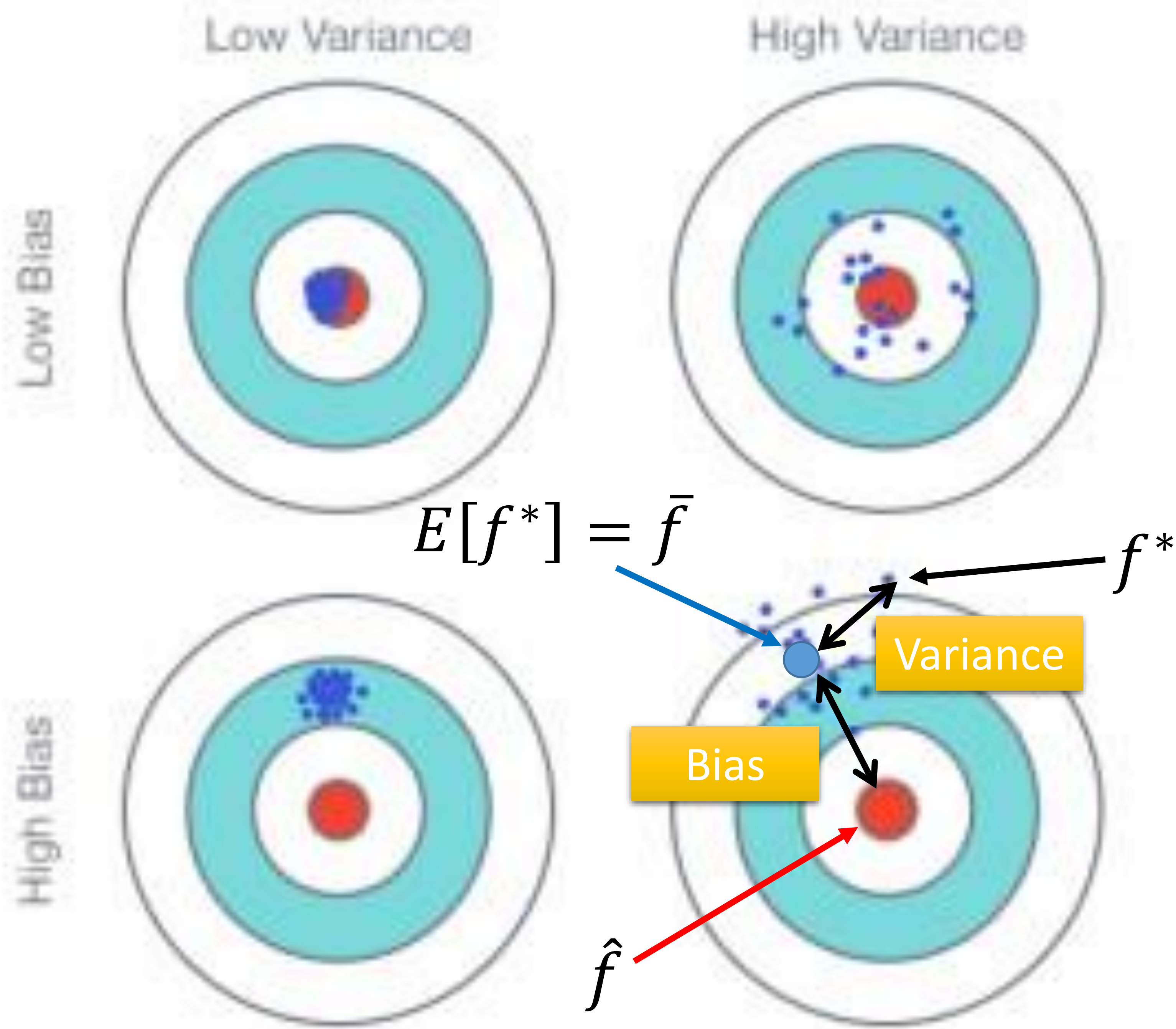
$$m = \frac{1}{N}\sum_n x^n \quad s = \frac{1}{N}\sum_n (x^n - m)^2$$

Biased estimator

$$E[s] = \frac{N-1}{N}\sigma^2 \quad \neq \sigma^2$$

Increase N

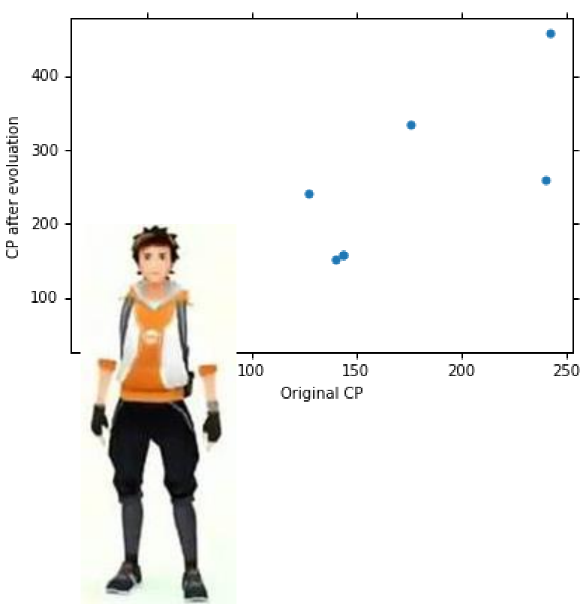



Low Variance
High Variance
Low Bias
High Bias
$E[f^*] = \bar{f}$
f^*
Variance
Bias
$\hat{f}$

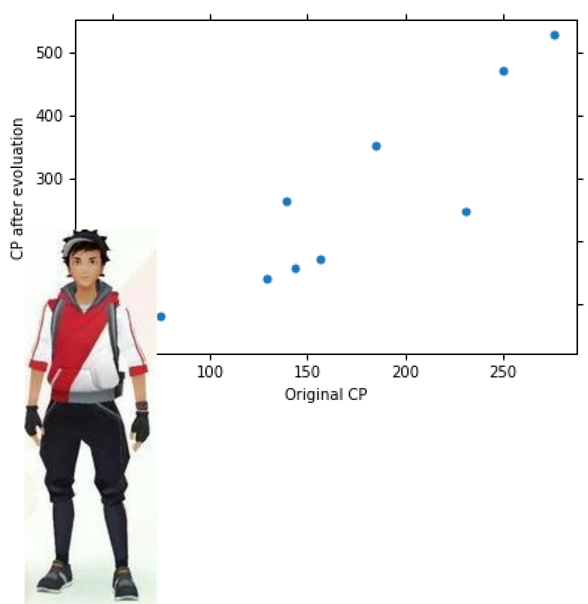
Parallel Universes

- In all the universes, we are collecting (catching) 10 Pokémons as training data to find f^*

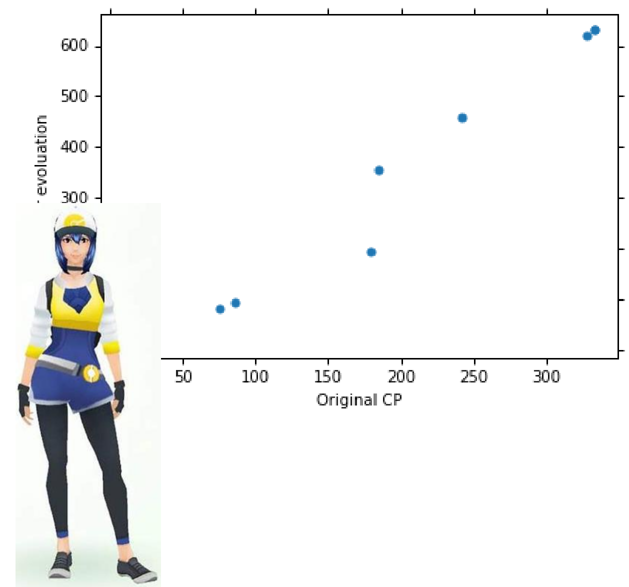
Universe 1



Universe 2



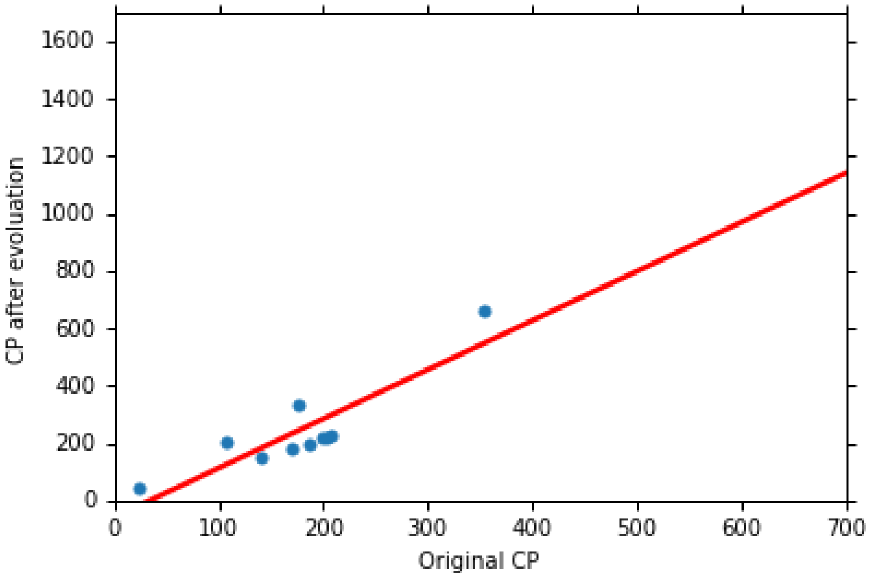
Universe 3



Parallel Universes

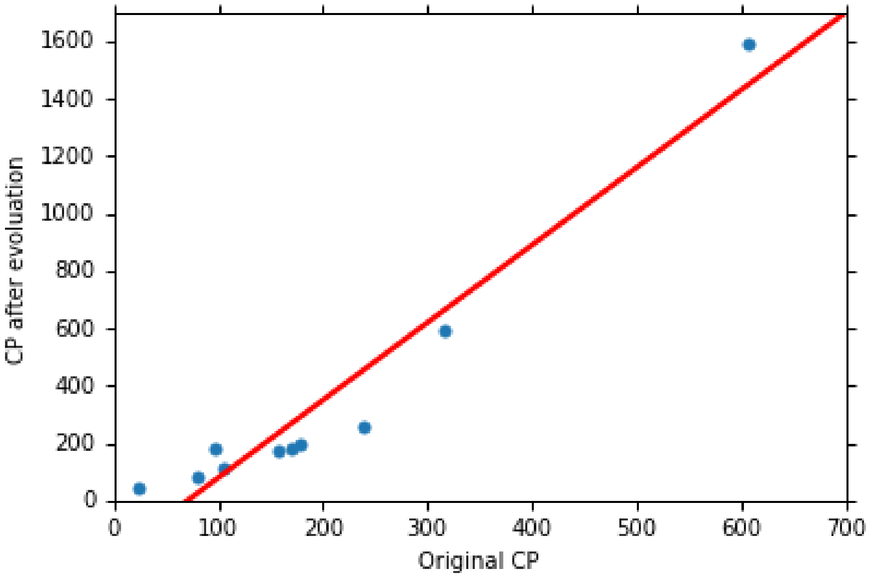
- In different universes, we use the same model, but obtain different f^*

Universe 123



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

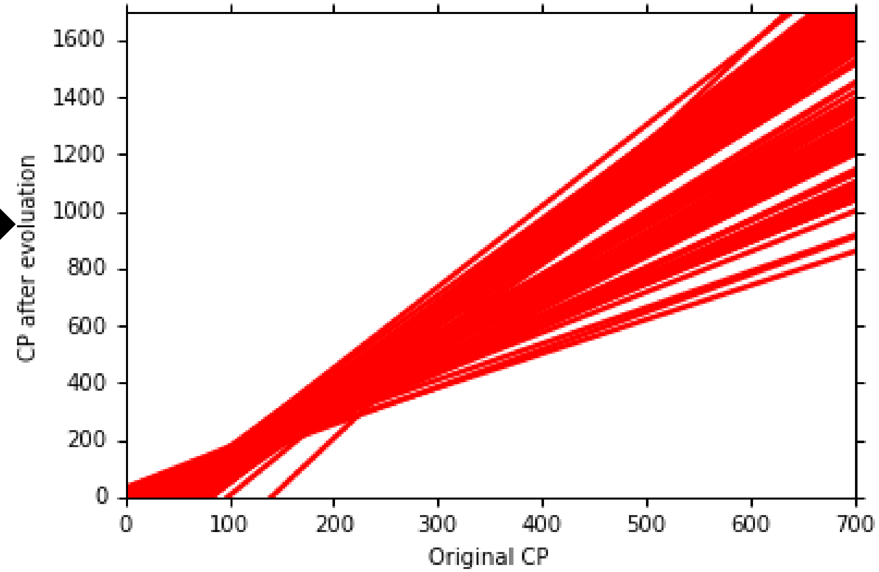
Universe 345



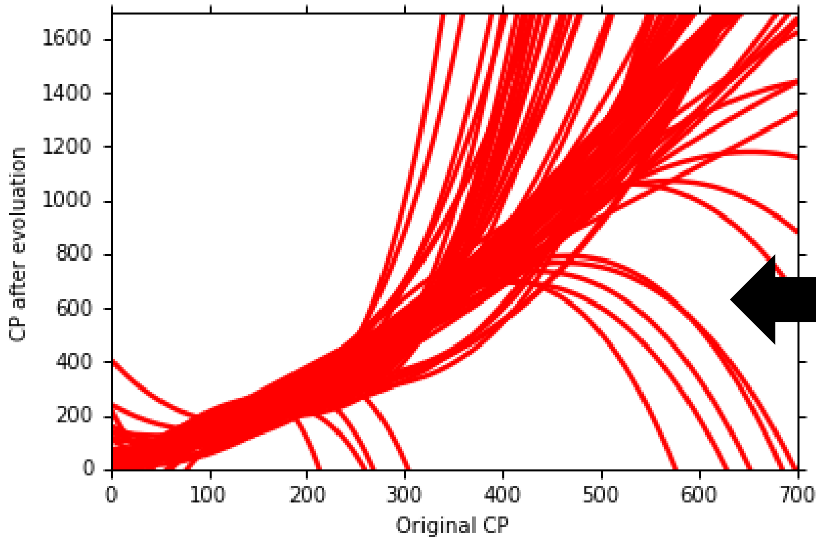
$$y = b + w \cdot x_{cp}$$

f^* in 100 Universes

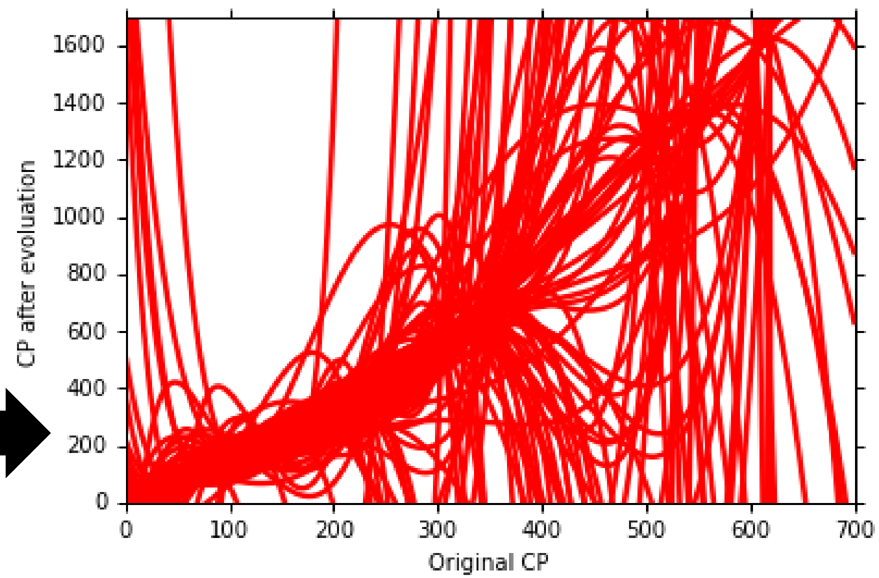
$$y = b + w \cdot x_{cp}$$



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

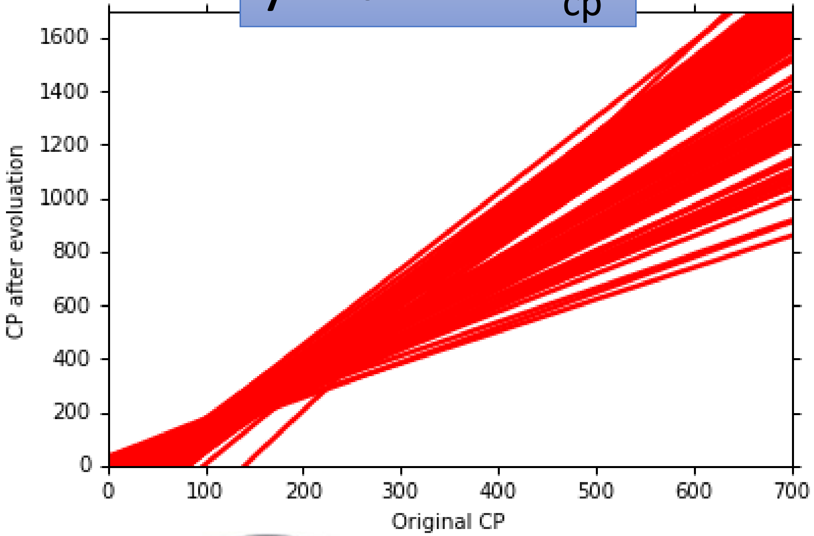


$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$

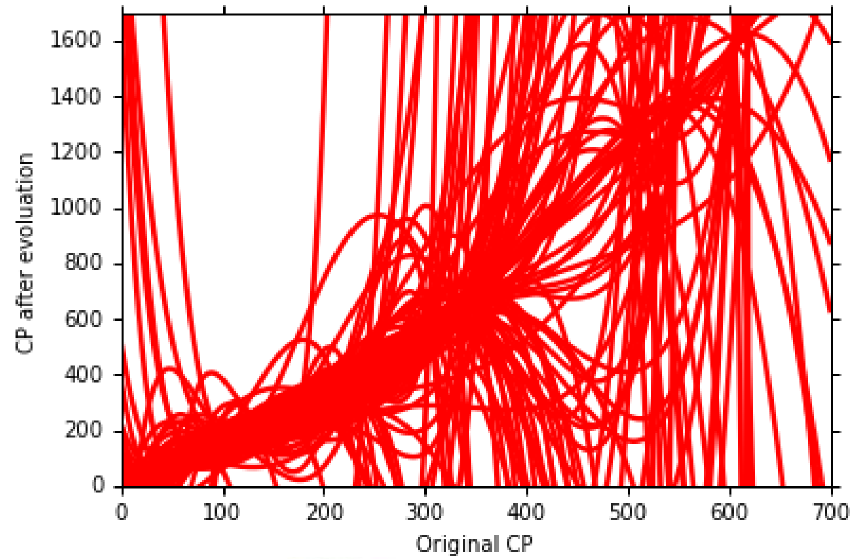


Variance

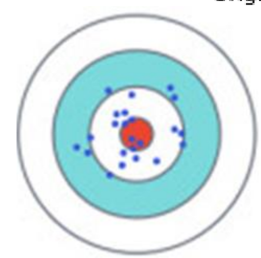
$$y = b + w \cdot x_{cp}$$



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



Small Variance



Large Variance

Simpler model is less influenced by the sampled data

Consider the extreme case f(x) = 5

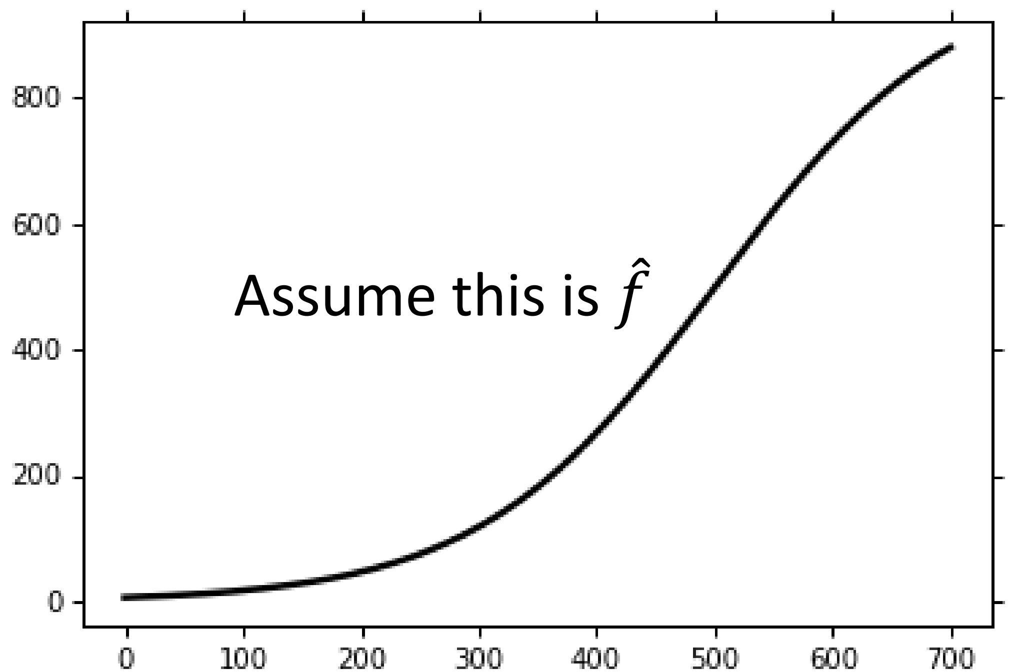
Bias

$$E[f^*] = \bar{f}$$

- Bias: If we average all the f^*, is it close to $\hat{f}$?

Large Bias

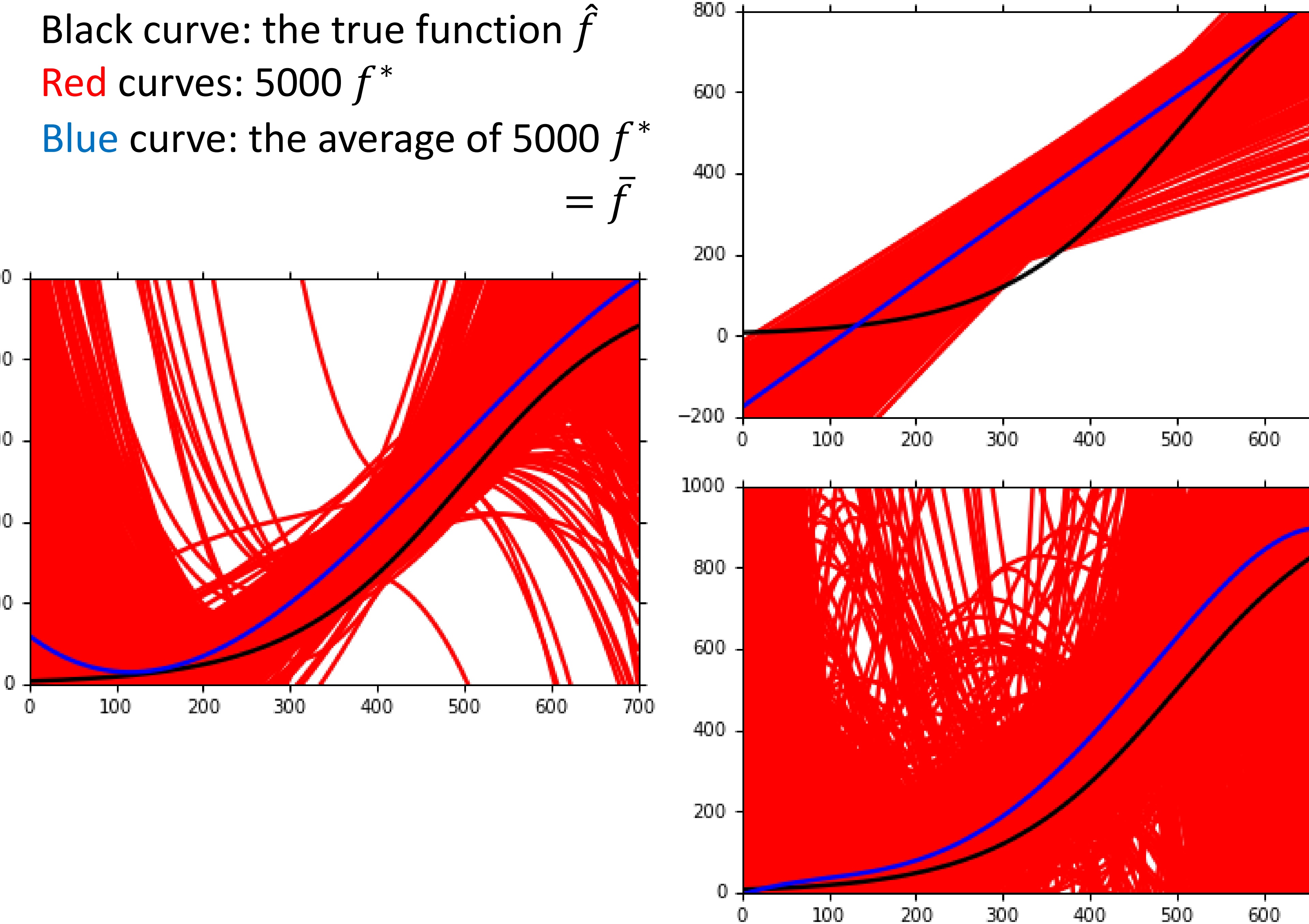
Small Bias



Black curve: the true function $\hat{f}$

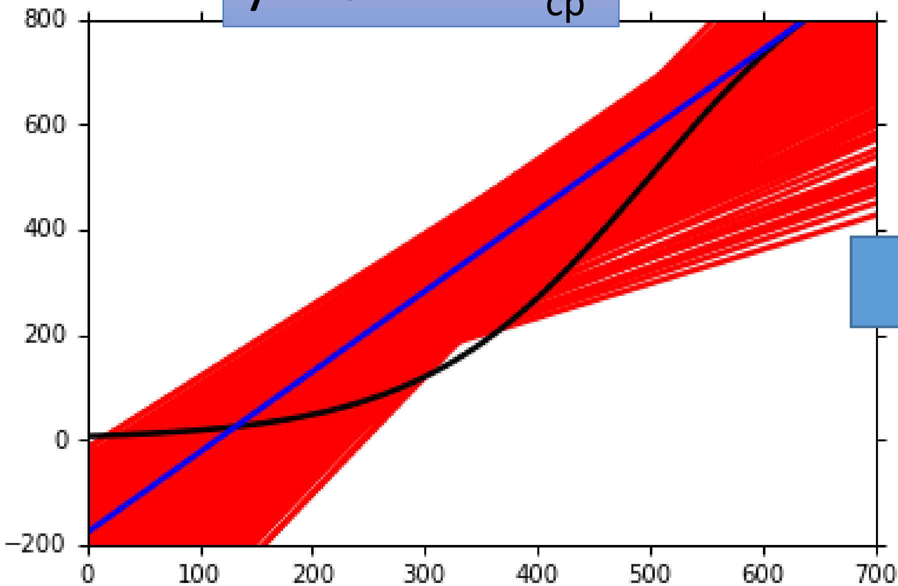
Red curves: 5000 f^*

Blue curve: the average of 5000 f^*
$= \bar{f}$

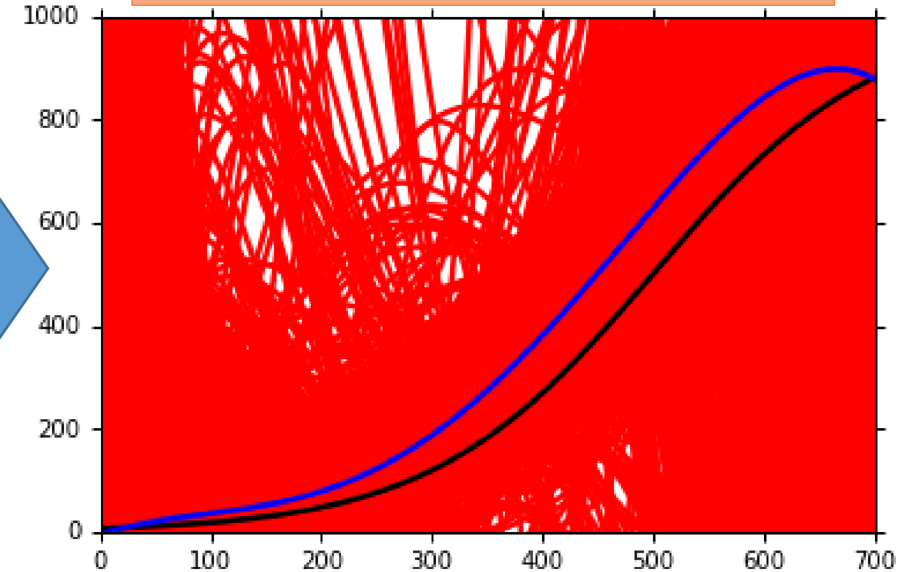


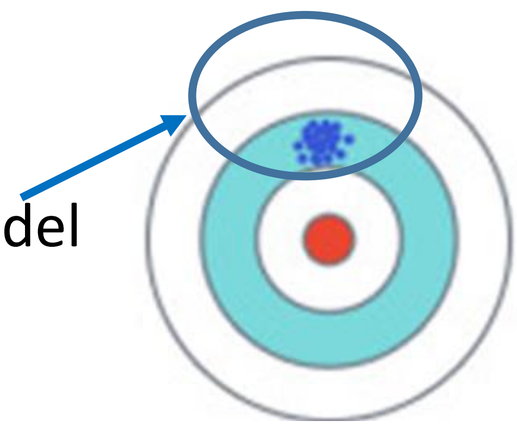
Bias

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



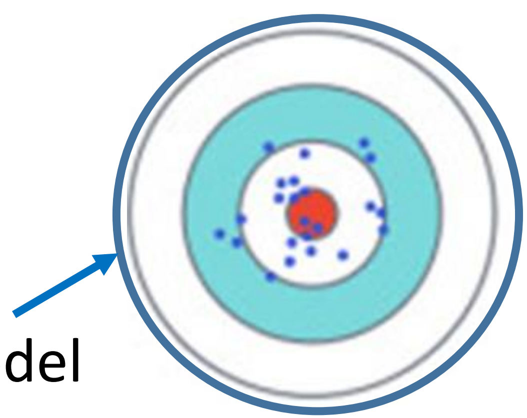
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$





model

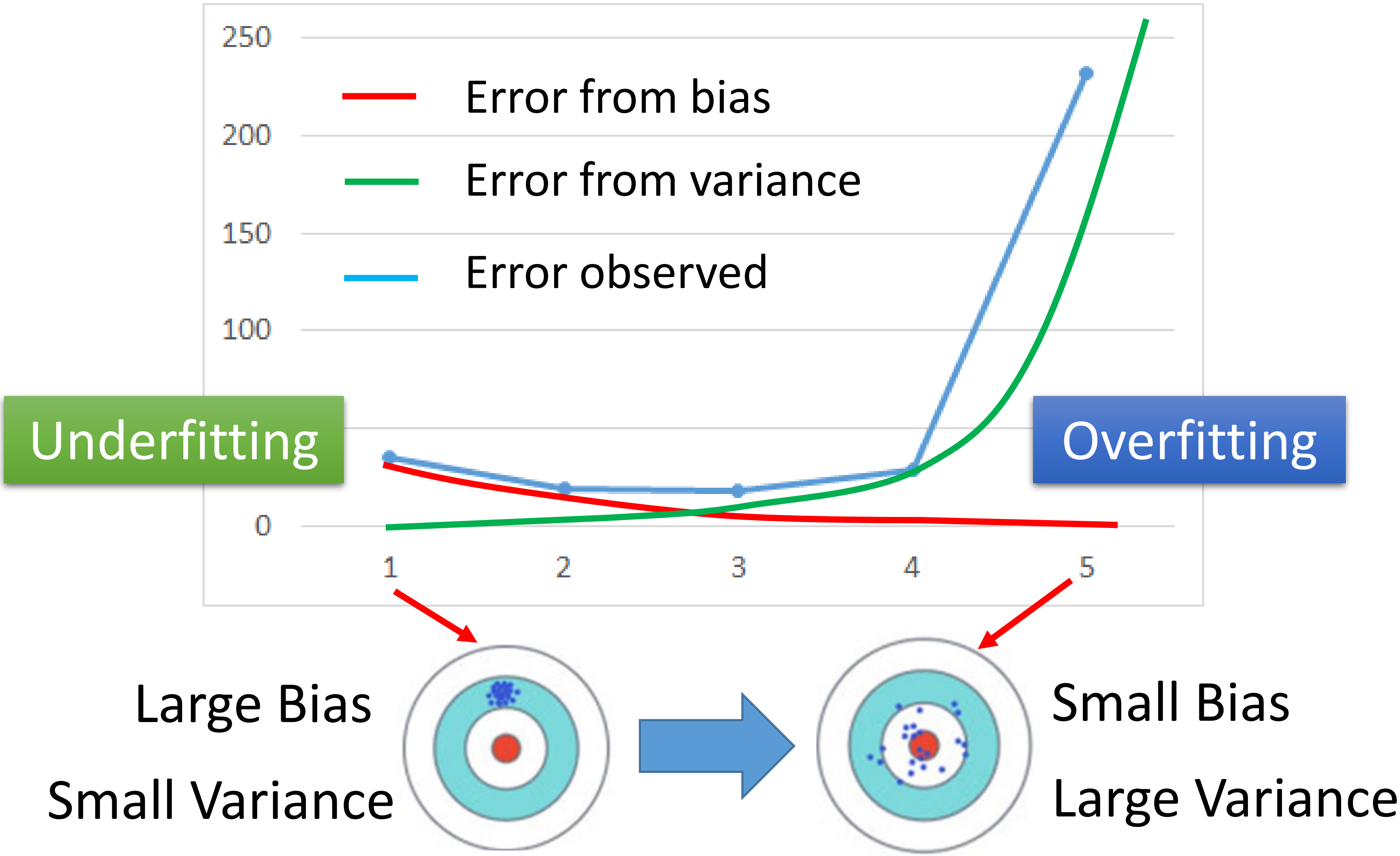
Large Bias



model

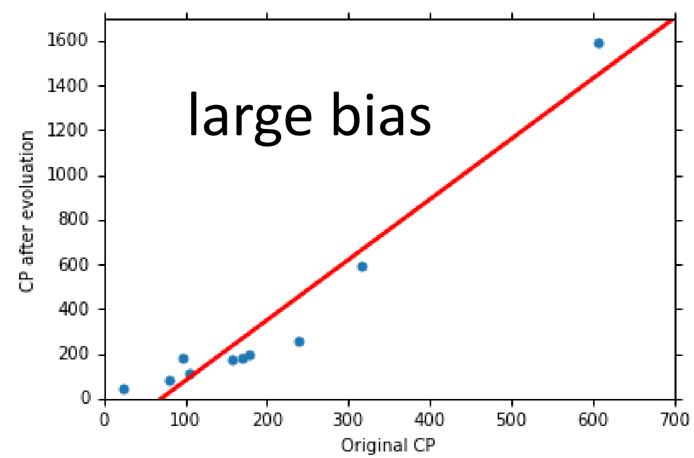
Small Bias

Bias v.s. Variance



What to do with large bias?

- Diagnosis:
  - If your model cannot even fit the training examples, then you have large bias **Underfitting**
  - If you can fit the training data, but large error on testing data, then you probably have large variance **Overfitting**
- For bias, redesign your model:
  - Add more features as input
  - A more complex model



Overfitting

- Small loss on training data, large loss on testing data. Why?

<u>An extreme example</u>

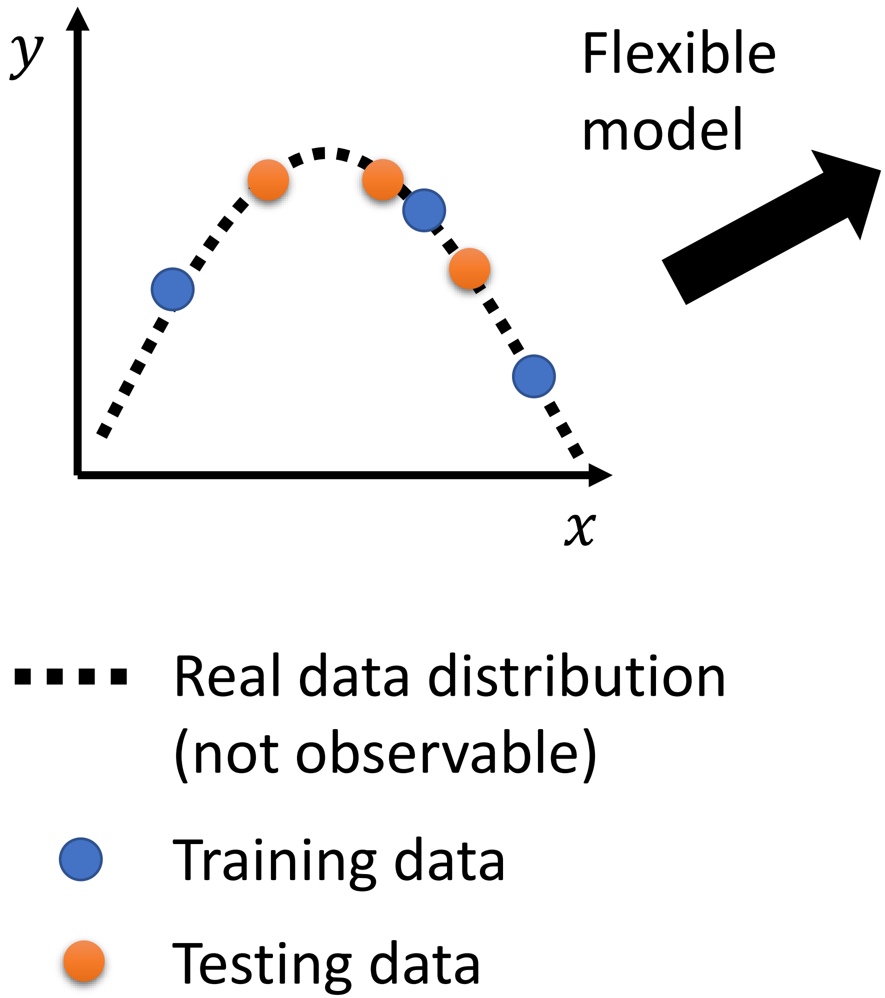
Training data: $\left\{\left(\boldsymbol{x}^{\mathbf{1}}, \hat{y}^{1}\right), \left(\boldsymbol{x}^{\mathbf{2}}, \hat{y}^{2}\right), \ldots, \left(\boldsymbol{x}^{\boldsymbol{N}}, \hat{y}^{N}\right)\right\}$

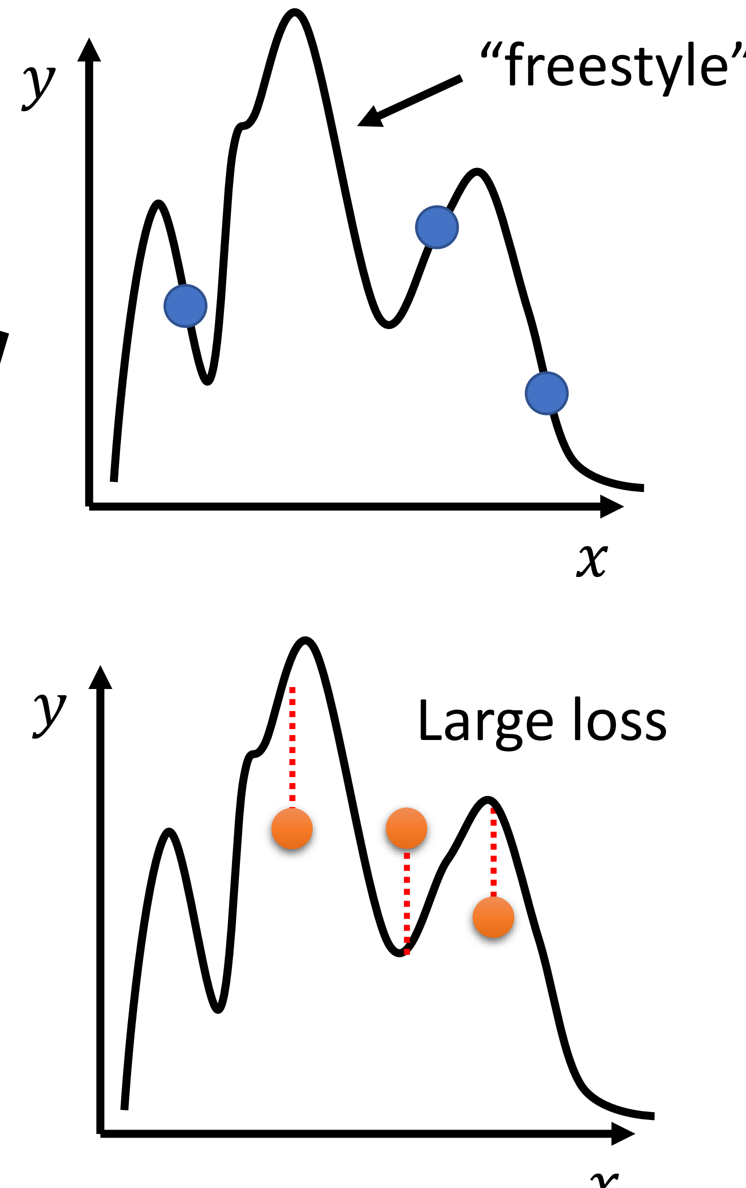
$$f(\boldsymbol{x}) = \begin{cases} \hat{y}^{i} & \exists \boldsymbol{x}^{\boldsymbol{i}} = \boldsymbol{x} \\ random & otherwise \end{cases}$$

Less than useless ...

This function obtains **zero training loss**, but **large testing loss**.

Overfitting

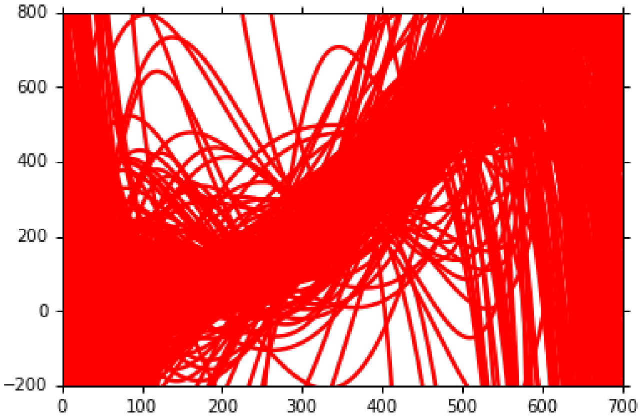




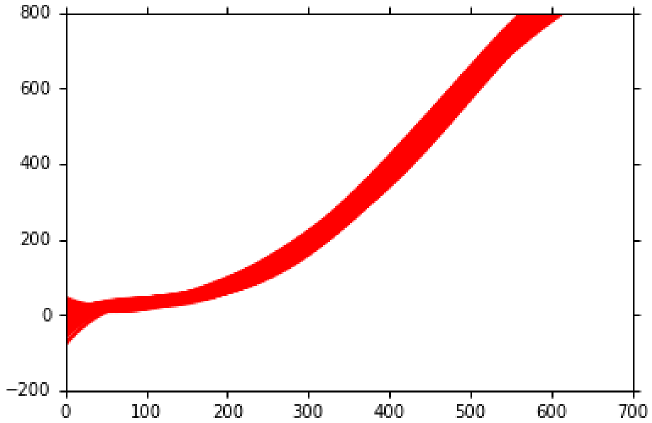
What to do with large variance?

- More data

Very effective, but not always practical



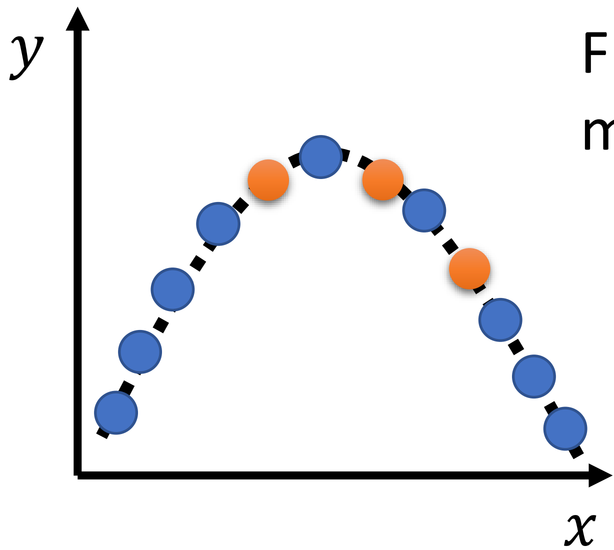
10 examples



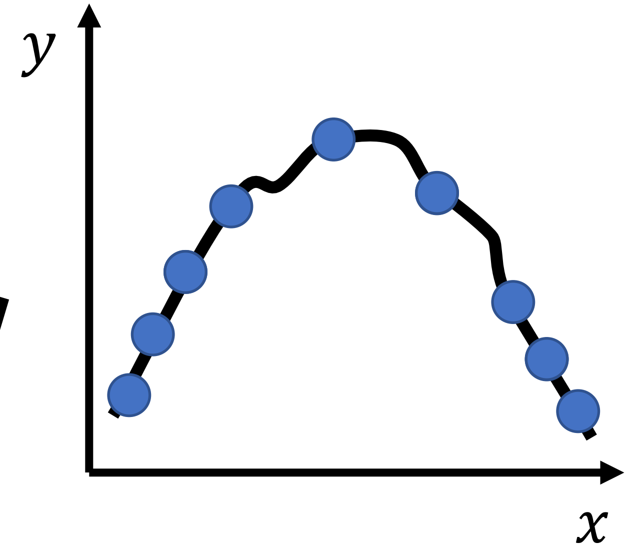
100 examples

- Add constraints

Overfitting



Flexible model

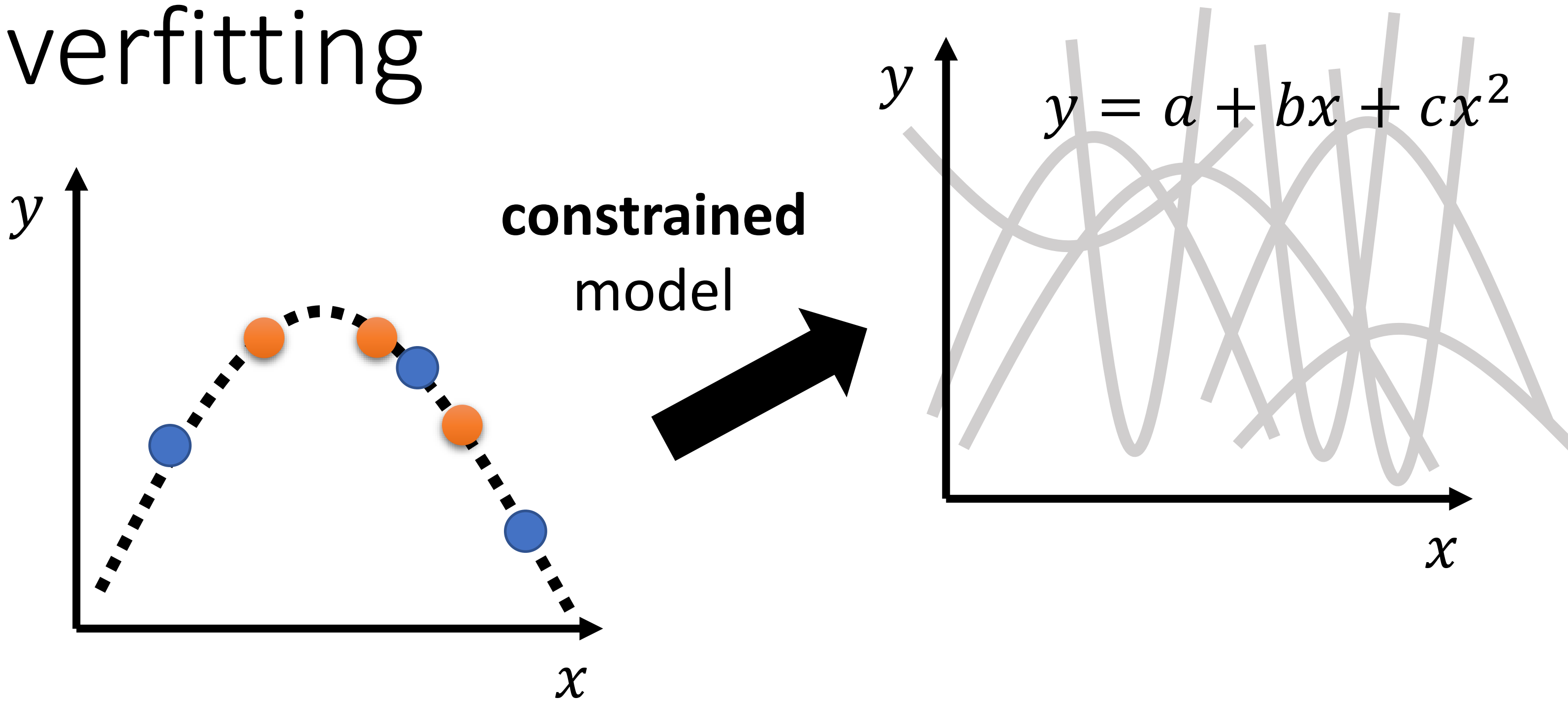


More training data

(cannot do it in HWs)

Data augmentation (you can do that in HWs)

Overfitting

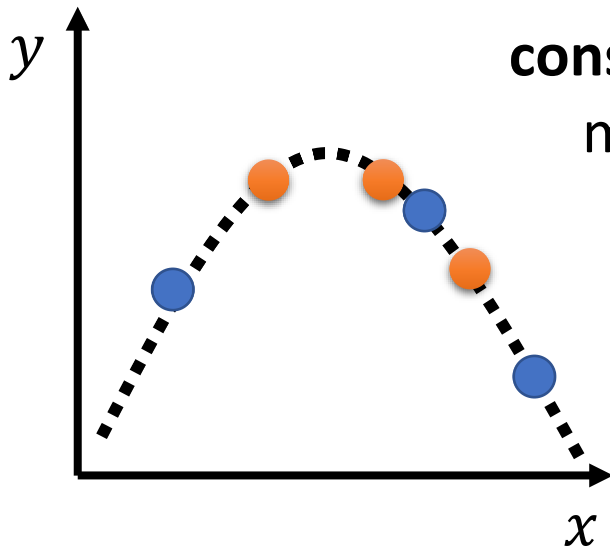


Real data distribution (not observable)

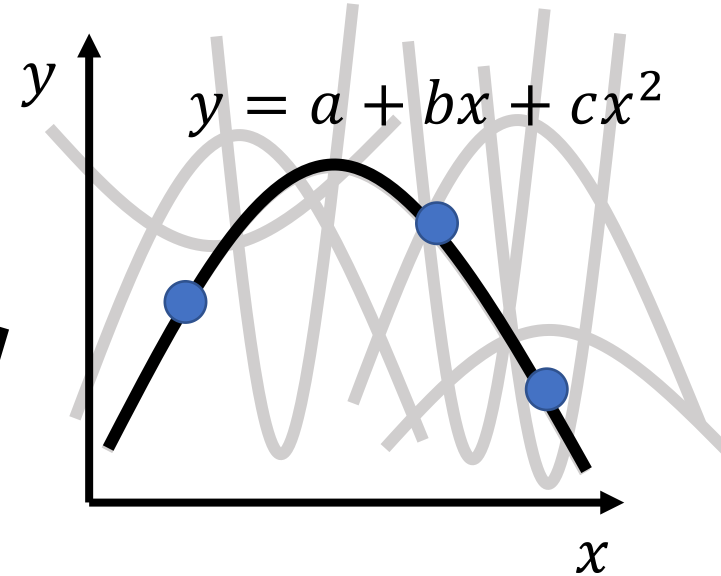
Training data

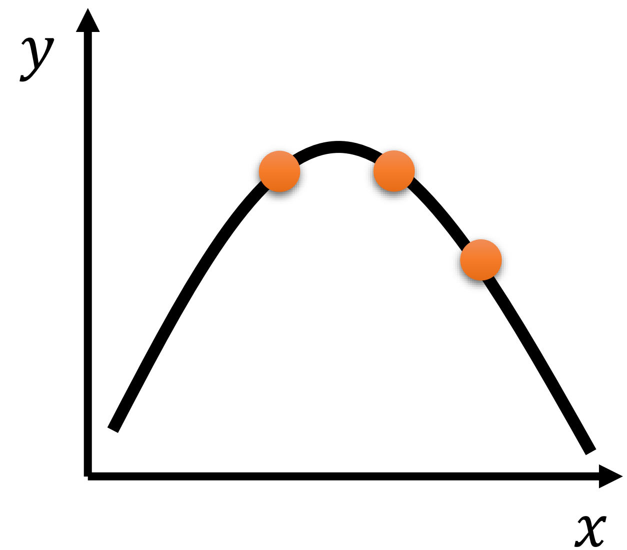
Testing data

Overfitting



constrained model



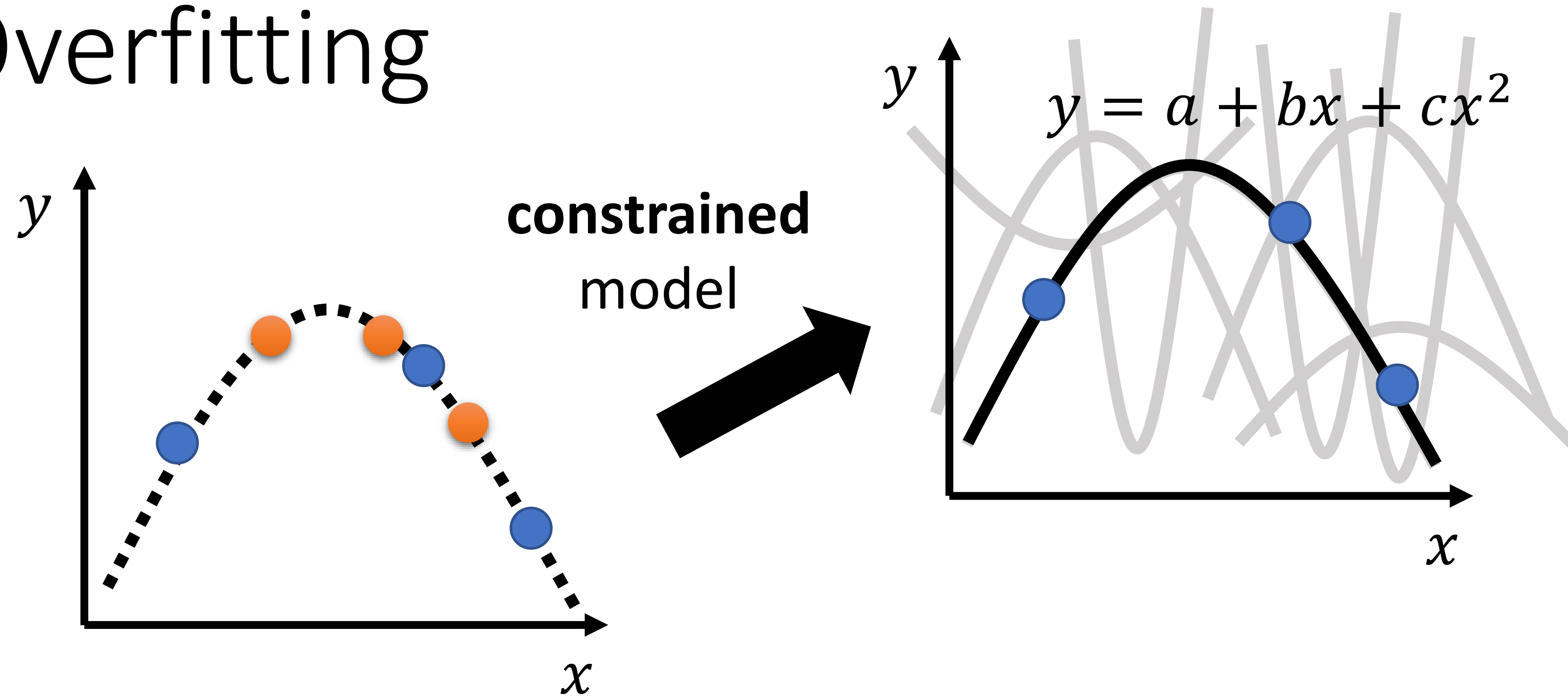


Real data distribution (not observable)

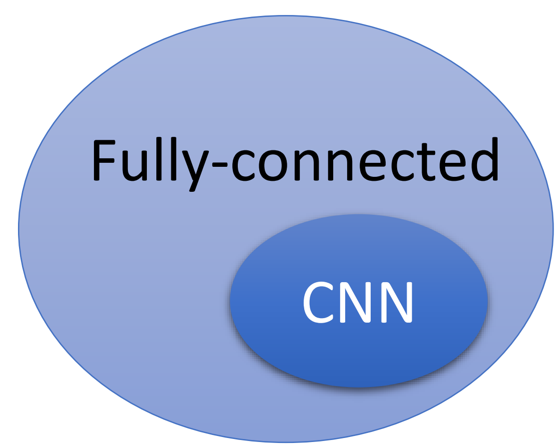
Training data

Testing data

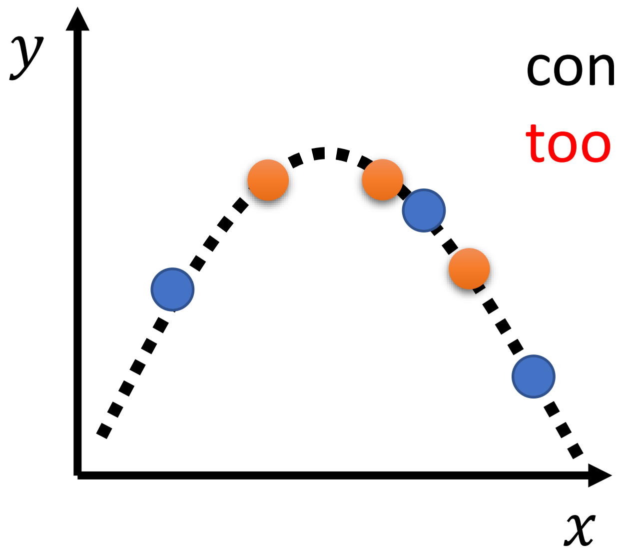
Overfitting



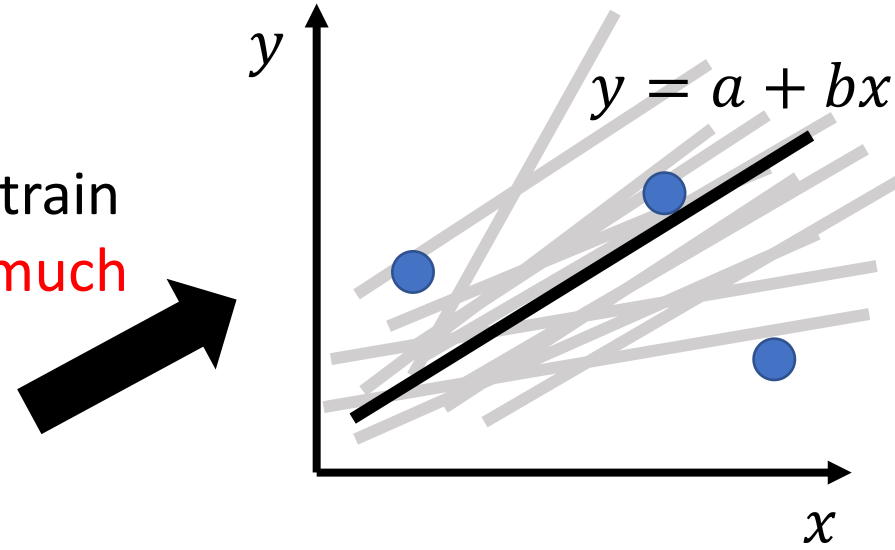
- Less parameters, sharing parameters
- Less features
- Early stopping
- Regularization
- Dropout

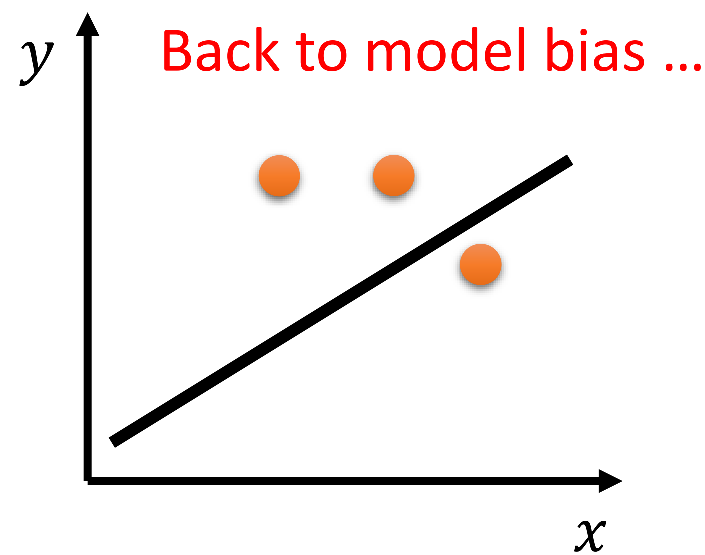


Overfitting



constrain
too much



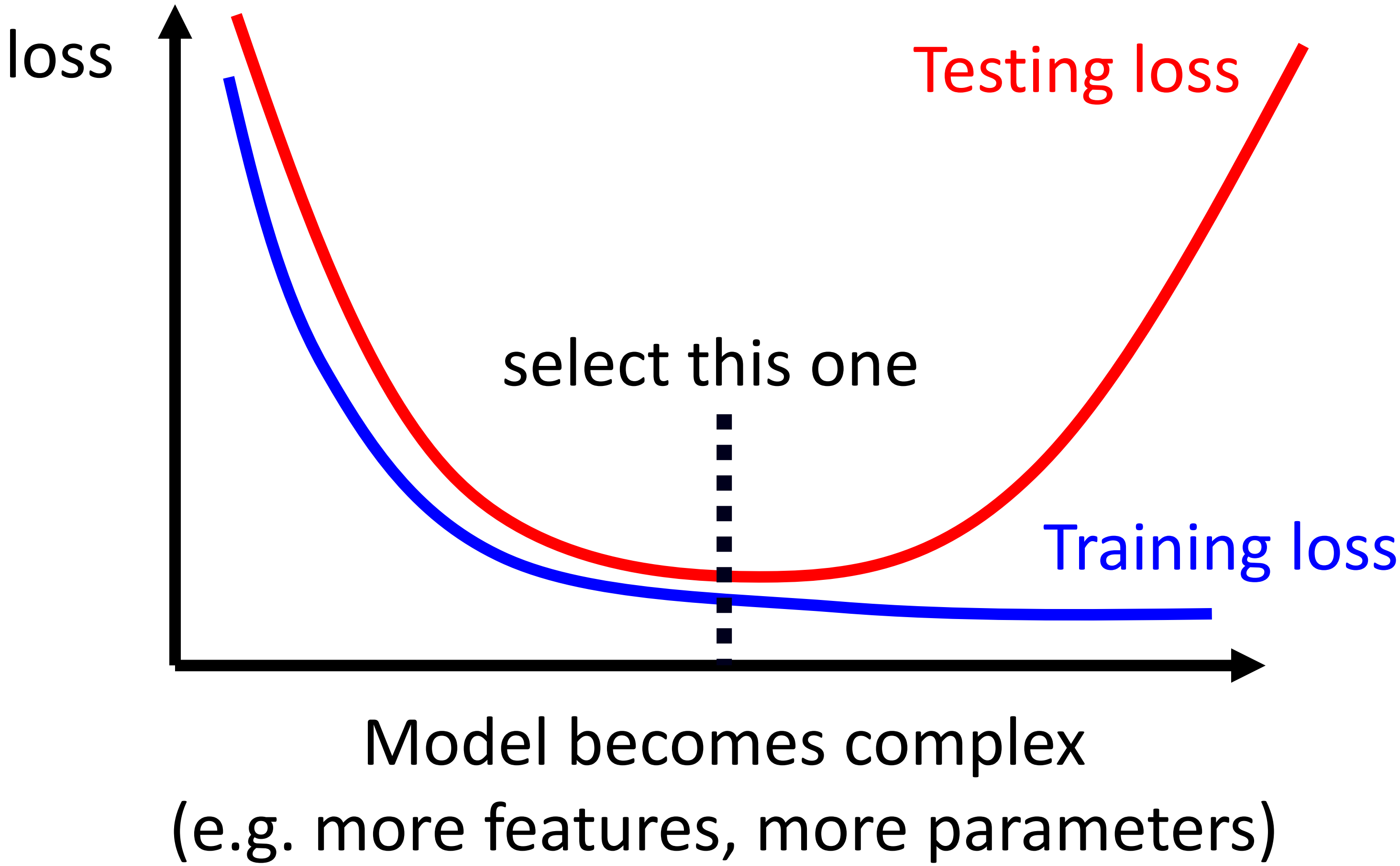


Real data distribution (not observable)

Training data

Testing data

Bias-Complexity Trade-off



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

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

奥卡姆剃刀

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

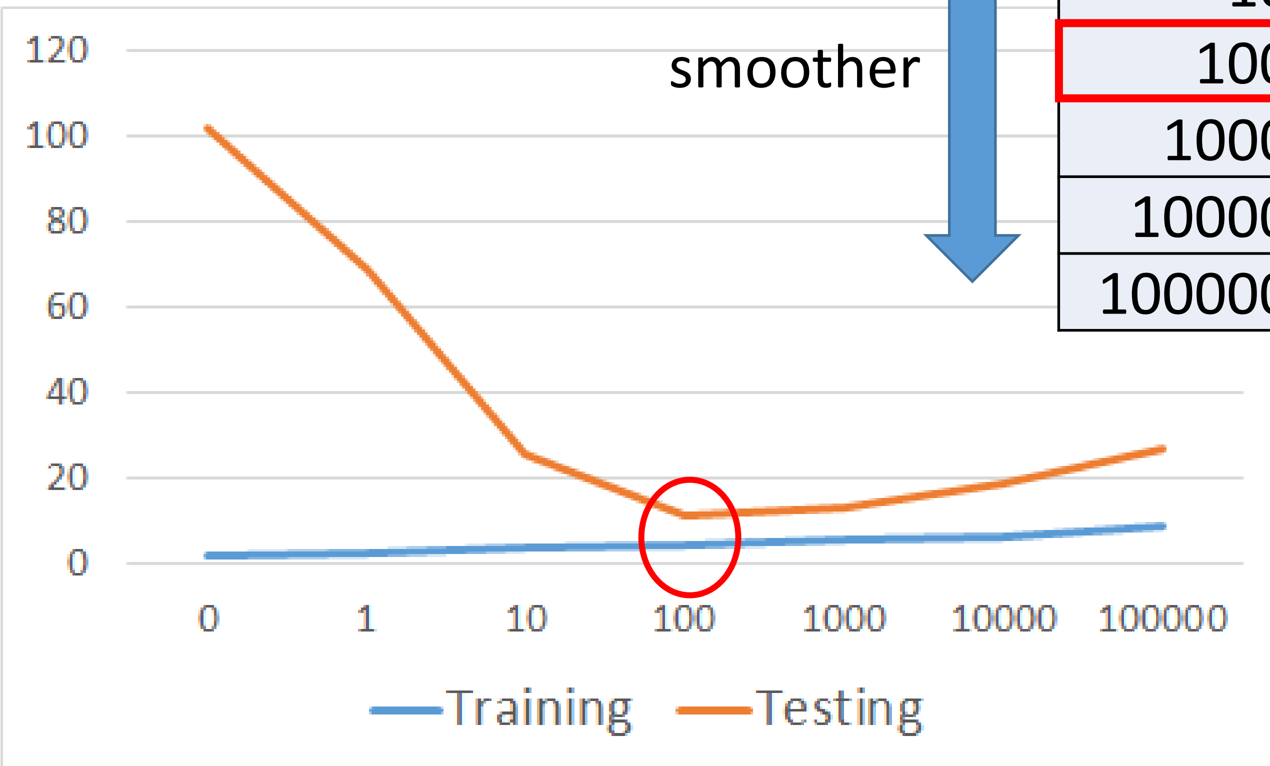
- We believe smoother function is more likely to be correct

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?

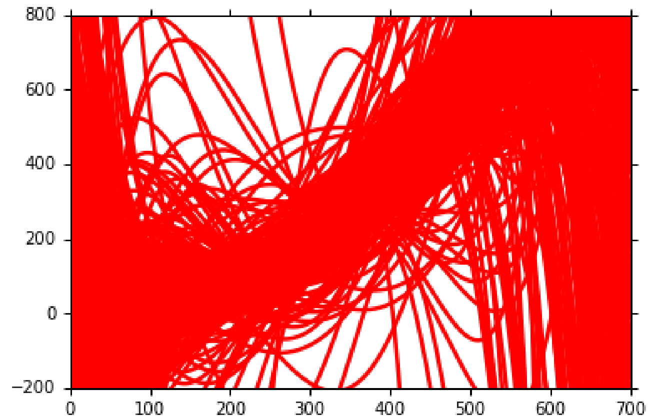
Select λ obtaining the best model

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

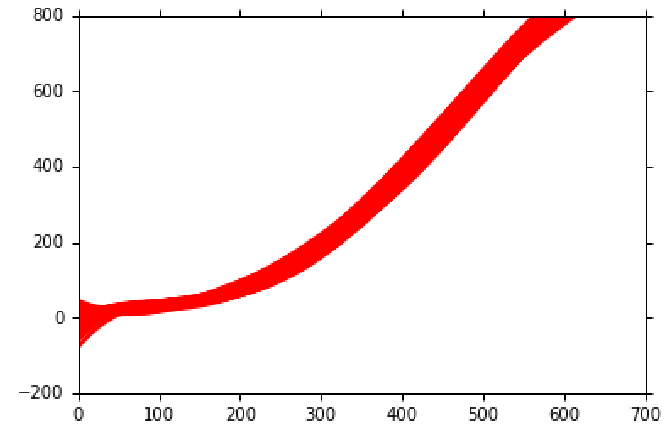
What to do with large variance?

- More data

Very effective, but not always practical



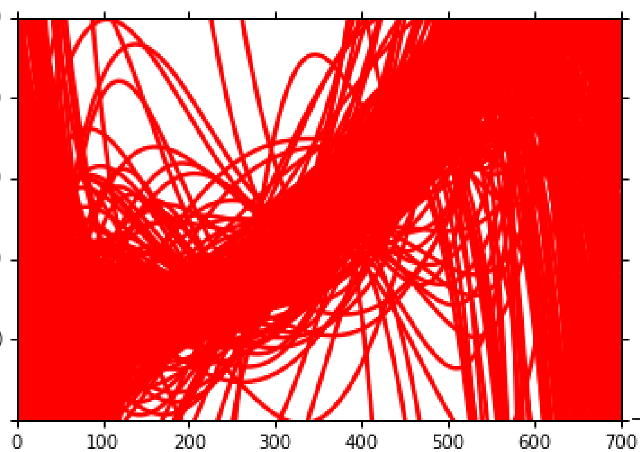
10 examples

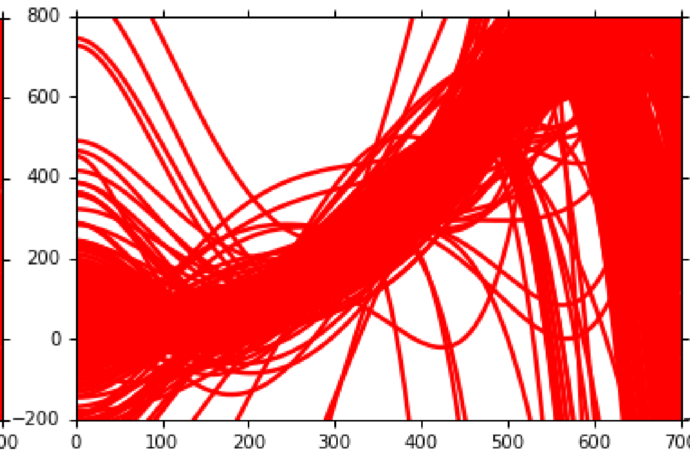


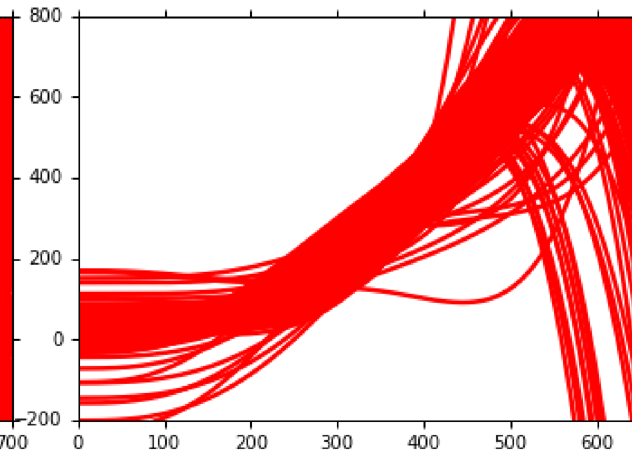
100 examples

- Regularization

May increase bias

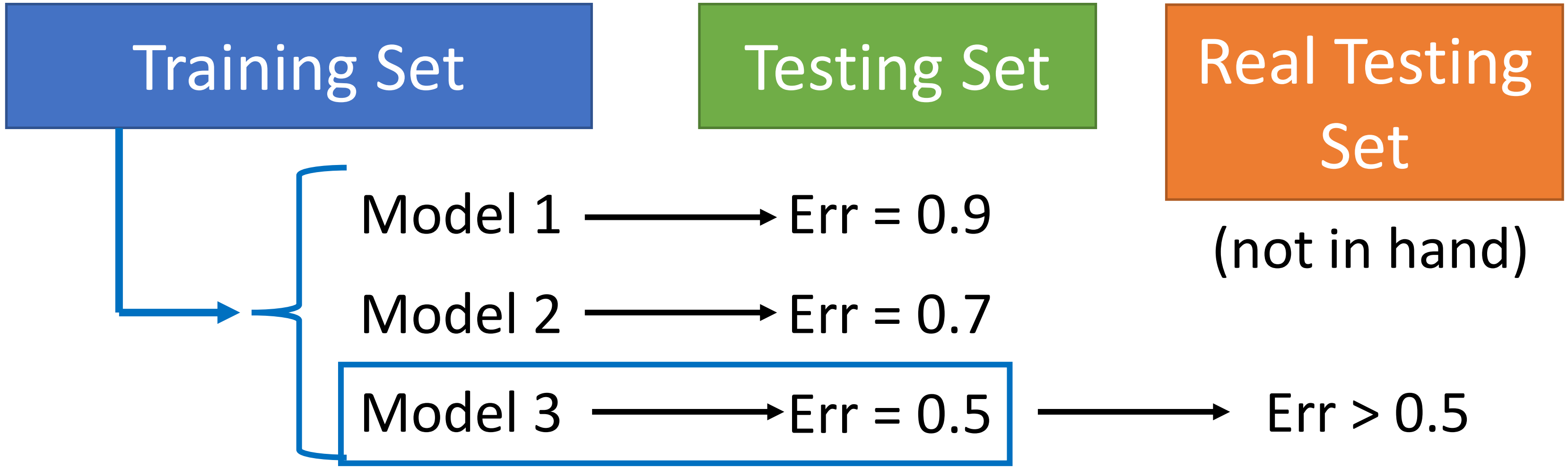






Model Selection

- There is usually a trade-off between bias and variance.
- Select a model that balances two kinds of error to minimize total error
- What you should NOT do:



Homework

public | private
Training Set | Testing Set | Testing Set

Model 1 → Err = 0.9

Model 2 → Err = 0.7

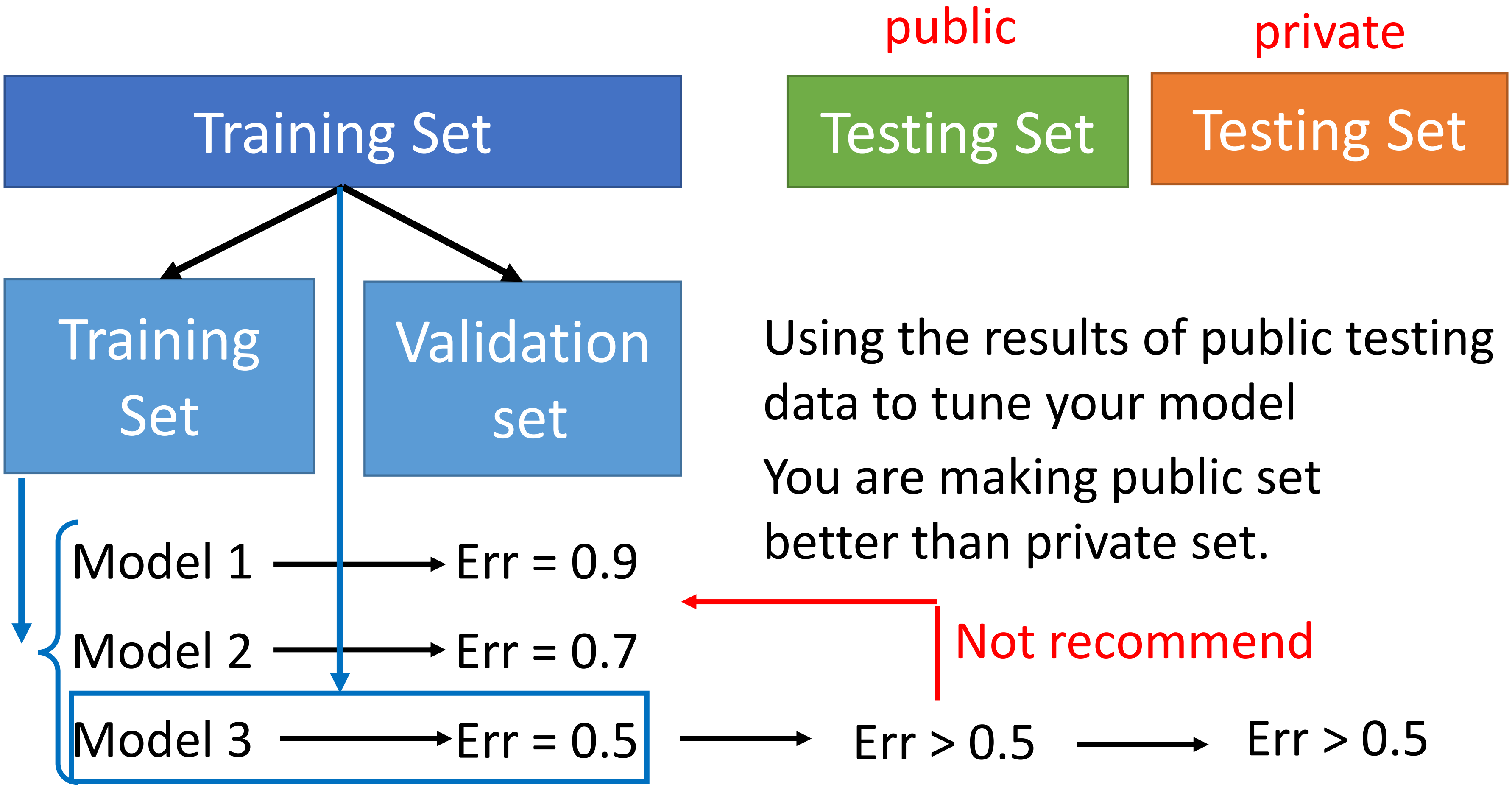
Model 3 → Err = 0.5 → Err > 0.5

I beat baseline! No, you don't

What will happen?

http://www.chioka.in/how-to-select-your-final-models-in-a-kaggle-competitio/

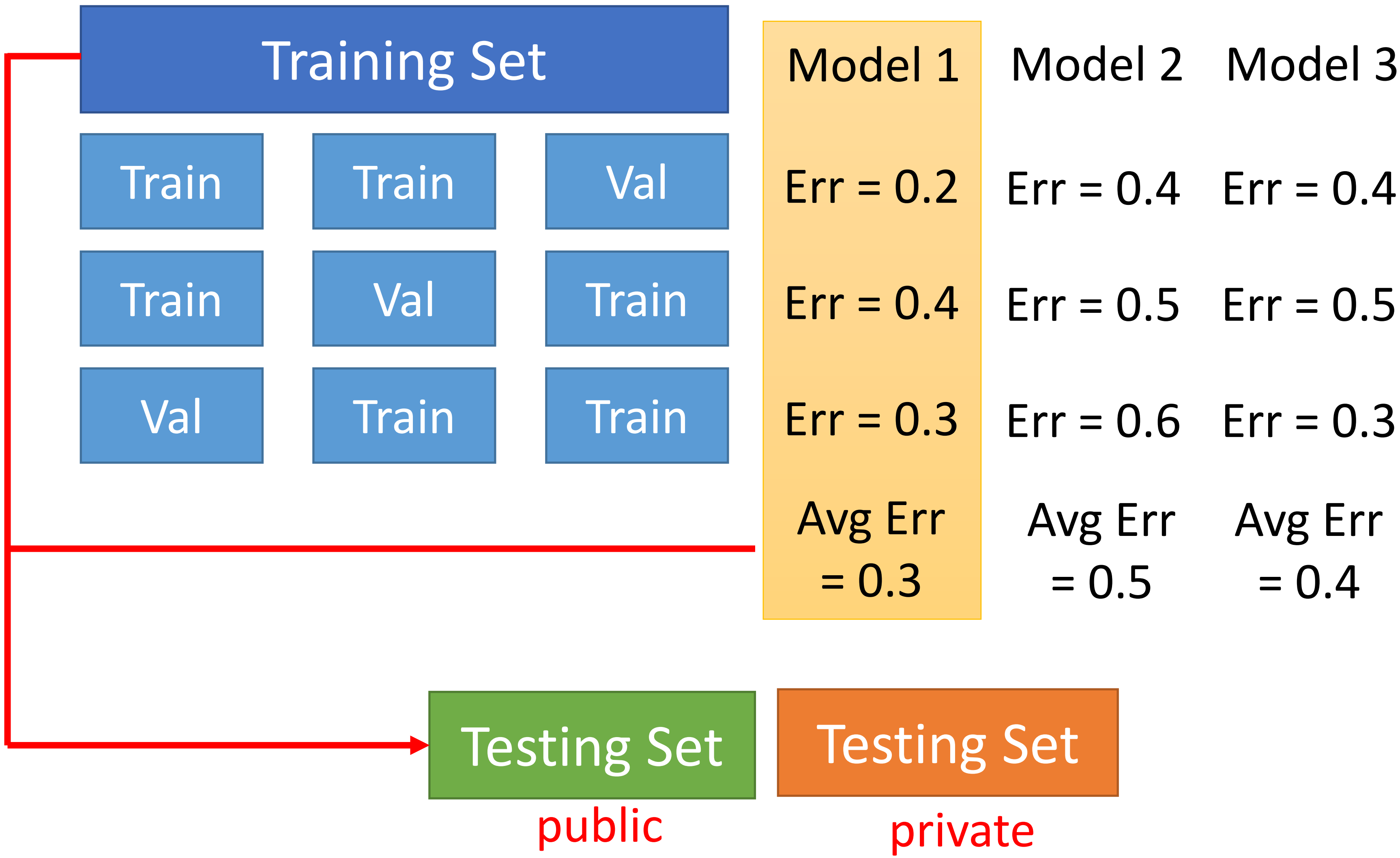
Cross Validation



Using the results of public testing data to tune your model

You are making public set better than private set.

N-fold Cross Validation



More about Validation Set

I used a validation set,

but my model still overfitted?

Validation Set

Training Set $\mathcal{D}_{train}$

Validation Set $\mathcal{D}_{val}$

Model $\mathcal{H}_1$ $\quad h_1^* = arg \min_{h \in \mathcal{H}_1} L(h, \mathcal{D}_{train})$ $\quad L(h_1^*, \mathcal{D}_{val}) = 0.9$

Model $\mathcal{H}_2$ $\quad h_2^* = arg \min_{h \in \mathcal{H}_2} L(h, \mathcal{D}_{train})$ $\quad L(h_2^*, \mathcal{D}_{val}) = 0.7$

Model $\mathcal{H}_3$ $\quad h_3^* = arg \min_{h \in \mathcal{H}_3} L(h, \mathcal{D}_{train})$ $\quad \boxed{L(h_3^*, \mathcal{D}_{val}) = 0.5}$

Testing Set $\mathcal{D}_{test}$

Approximation of $\mathcal{D}_{all}$

Training Set $\mathcal{D}_{train}$

Validation Set $\mathcal{D}_{val}$

Model $\mathcal{H}_1$ $\quad h_1^* = arg \min_{h \in \mathcal{H}_1} L(h, \mathcal{D}_{train})$ $\quad L(h_1^*, \mathcal{D}_{val}) = 0.9$

Model $\mathcal{H}_2$ $\quad h_2^* = arg \min_{h \in \mathcal{H}_2} L(h, \mathcal{D}_{train})$ $\quad L(h_2^*, \mathcal{D}_{val}) = 0.7$

Model $\mathcal{H}_3$ $\quad h_3^* = arg \min_{h \in \mathcal{H}_3} L(h, \mathcal{D}_{train})$ $\quad \boxed{L(h_3^*, \mathcal{D}_{val}) = 0.5}$

$$\mathcal{H}_{val} = \{h_1^*, h_2^*, h_3^*\} \qquad h^* = arg \min_{h \in \mathcal{H}_{val}} L(h, \mathcal{D}_{val})$$

Using validation set to select model =

considered as "*training*" by $\mathcal{D}_{val}$

Your model is $\mathcal{H}_{val} = \{h_1^*, h_2^*, h_3^*\}$

Using validation set to select model =

considered as "*training*" by $\mathcal{D}_{val}$

Your model is $\mathcal{H}_{val} = \{h_1^*, h_2^*, h_3^*\}$

$$L(h^{train}, \mathcal{D}_{all}) - L(h^{all}, \mathcal{D}_{all}) \leq \delta$$

$$P(\mathcal{D}_{train}\ is\ \boldsymbol{bad}) \leq |\mathcal{H}| \cdot 2exp(-2N\varepsilon^2)$$

$$L(h^{val}, \mathcal{D}_{all}) - L(h^{all}, \mathcal{D}_{all}) \leq \delta$$

$$P(\mathcal{D}_{val}\ is\ \boldsymbol{bad}) \leq |\mathcal{H}_{val}| \cdot 2exp(-2N_{val}\varepsilon^2)$$

It is small.

Hopefully …… ☺