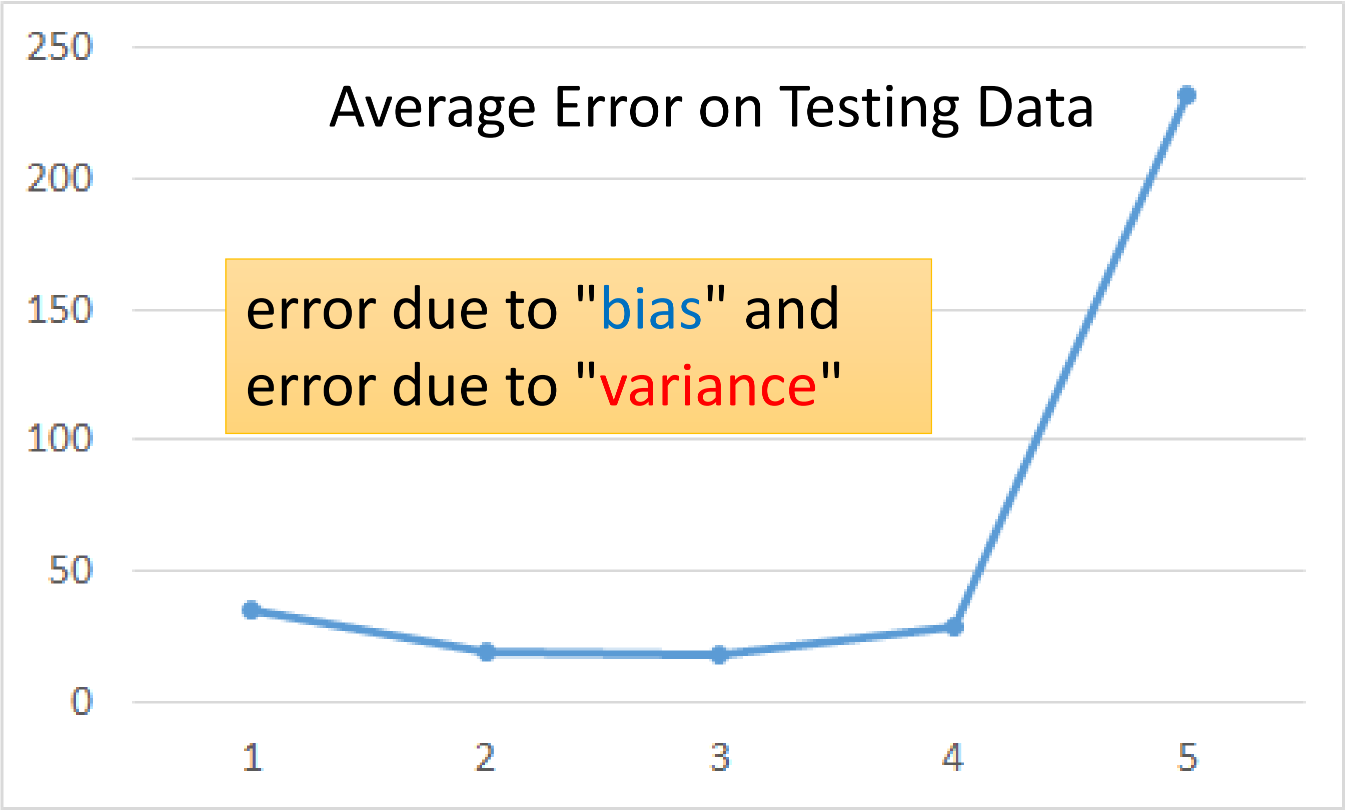
Where does the error come from?

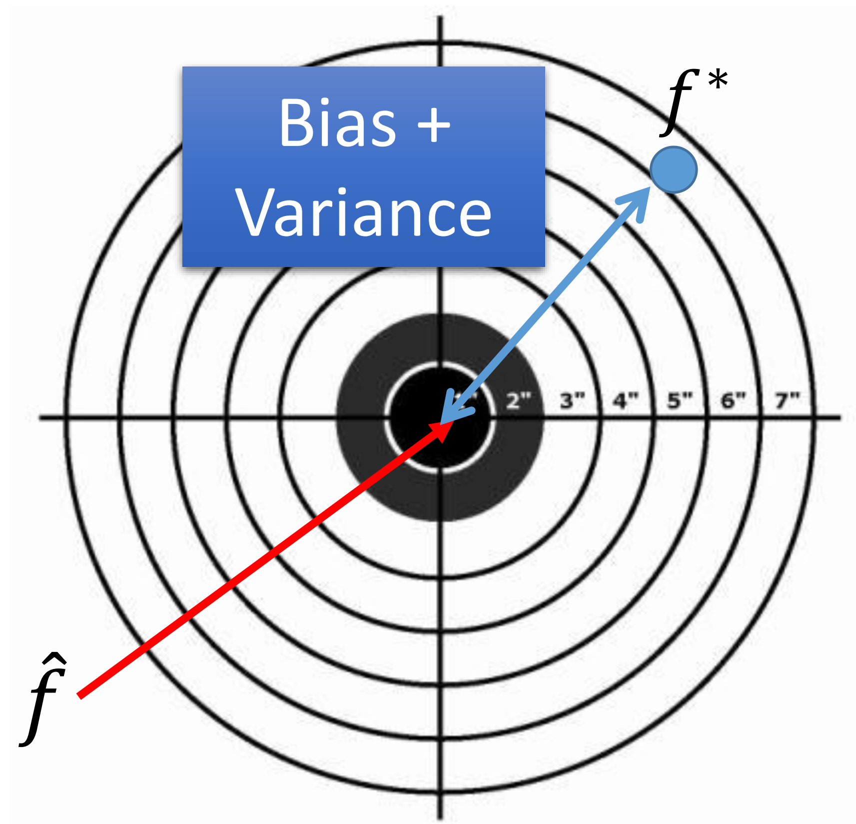
Review



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^*

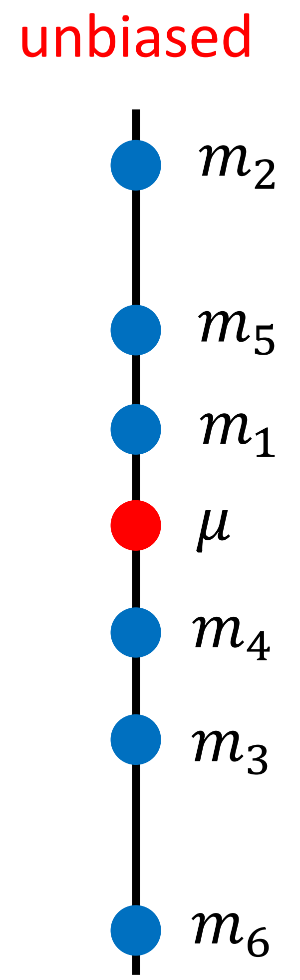
f^* is an estimator of $\hat{f}$

Bias and Variance of Estimator

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

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

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



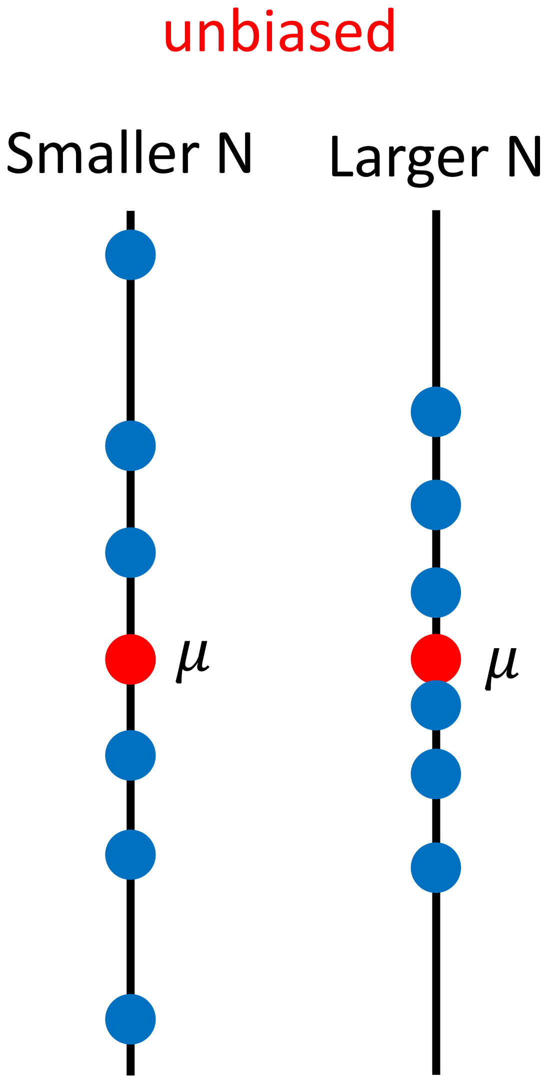
Bias and Variance of Estimator

- 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: $\{x^1, x^2, \dots, x^N\}$

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

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

Variance depends on the number of samples



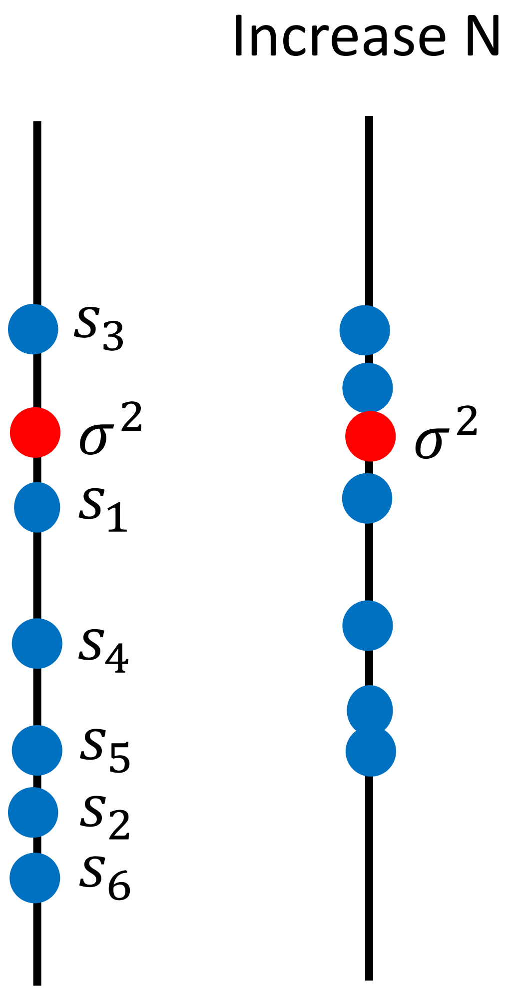
Bias and Variance of Estimator

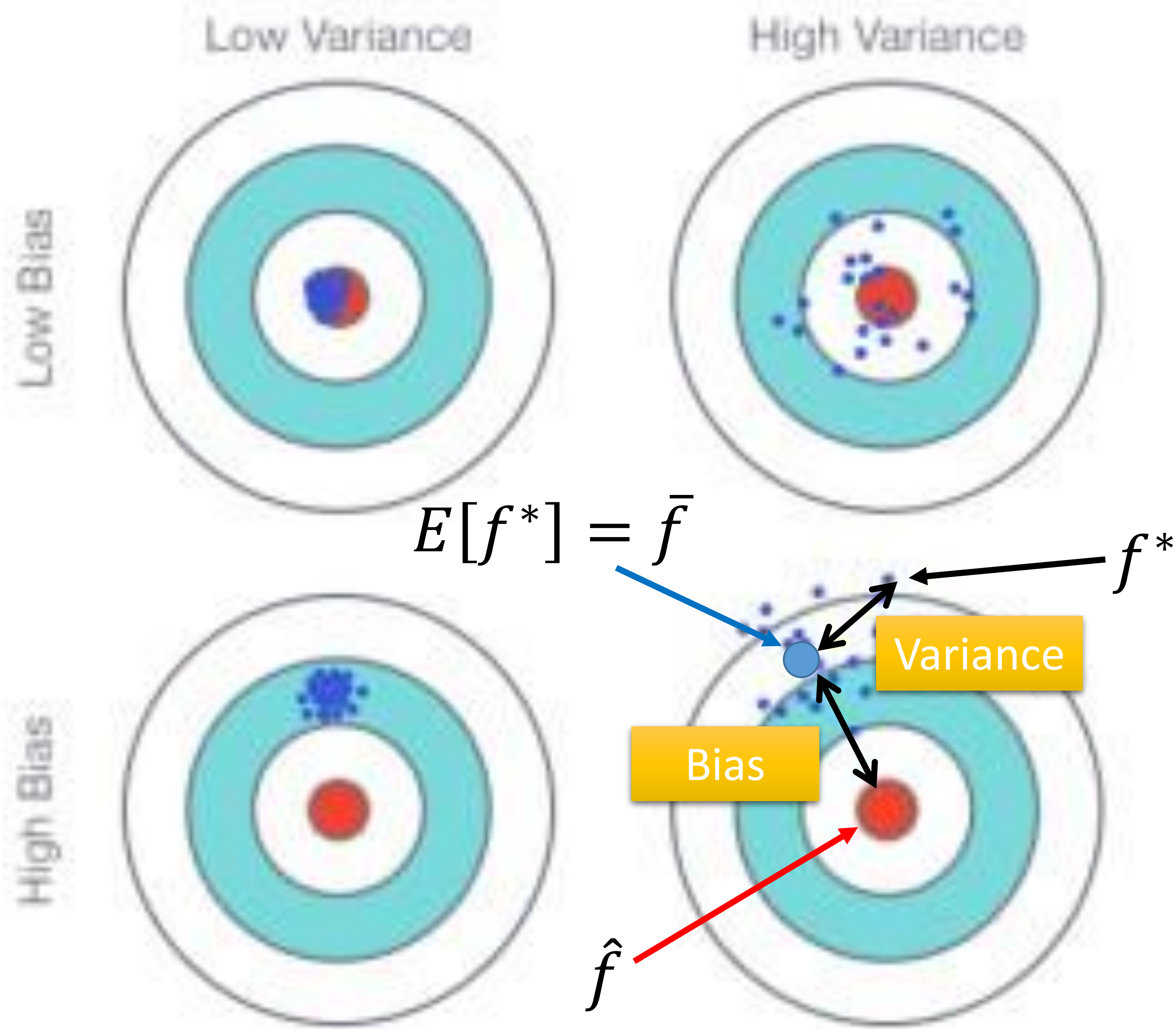
- Estimate the mean of a variable x
  - assume the mean of x is μ
  - assume the variance of x is σ^2
- Estimator of variance σ^2
  - Sample N points: $\{x^1, x^2, \ldots, x^N\}$

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

Biased estimator

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



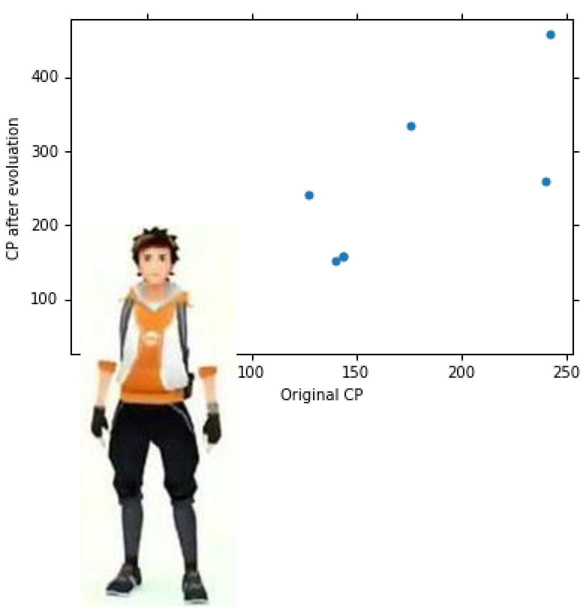


Low Variance
High Variance
Low Bias
High Bias
$E[f^*] = \bar{f}$
f^*
Variance
Bias
$\hat{f}$

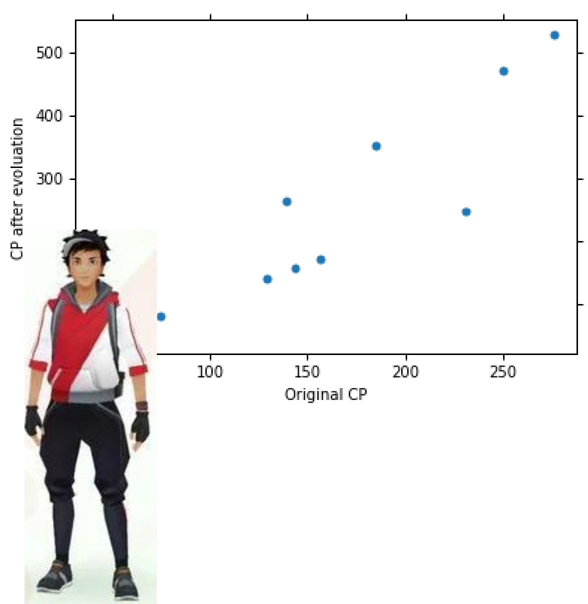
Parallel Universes

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

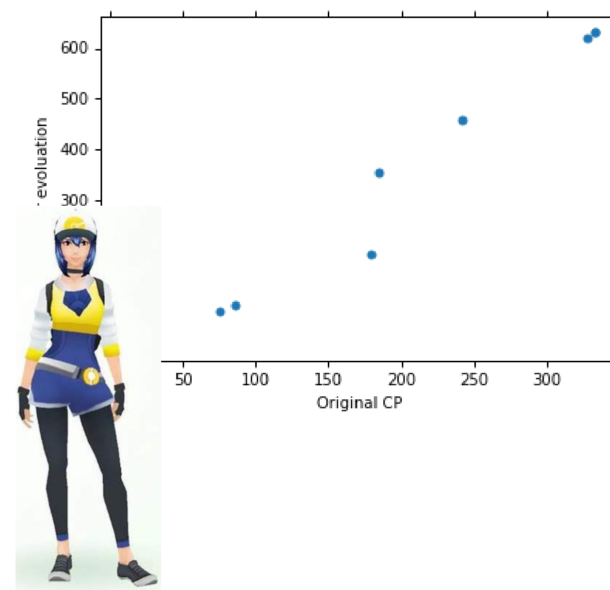
Universe 1



Universe 2



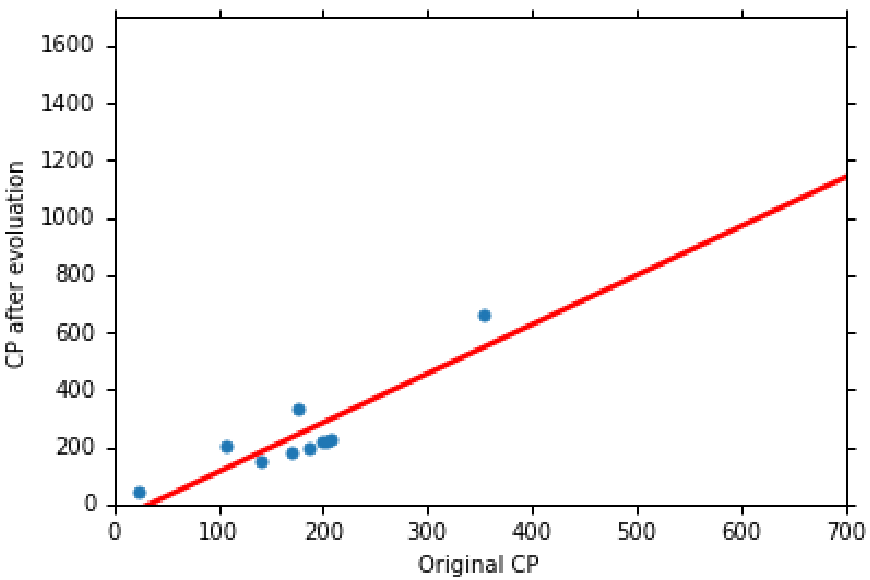
Universe 3



Parallel Universes

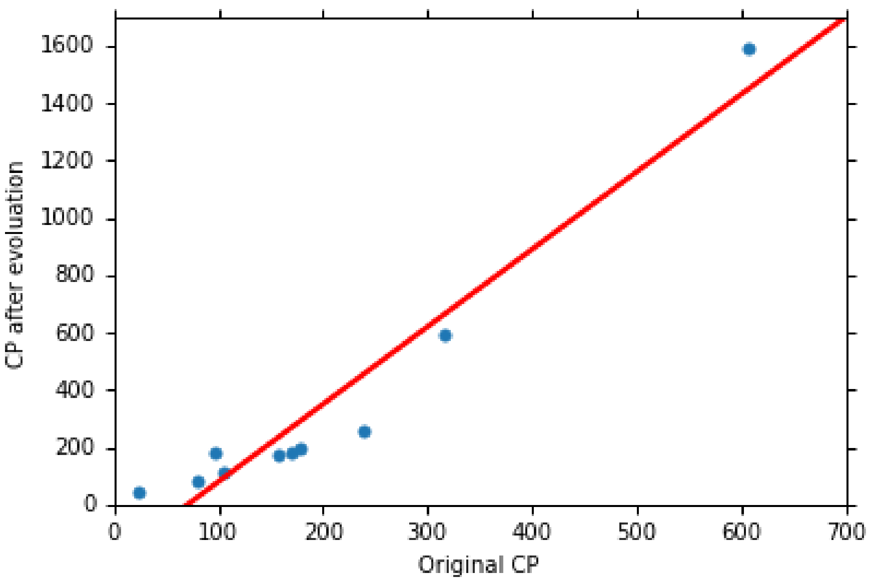
- In different universes, we use the same model, but obtain different f^*

Universe 123



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

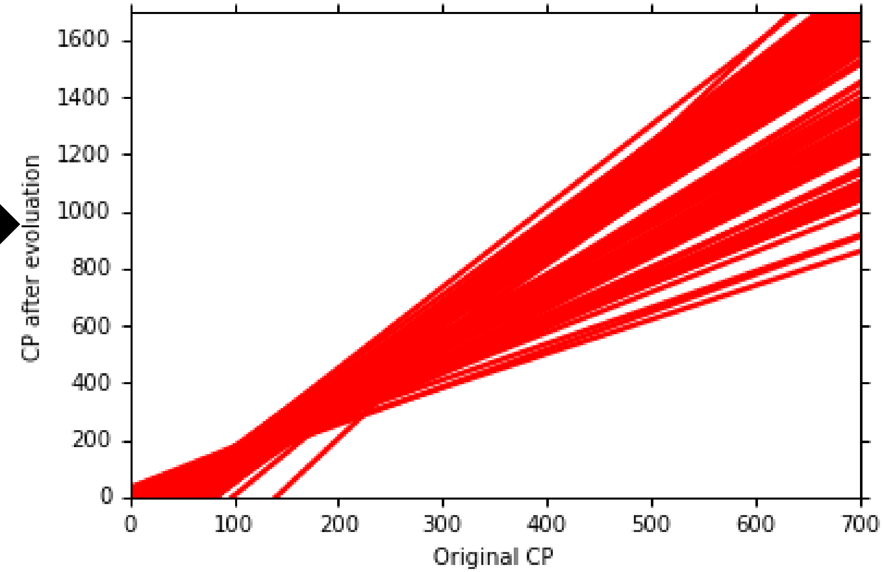
Universe 345



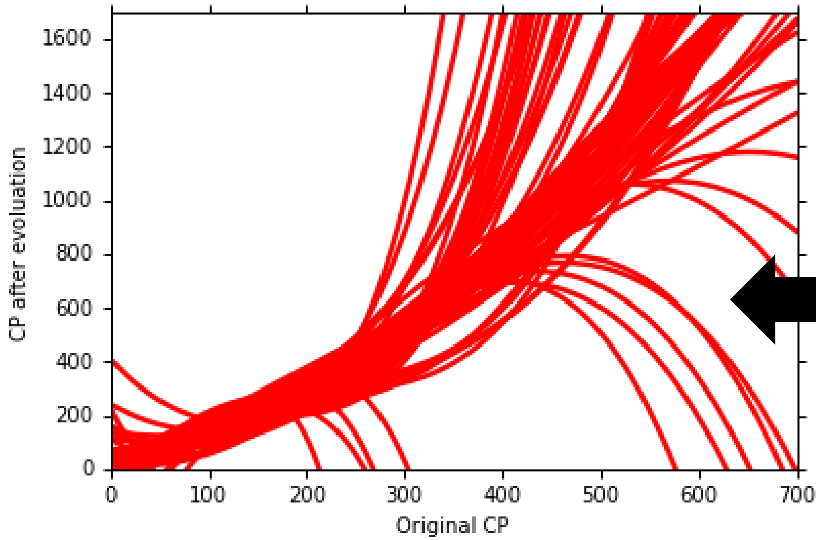
$y = b + w \cdot x_{cp}$

f^* in 100 Universes

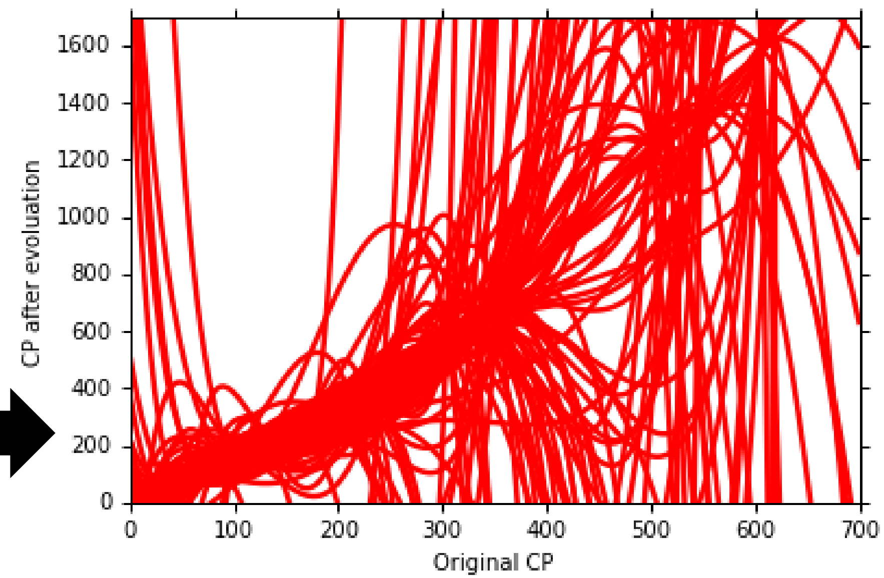
$$y = b + w \cdot x_{cp}$$



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

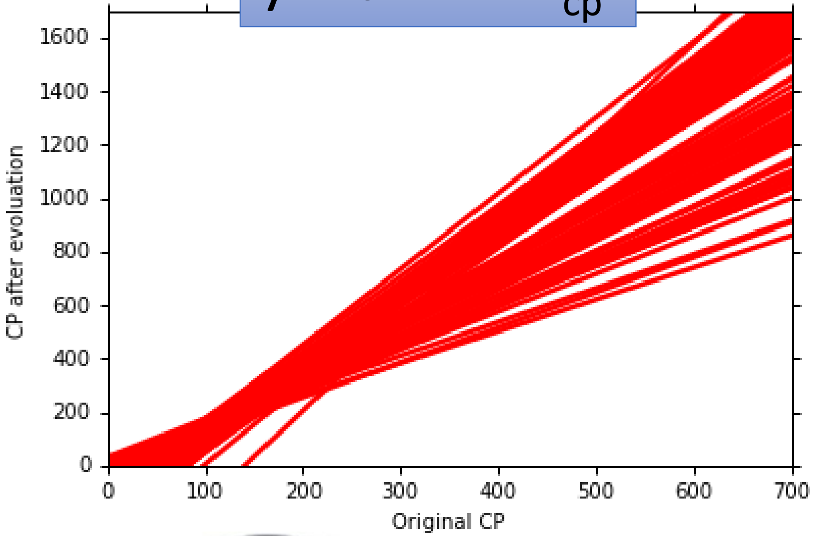


$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$

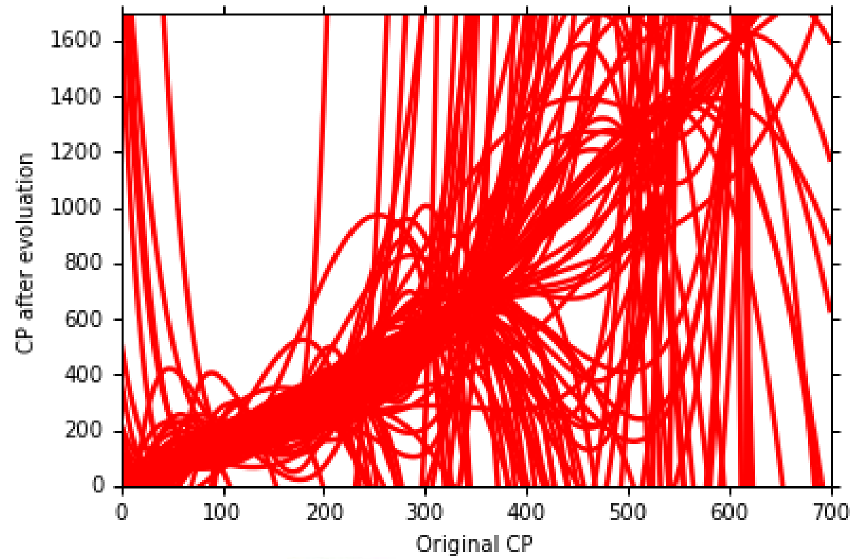


Variance

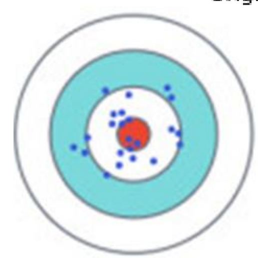
$y = b + w \cdot x_{cp}$



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



Small Variance



Large Variance

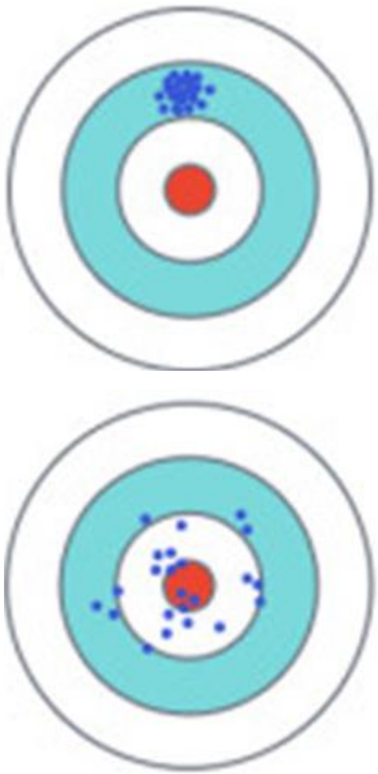
Simpler model is less influenced by the sampled data

Consider the extreme case f(x) = 5

Bias

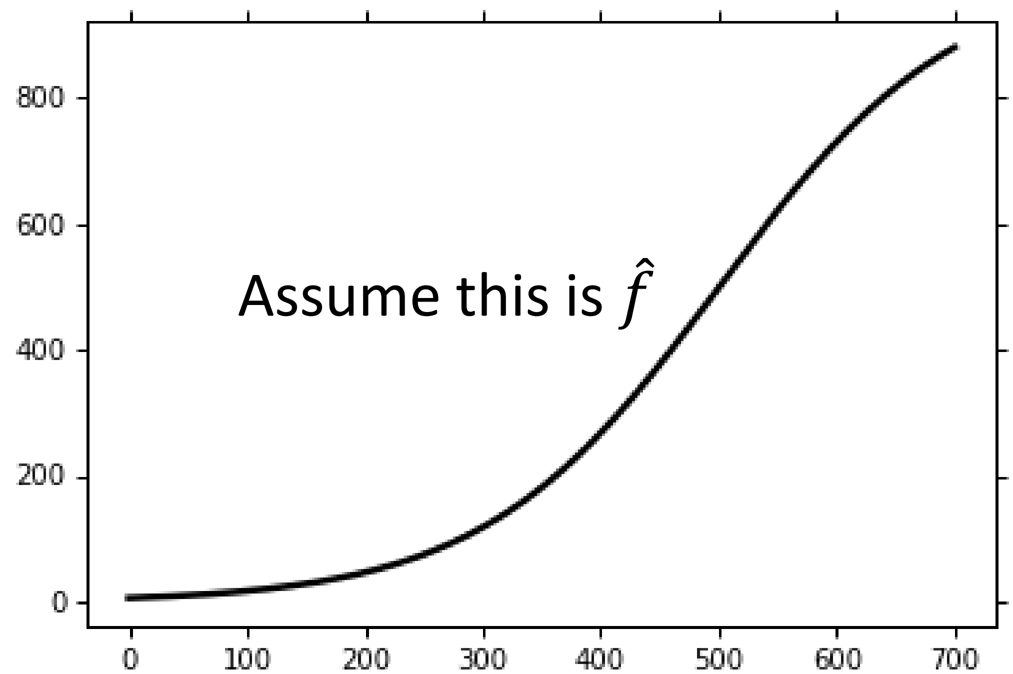
$$E[f^*] = \bar{f}$$

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



Large Bias

Small Bias

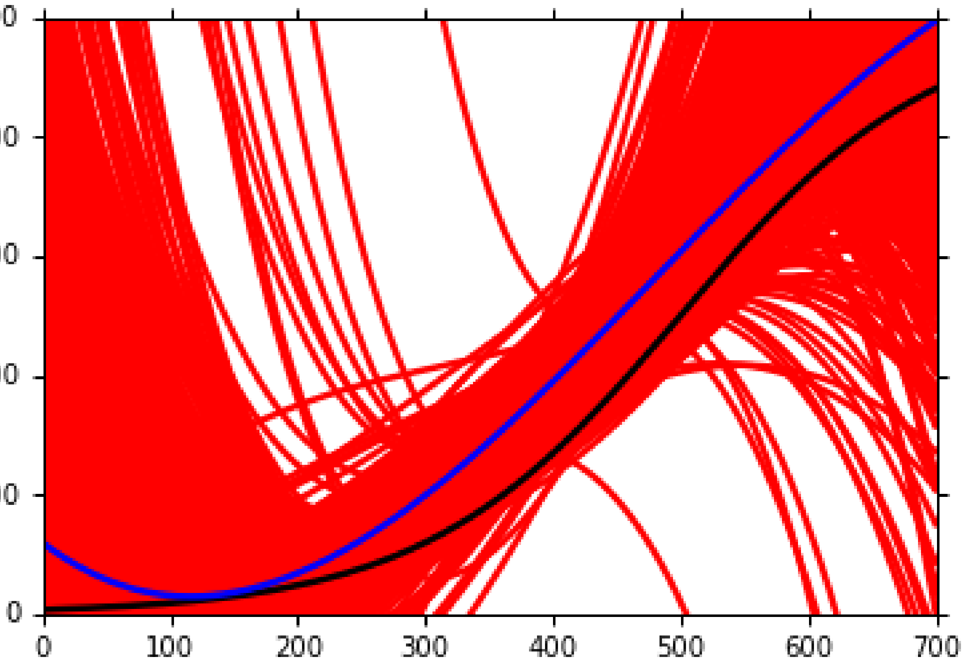


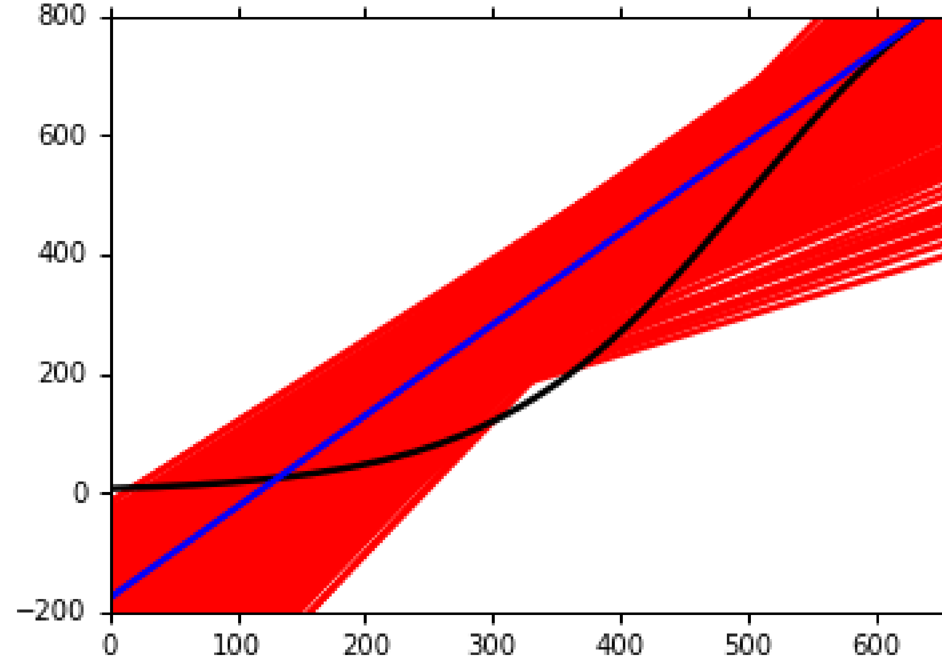
Black curve: the true function $\hat{f}$

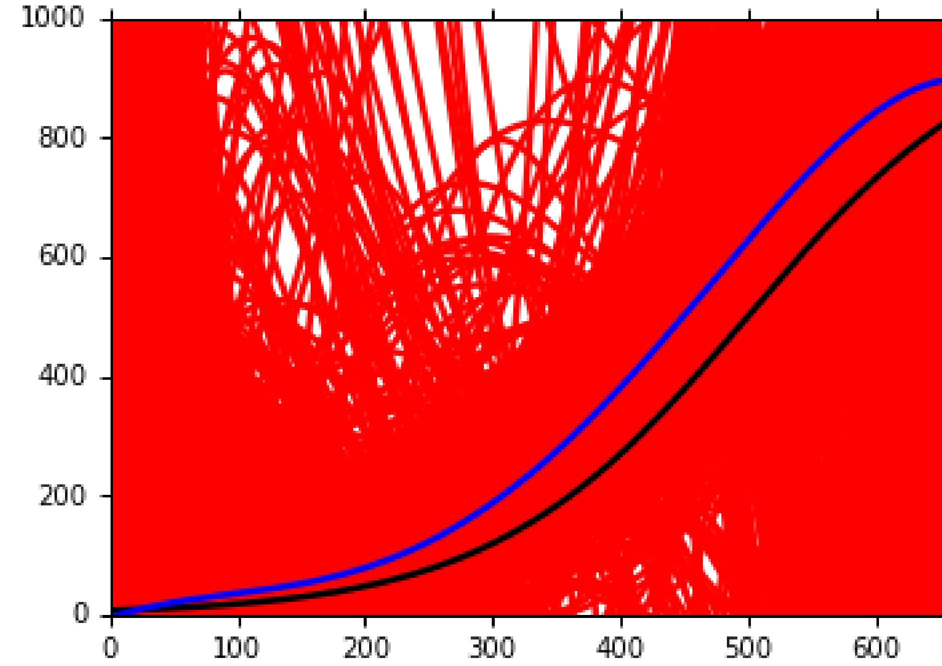
Red curves: 5000 f^*

Blue curve: the average of 5000 f^*

$= \bar{f}$



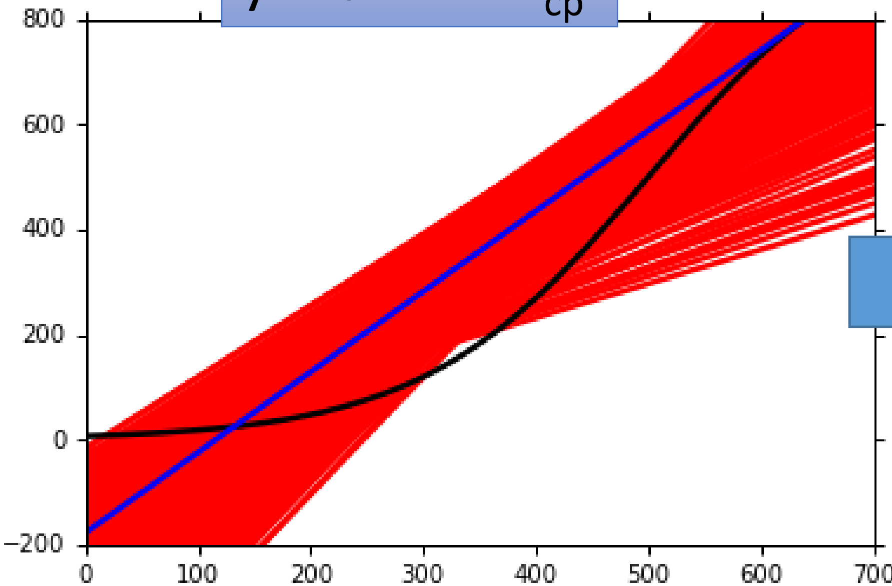


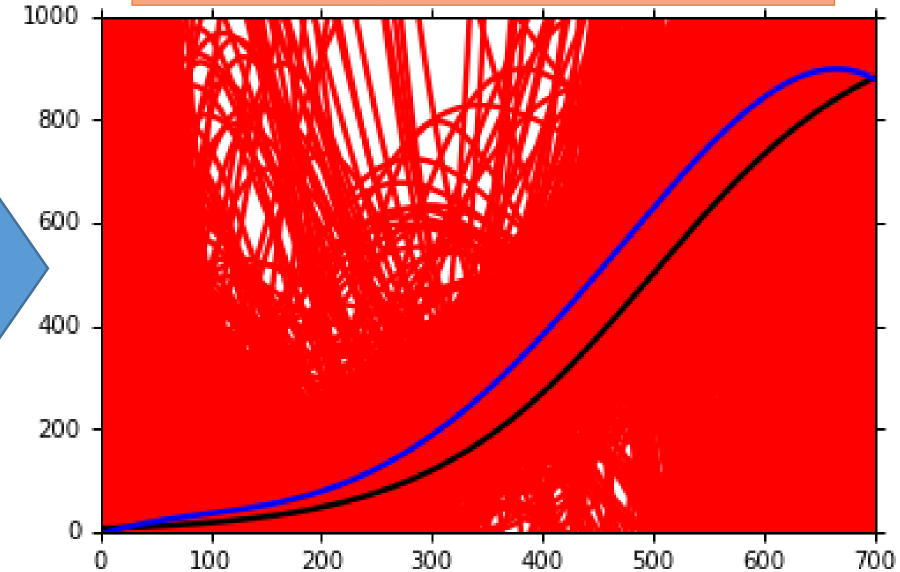


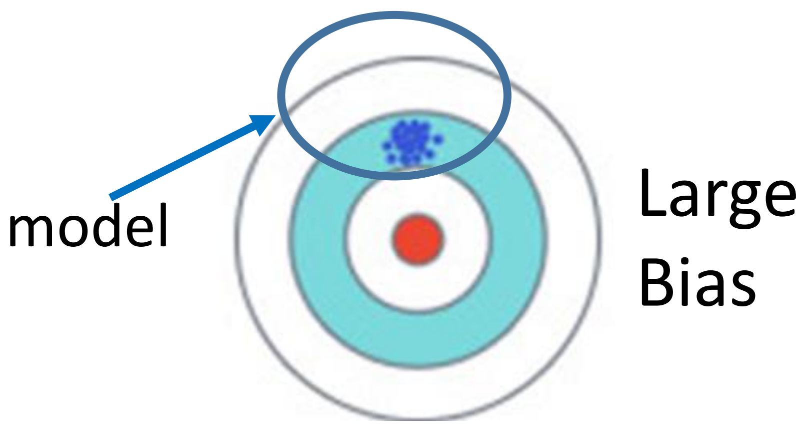
Bias

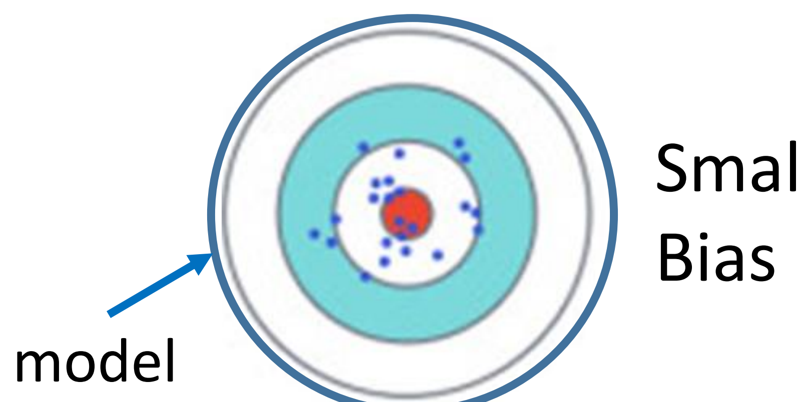
$$y = b + w_1 \cdot x_{cp} + w_2 \cdot (x_{cp})^2 + w_3 \cdot (x_{cp})^3 + w_4 \cdot (x_{cp})^4 + w_5 \cdot (x_{cp})^5$$

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

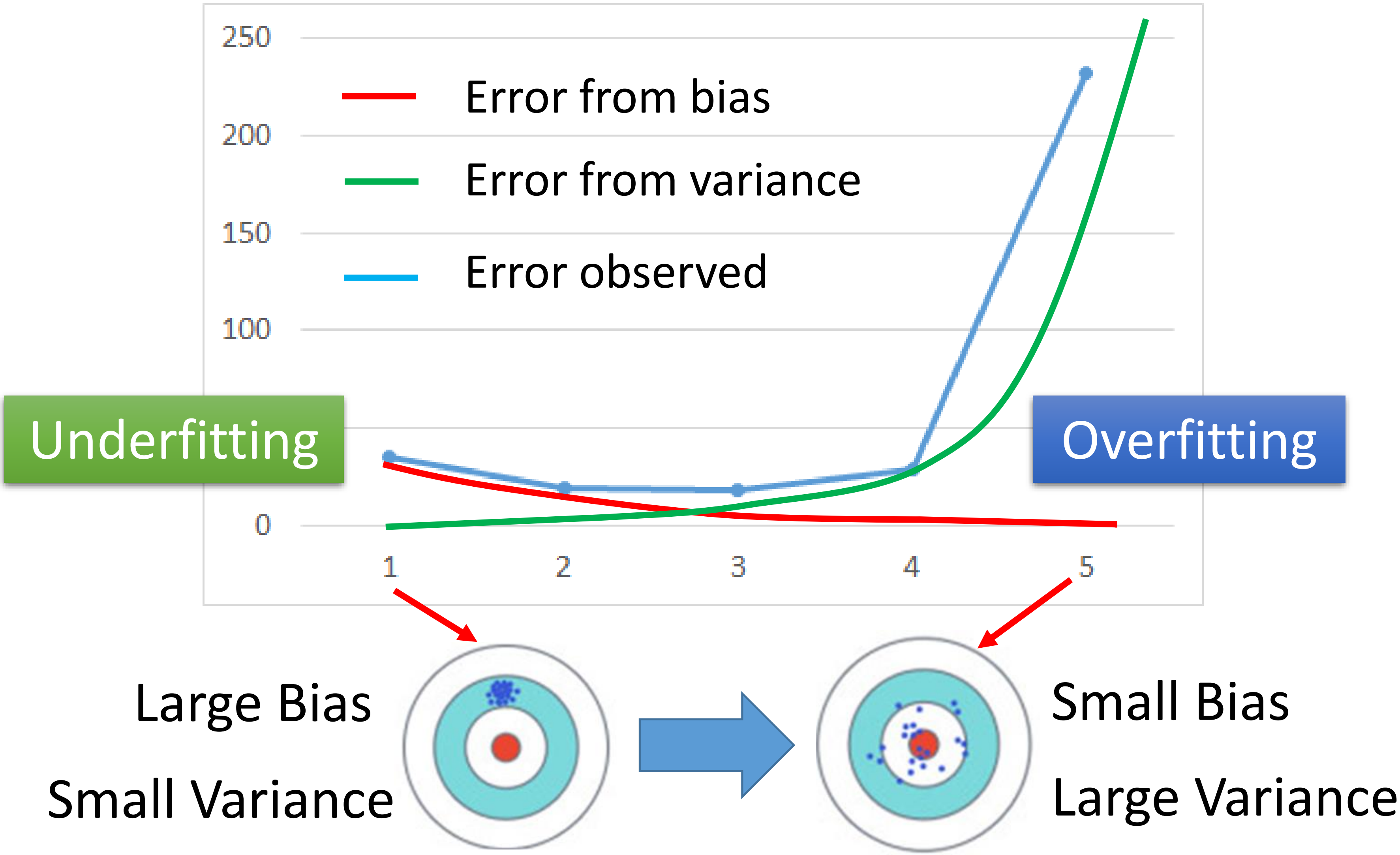






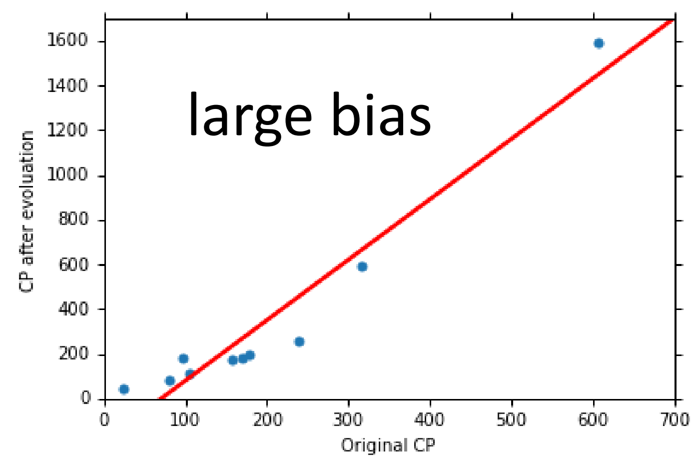


Bias v.s. Variance



What to do with large bias?

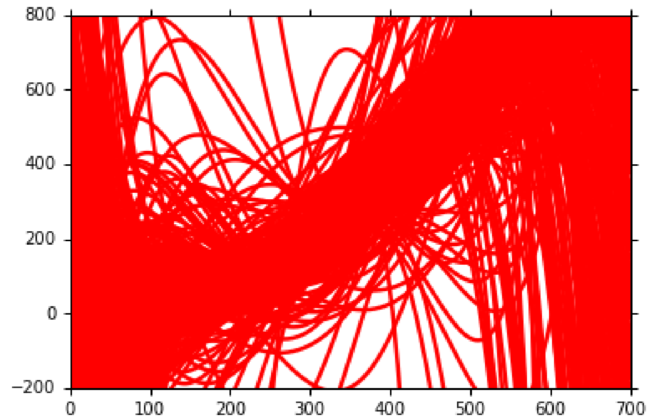
- Diagnosis:
  - If your model cannot even fit the training examples, then you have large bias **Underfitting**
  - If you can fit the training data, but large error on testing data, then you probably have large variance **Overfitting**
- For bias, redesign your model:
  - Add more features as input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



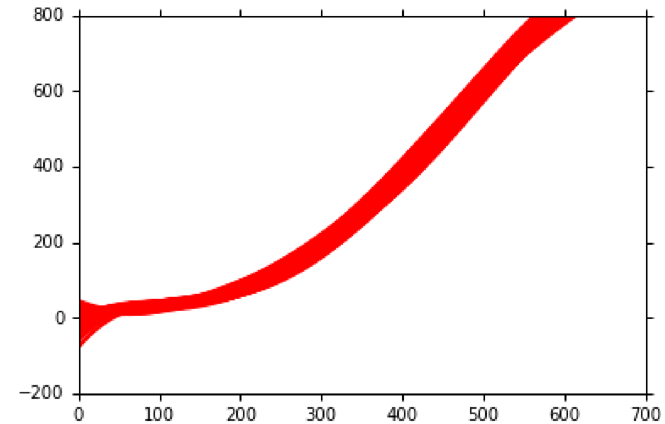
What to do with large variance?

- More data

Very effective, but not always practical



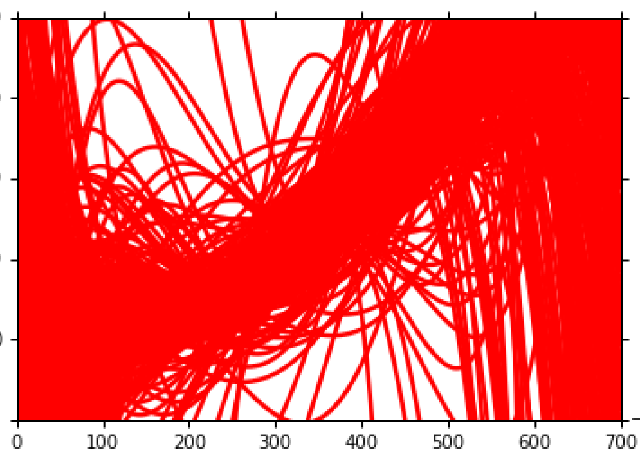
10 examples

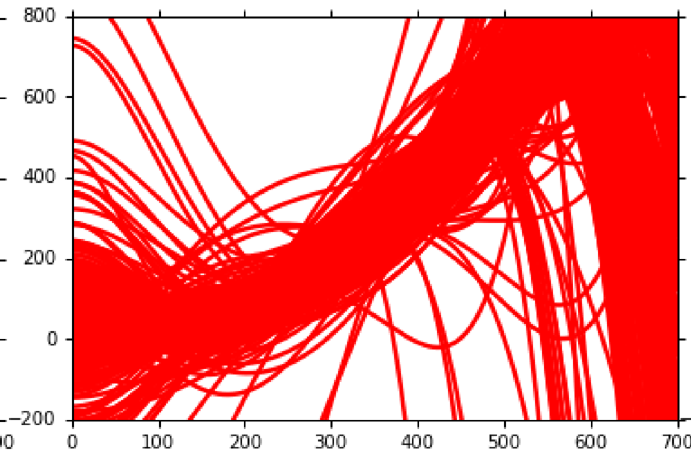


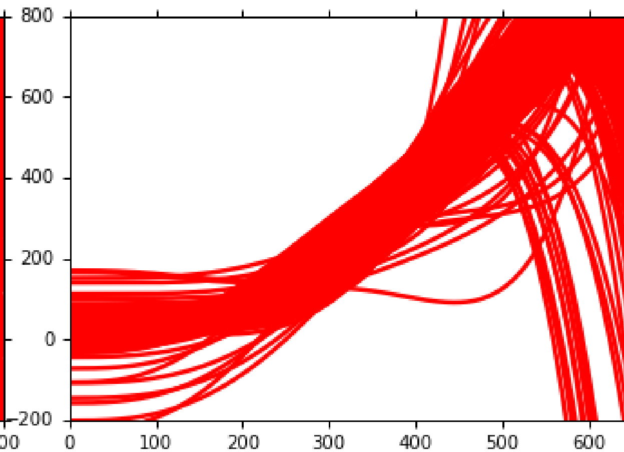
100 examples

- Regularization

May increase bias

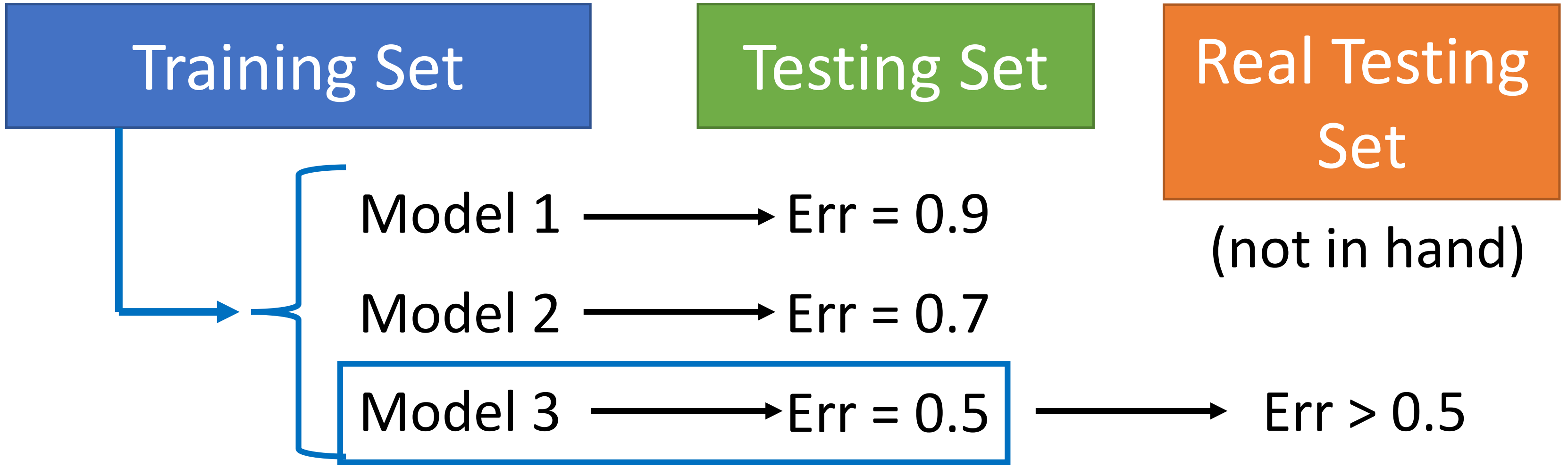






Model Selection

- 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

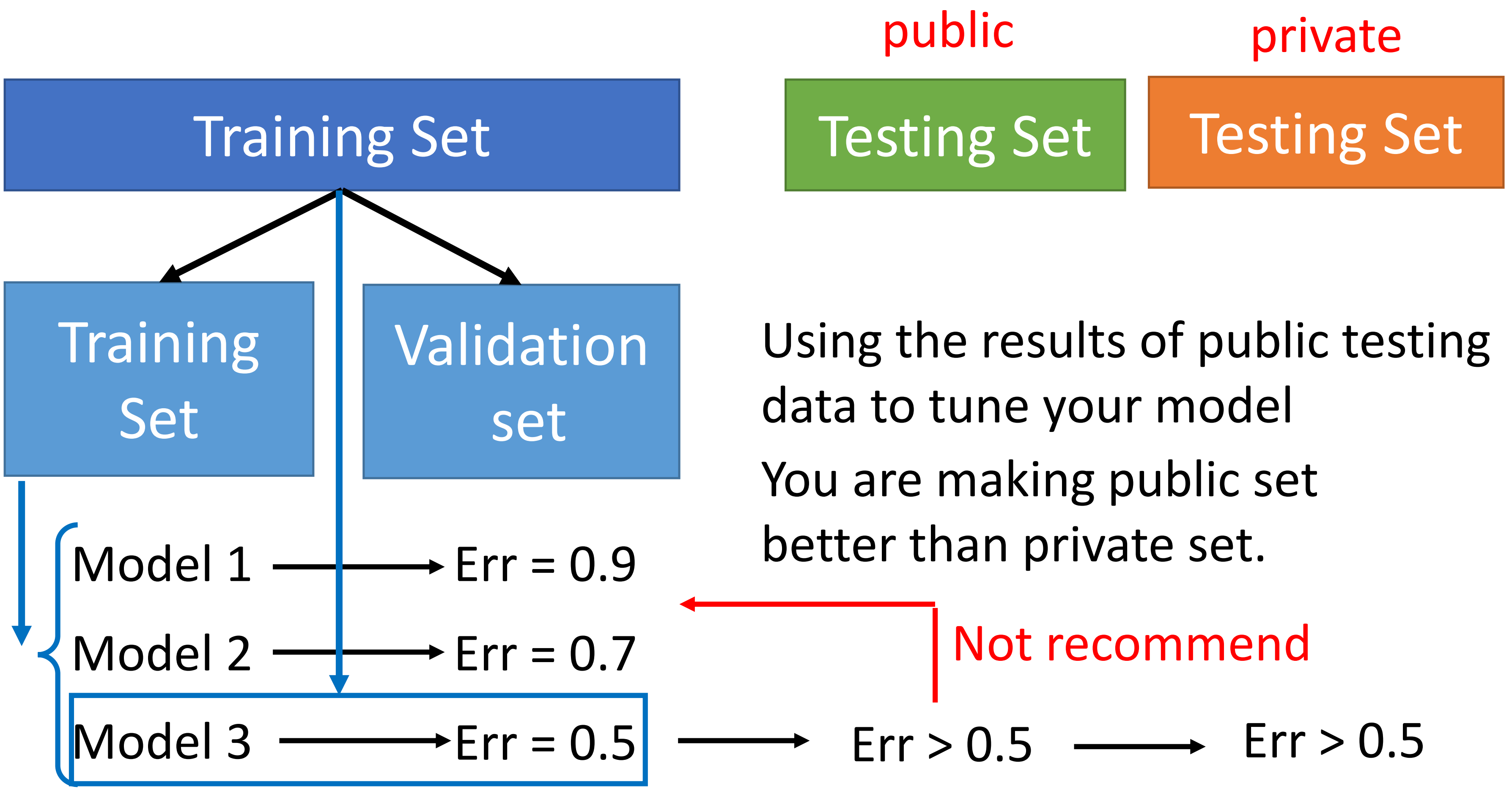
I beat baseline!

No, you don't

What will happen?

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

Model Selection Do and Don’t



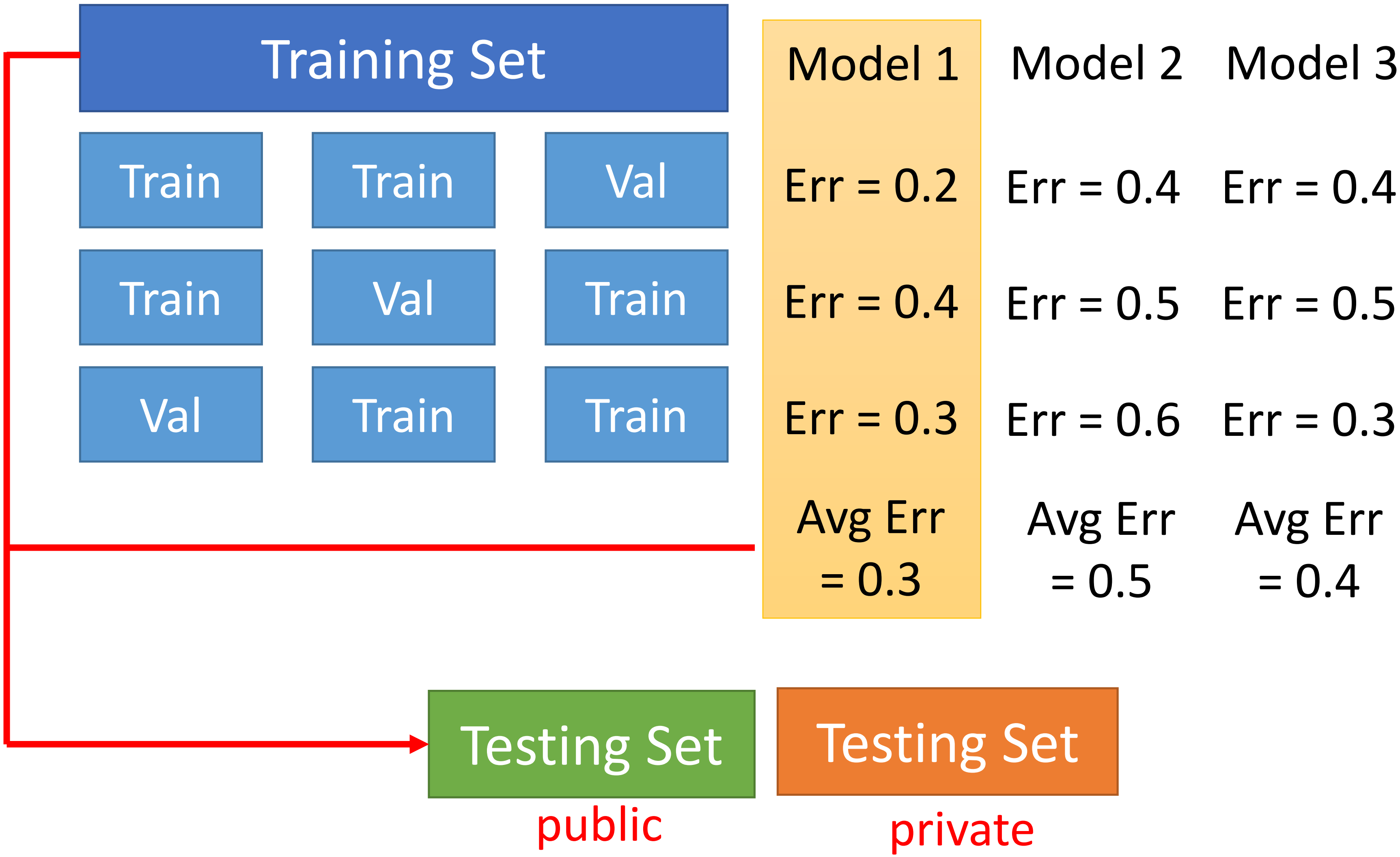
Using the results of public testing data to tune your model

You are making public set better than private set.

Testing data should never involve in model training nor model selection!!

K-fold Cross Validation

3-fold cross validation



Leave One Out (LOO) Cross Validation

Definition 1. *Let H be a family of functions mapping from input space $\mathcal{X}$ to output space $\mathcal{Y}$. Define the Leave One Out (LOO) cross validation error of algorithm $\mathcal{A} : \bigcup_{m \in \mathbb{N}} (\mathcal{X} \times \mathcal{Y})^m \to H$ on sample $S = ((x_i, y_i))_{i=1}^m \in (\mathcal{X} \times \mathcal{Y})^m$ as*

$$\hat{\mathcal{R}}_S^{LOO}(\mathcal{A}) = \frac{1}{m} \sum_{i=1}^{m} \ell(h_{S_i}(x_i), y_i)$$

where $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_{\geq 0}$ is the loss function, $S_i = S \setminus \{(x_i, y_i)\}$, $h_{S_i} = \mathcal{A}(S_i)$.

Unbiased Estimation of Testing Error

Theorem 2. *Let H be a family of functions mapping from input space $\mathcal{X}$ to output space $\mathcal{Y}$, and let $\mathcal{A} : \bigcup_{m\in\mathbb{N}}(\mathcal{X}\times\mathcal{Y})^m \to H$. Let D be the unknown underlying distribution on $\mathcal{X}\times\mathcal{Y}$, then*

$$\mathbb{E}_{S\sim D^m}[\hat{\mathcal{R}}_S^{LOO}(\mathcal{A})] = \mathbb{E}_{S'\sim D^{m-1},(x,y)\in D}[\ell(\mathcal{A}(S')(x), y)]$$

In other words, LOO cross validation (on m instances) is an unbiased estimate of the algorithm's testing error (after training on $m-1$ instances).

Proof. For $S = ((x_i, y_i))_{i=1}^m \in (\mathcal{X}\times\mathcal{Y})^m$, denote $S_i = S \setminus \{(x_i, y_i)\}$, $h_S = \mathcal{A}(S)$. Then

$$\begin{aligned}
\mathbb{E}_{S\sim D^m}[\hat{\mathcal{R}}_S^{LOO}(\mathcal{A})] &= \frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{S\sim D^m}\left[\ell(h_{S_i}(x_i), y_i)\right] \\
&= \frac{1}{m}\sum_{i=1}^{m}\mathbb{E}_{S_i\sim D^{m-1},(x_i,y_i)\sim D}\left[\ell(h_{S_i}(x_i), y_i)\right] \\
&= \mathbb{E}_{S'\sim D^{m-1},(x,y)\in D}[\ell(h_{S'}(x), y)].
\end{aligned}$$