Aprendizado de Máquina e Reconhecimento de Padrões 2021.2

The Bias-Variance Trade-off

Based on videos from StatQuest, the course 'Machine Learning' from Andrew Ng, and the book 'Hands-on machine learning with Scikit-Learn, Keras and TensorFlow' from A. Géron

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Generalization Error

The **Generalization Error** for any machine learning algorithm can be broken down into three parts:

- Bias Error
- Variance Error
- Irreducible Error
    - This part is due to the noisiness of the data itself.
    - The only way to reduce this part of the error is to **clean up the data**
        - Fix the data sources (e.g., broken sensors), or
        - Detect and remove outliers.

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Let’s see these errors

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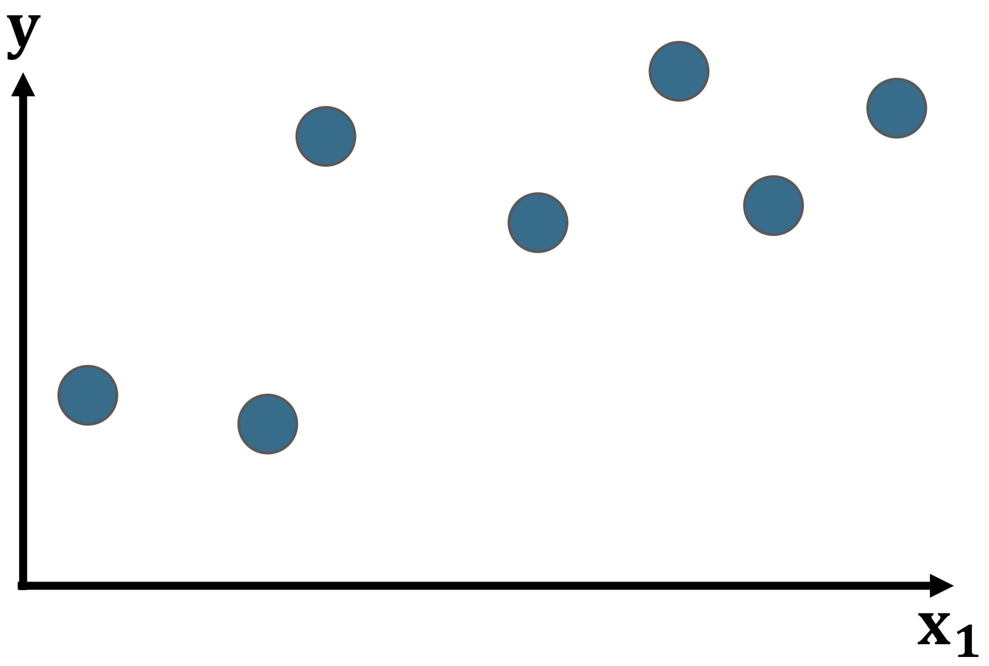
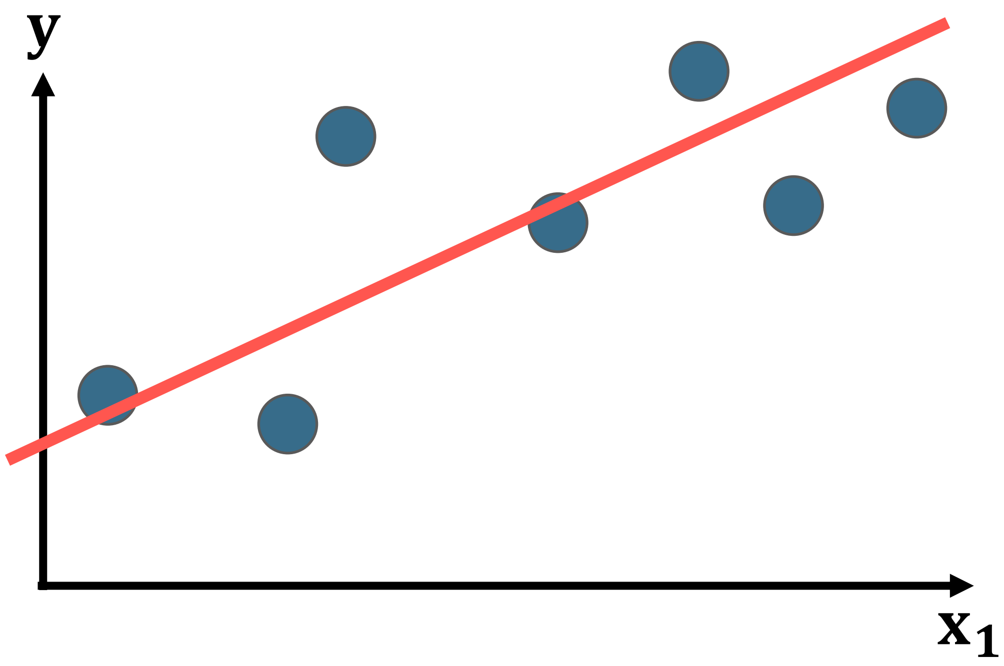

y
x1

e.g., Linear Regression

Straight Line



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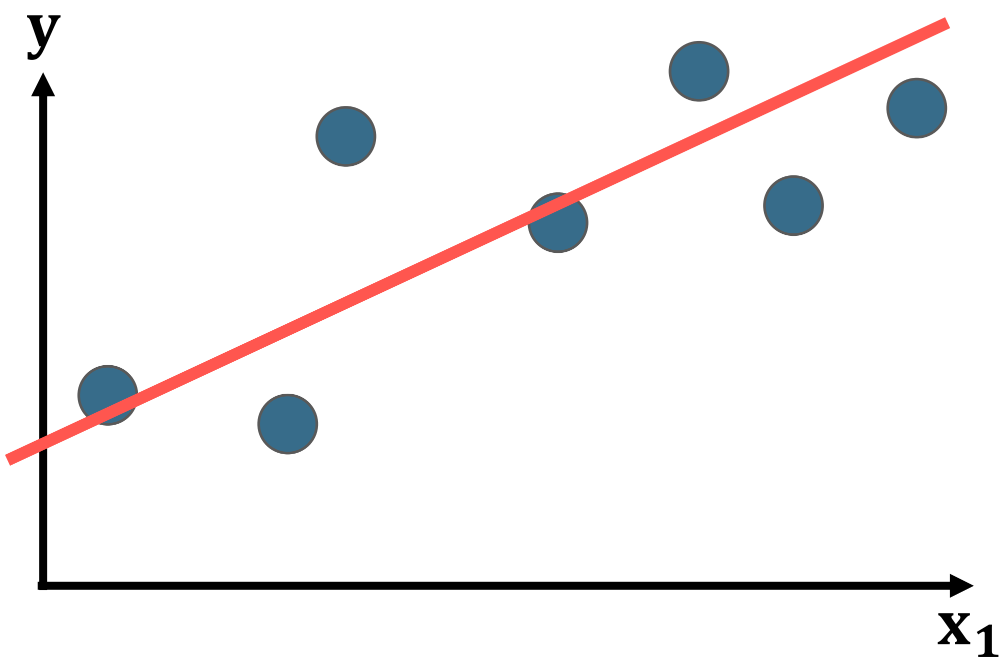

The **linear model** (straight line) **cannot** capture the **true relationship** between $\mathbf{x_1}$ and $\mathbf{y}$.

In ML, this inability is called **bias**.

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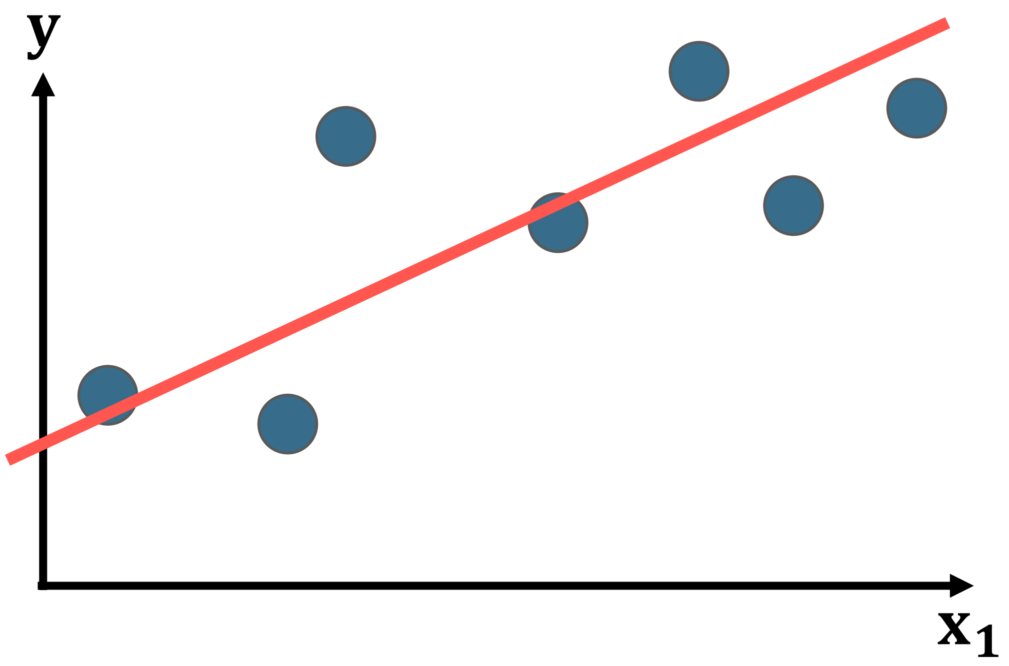

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Bias
Error associated to **wrong assumptions (simplifications)** made by a model (e.g., assuming that the data is linear when it is quadratic) to make it **easier to learn**.

Bias
'Average distance' between **predictions** and the **truth**.

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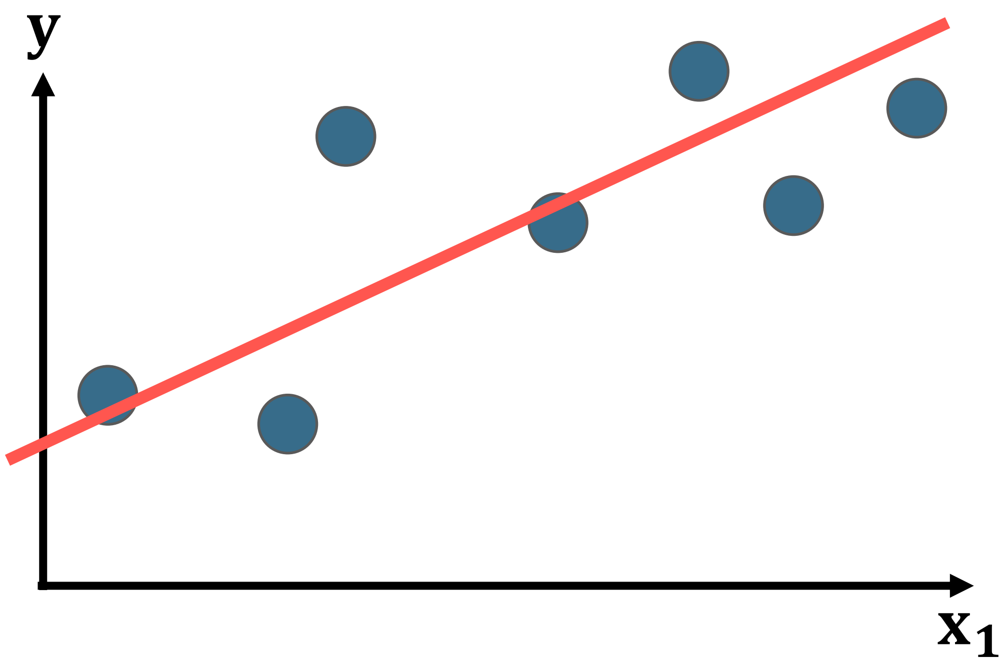

(relatively) **high** bias

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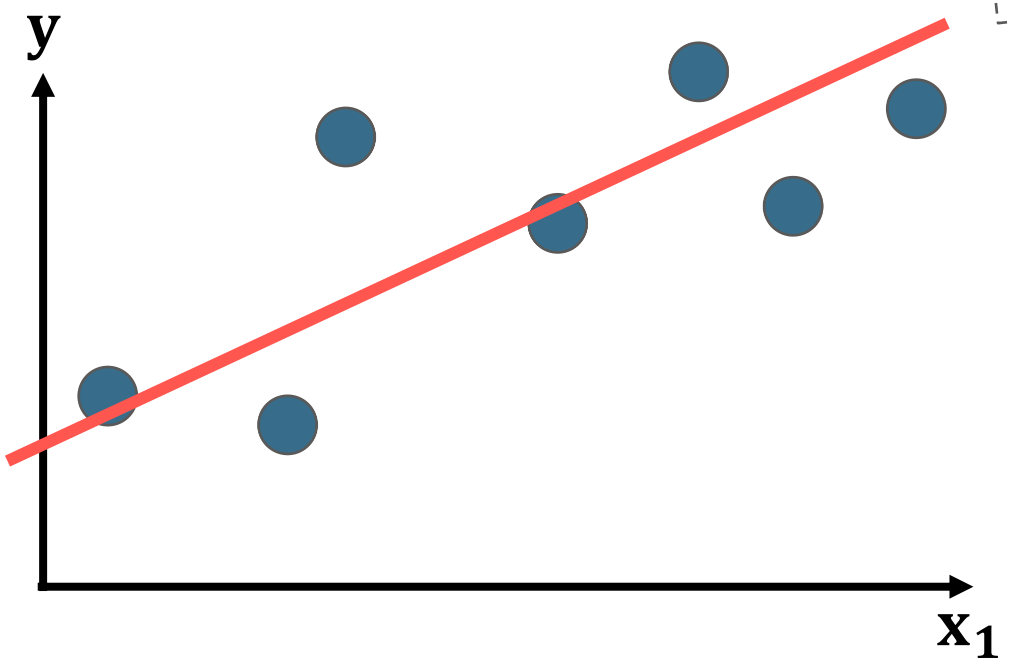

A **high-bias model** is most likely to **underfit** the training data.

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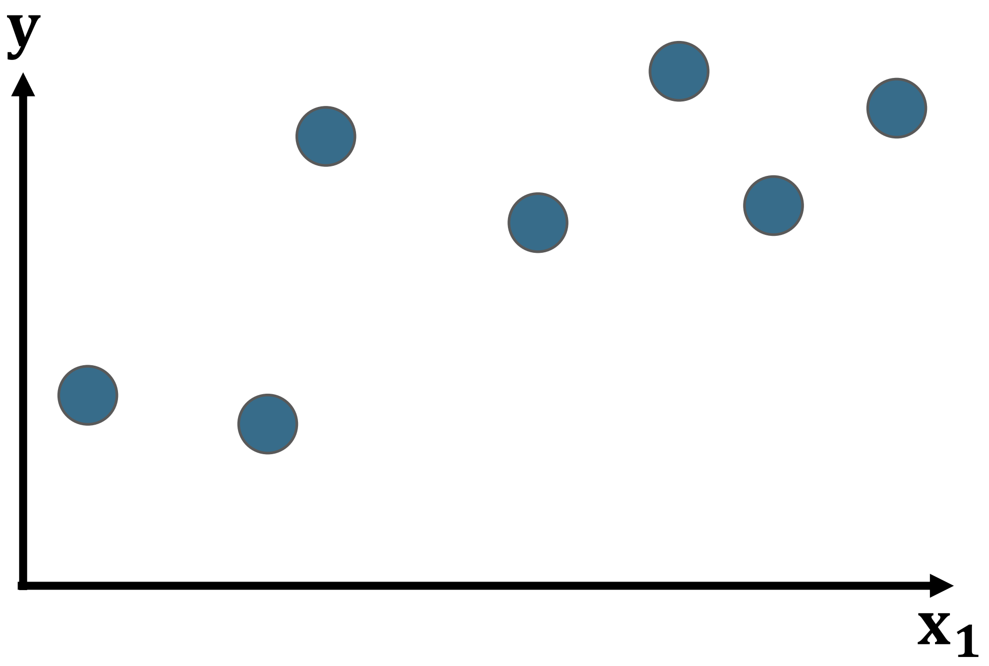
y
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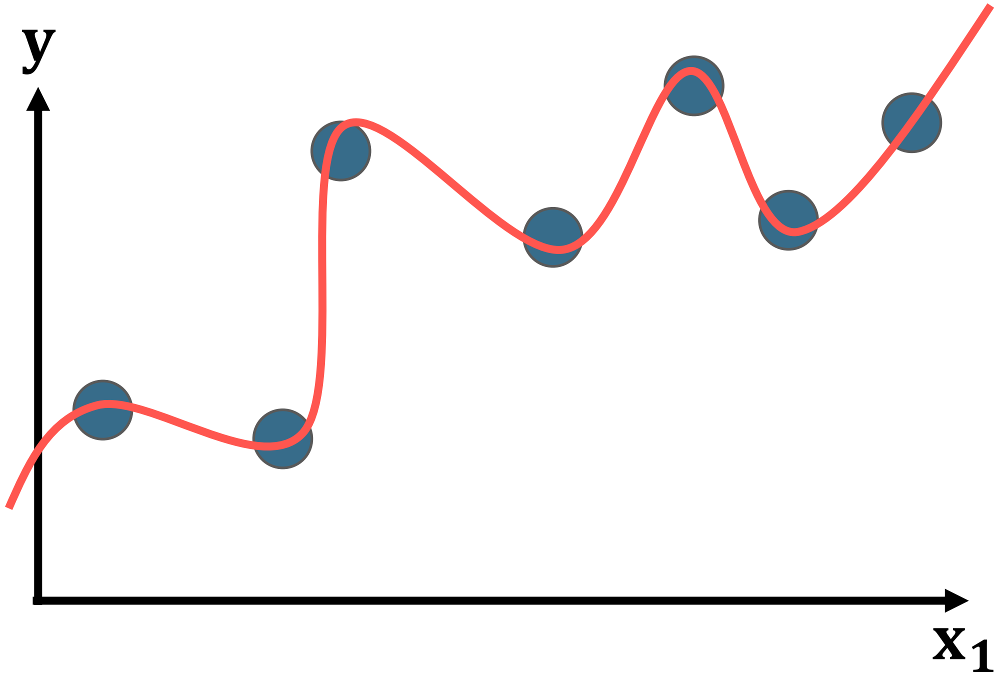
a more complex model ➔ *e.g.,* high-degree polynomial model

Squiggly Line



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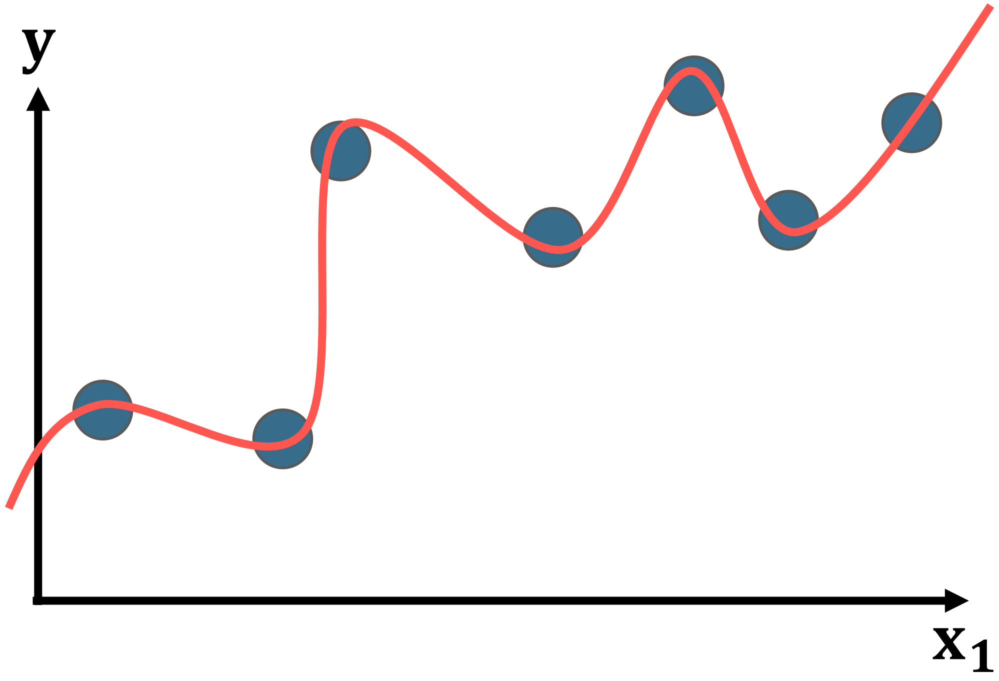

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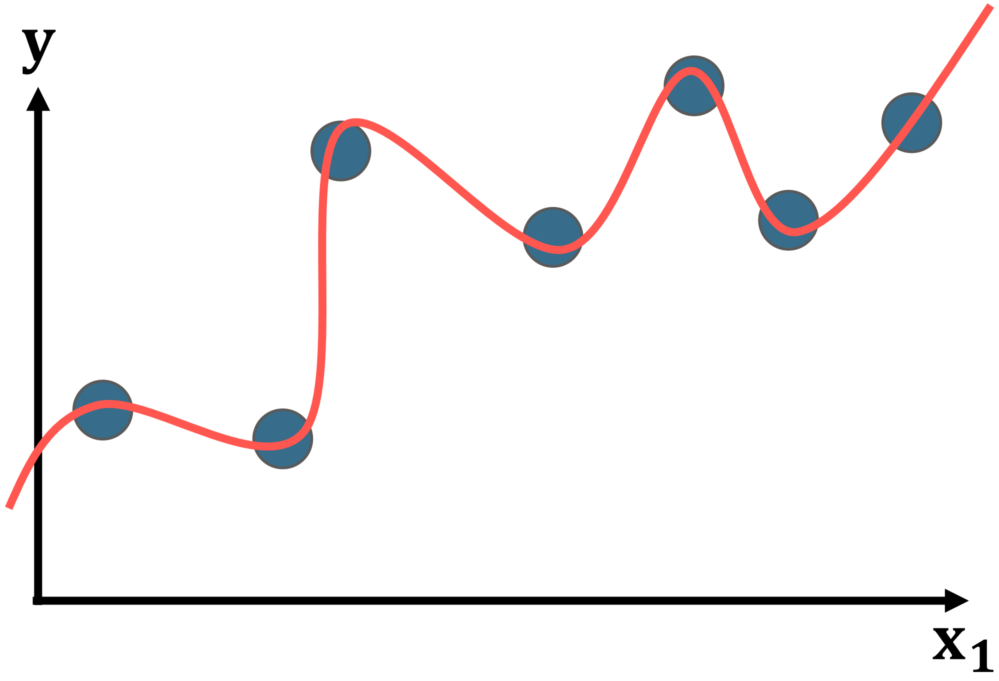
Squiggly Line



(very) **low bias**

'Average distance' between predictions and the **truth** is **close to zero**.

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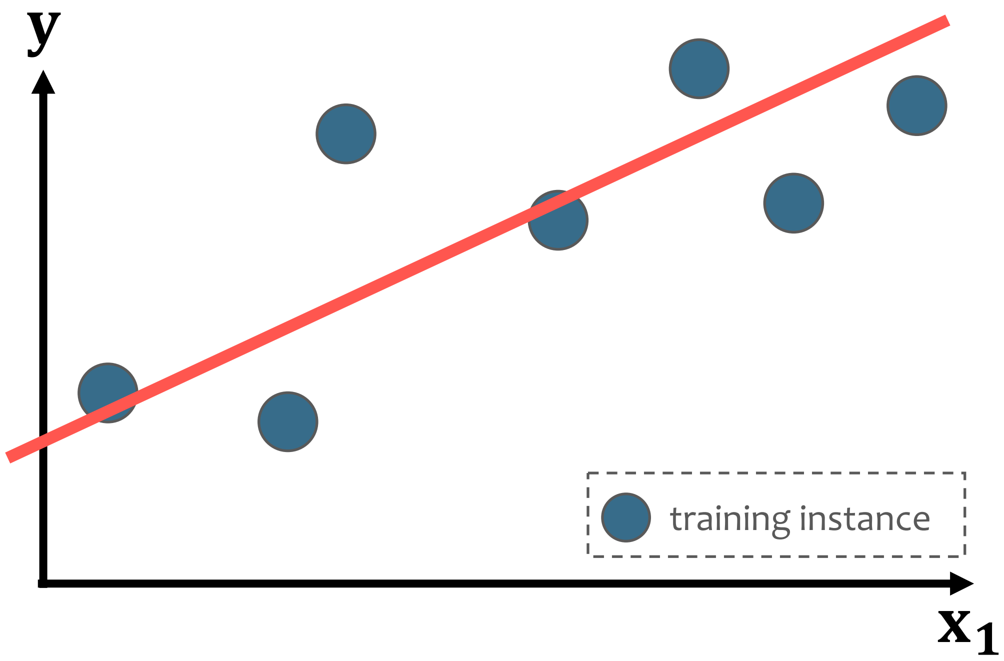
Straight Line



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Squiggly Line

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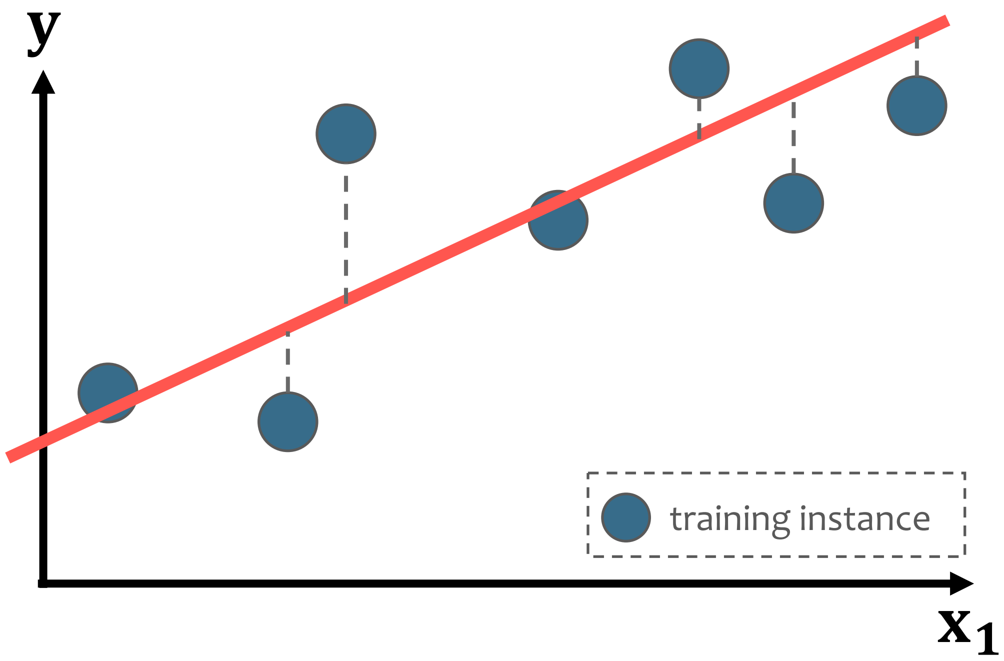
By considering *only* the **training set errors**, we would pick the **squiggly line** below.

Straight Line

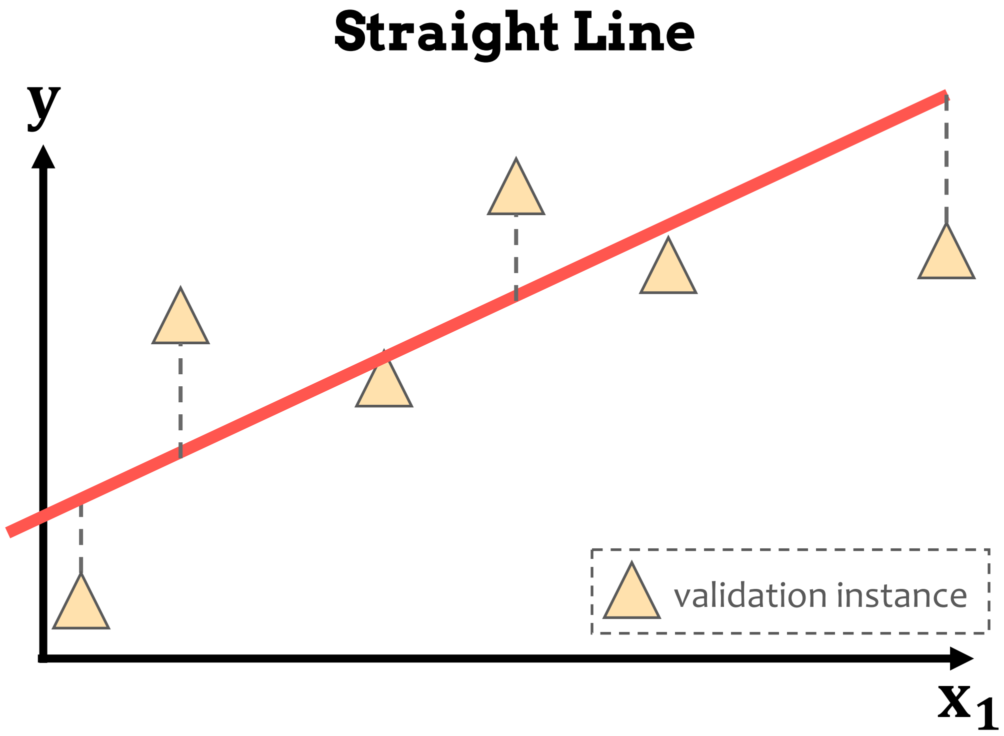


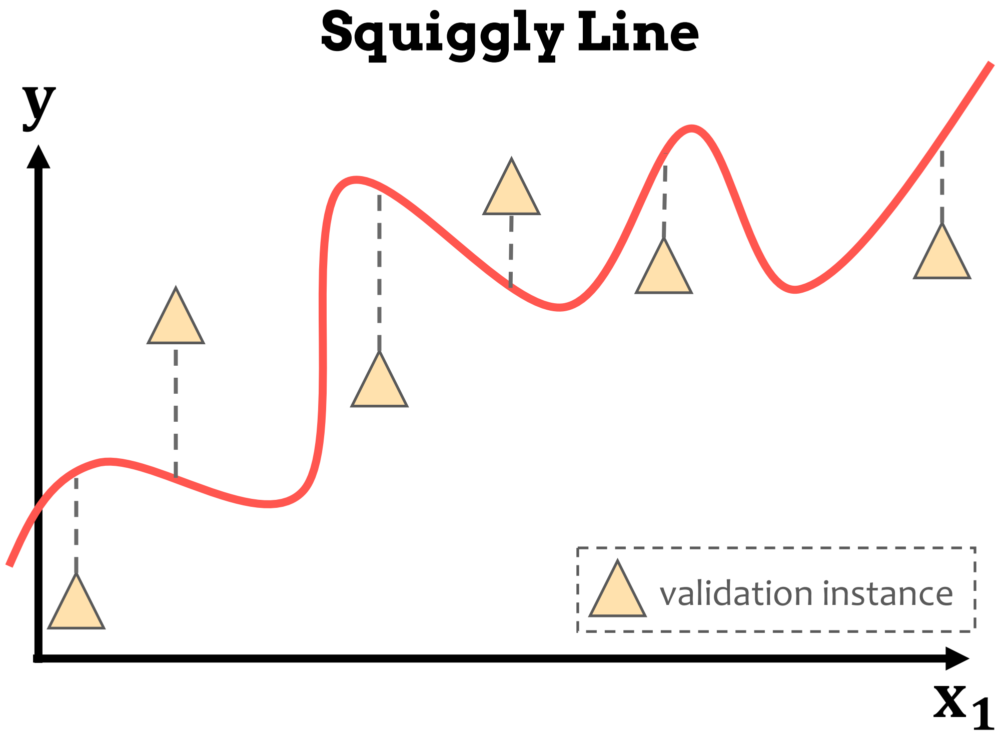
(relatively) **high bias**

Squiggly Line

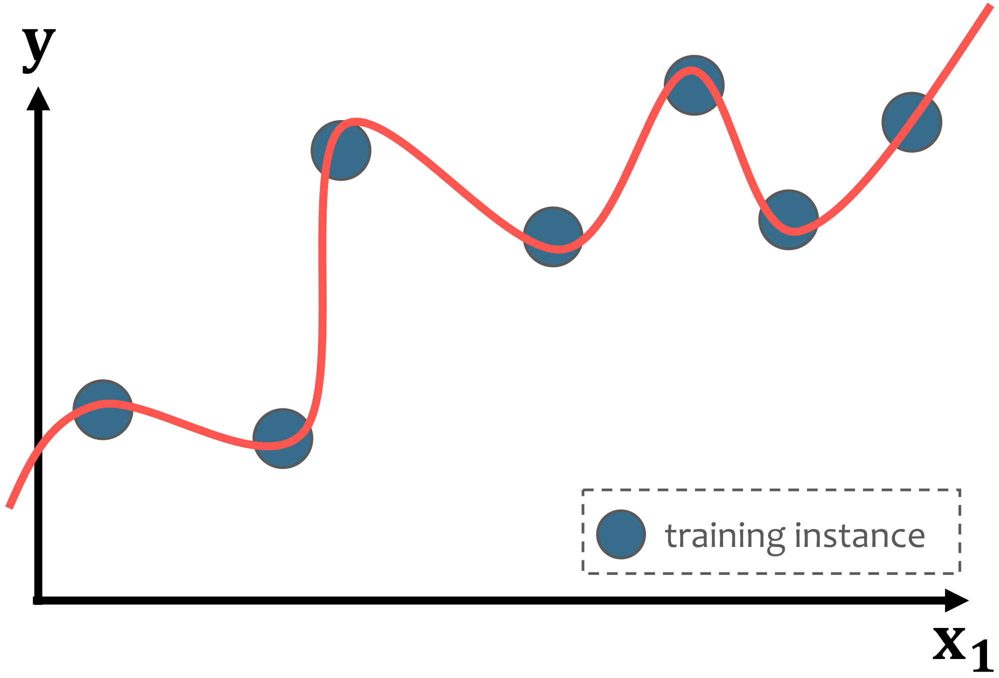
(very) **low bias**

In contrast, the considered **straight line** fits the validation set (unseen data) **better** than squiggly line → better generalization

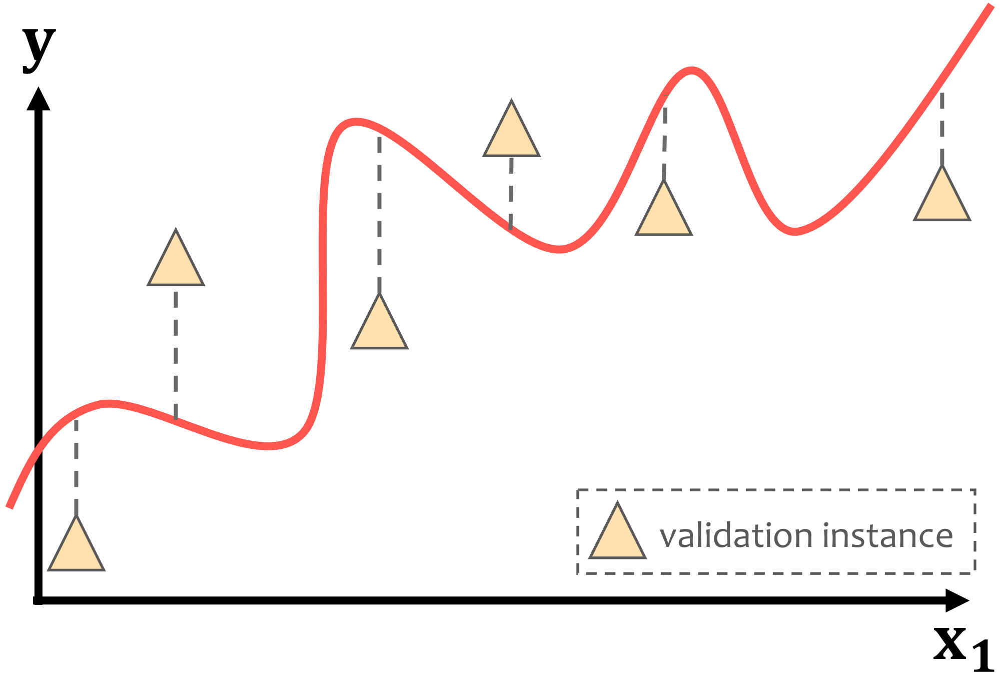




Great job fitting the **training set**



Terrible job fitting the **validation set** → **not generalize well**



In ML, the **difference in fits between datasets** is called **variance.**

Great job fitting the **training set**

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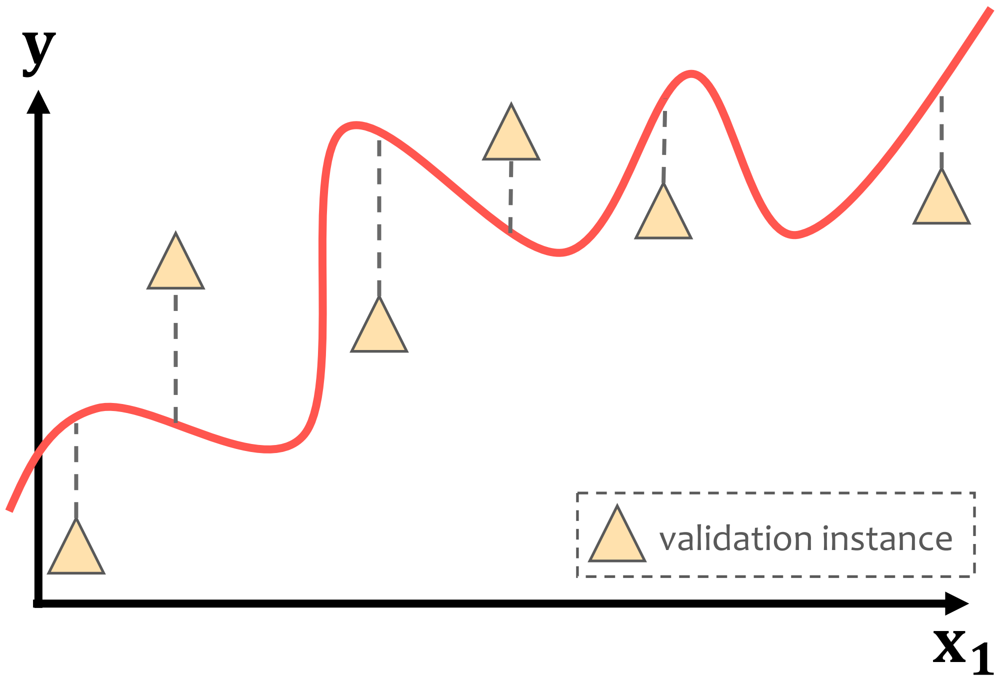

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Variance

The amount that the **estimate** of the model will **change** if **different training data** was used.

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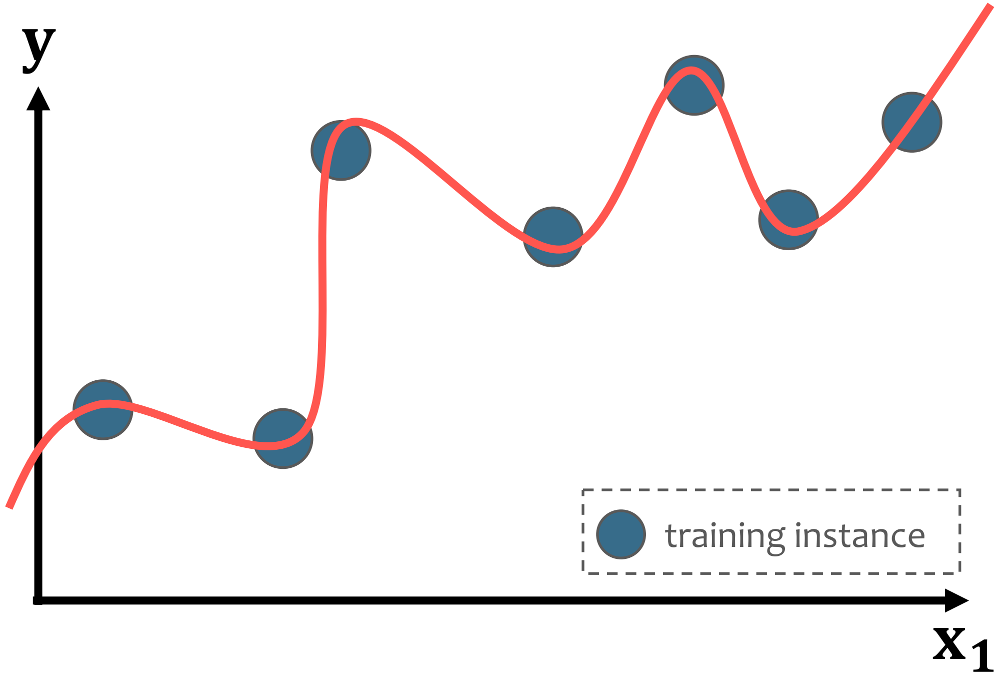

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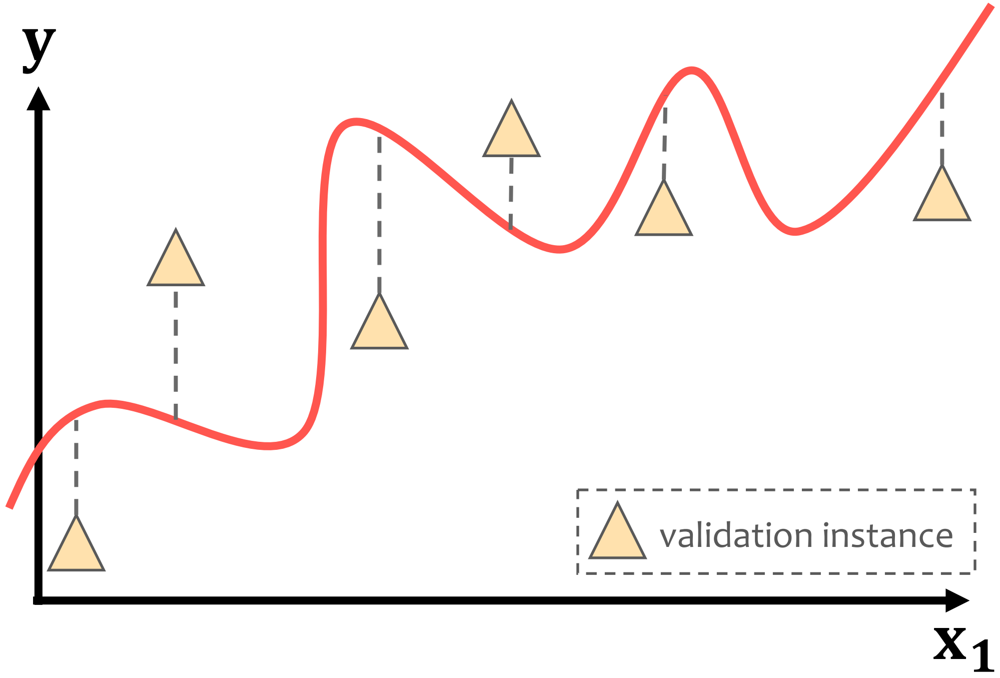

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A **high-variance model** is most likely to **overfit** the training data.

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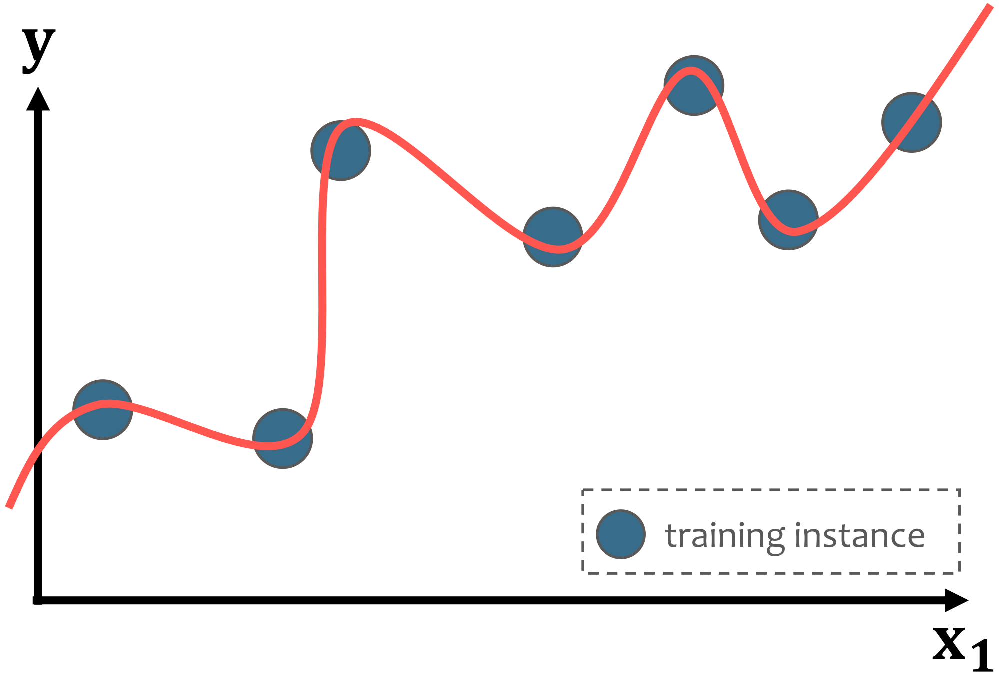

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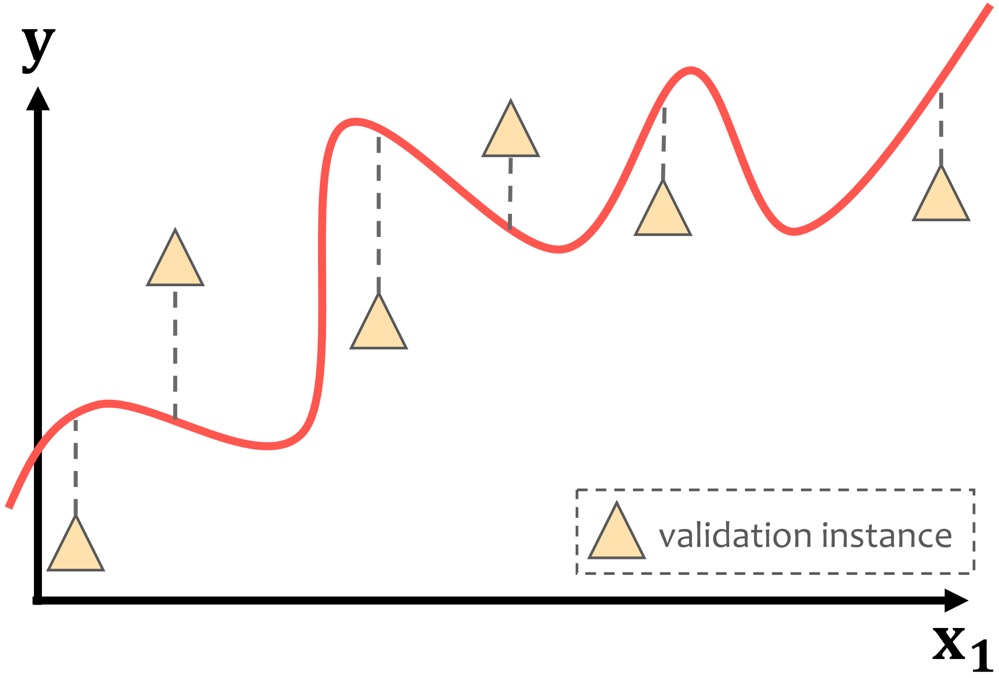
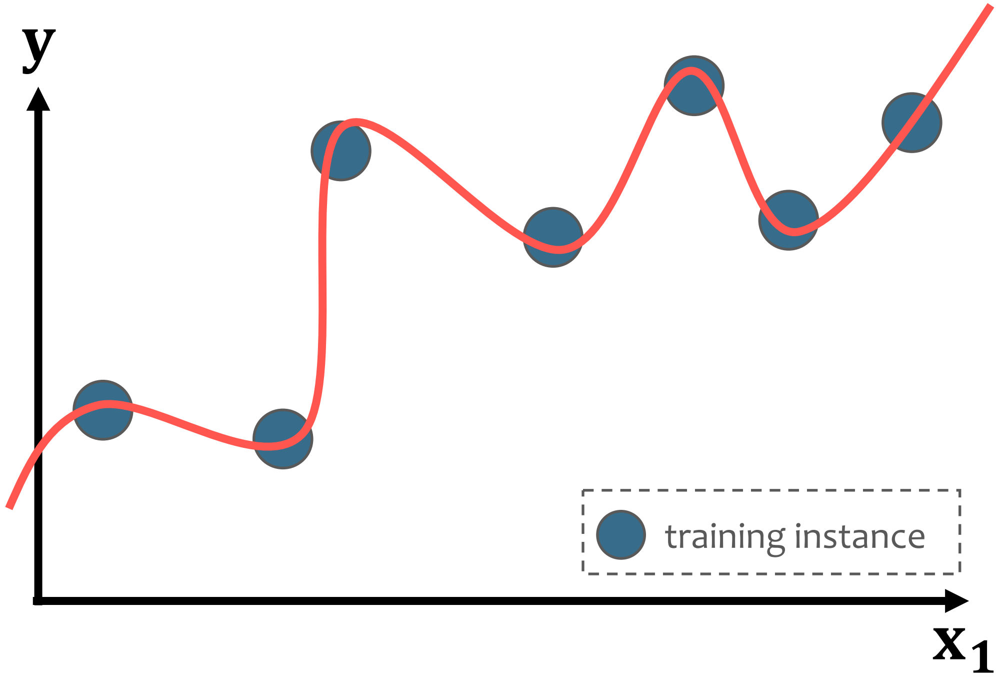
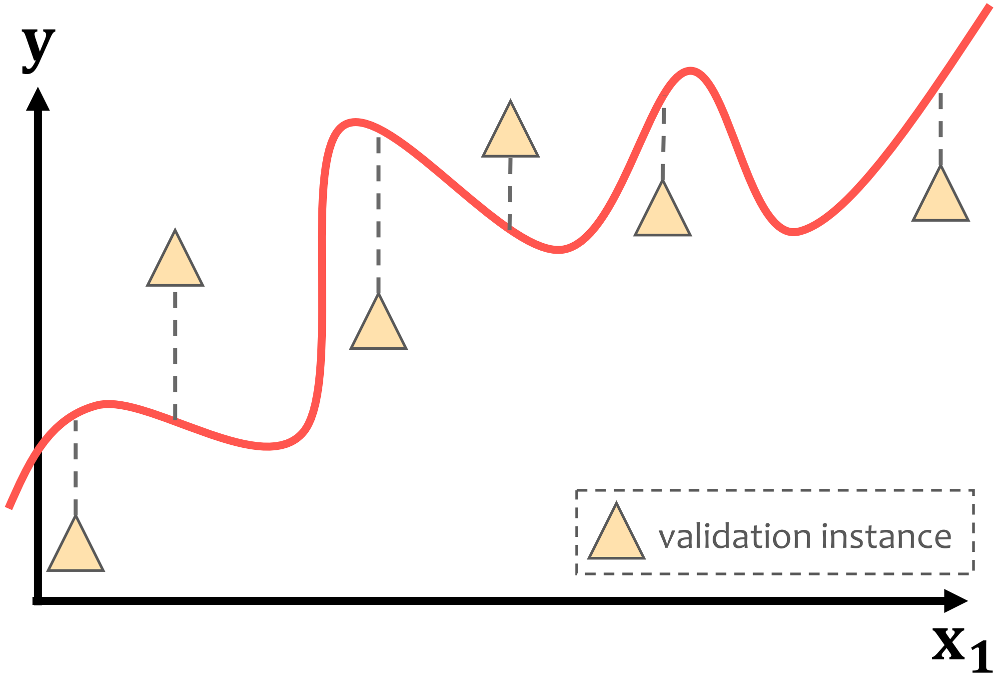
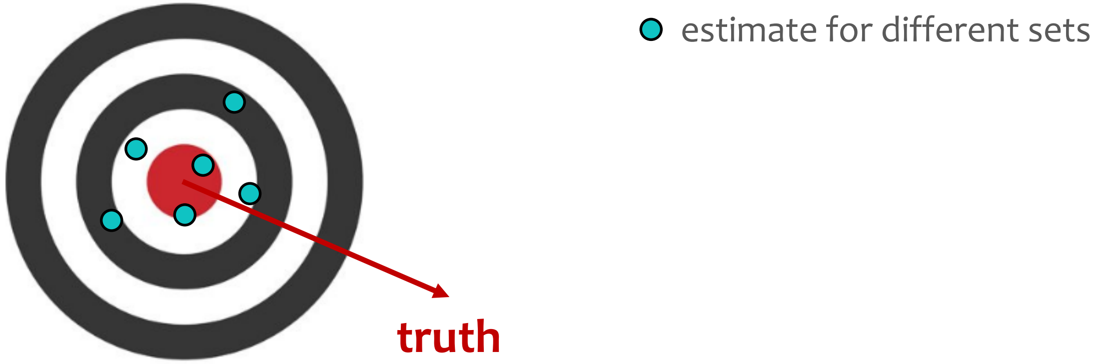


Squiggly Line





low bias
high variance



Straight Line

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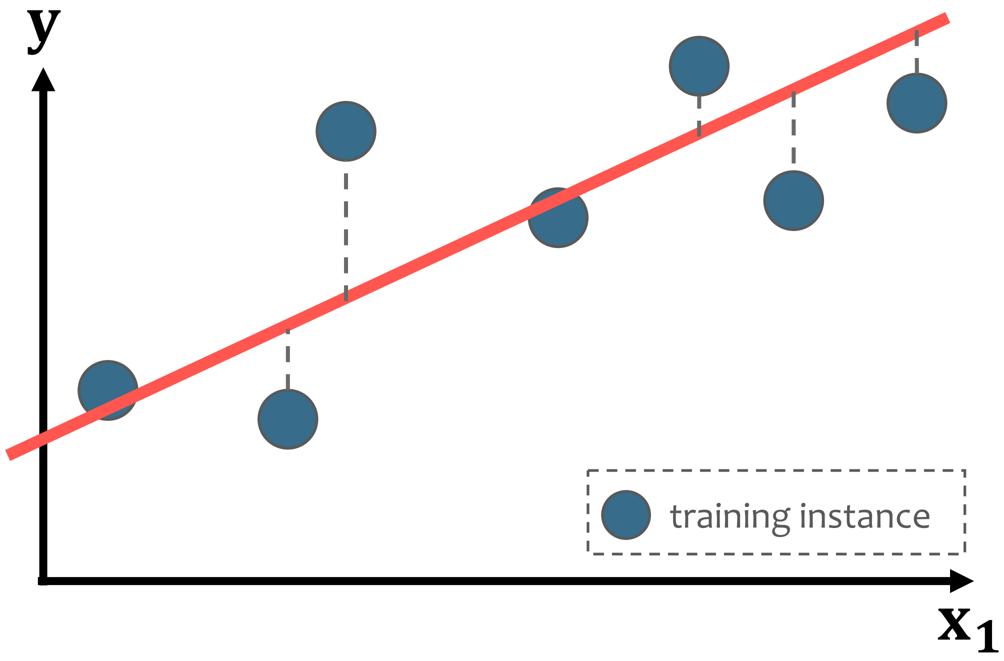
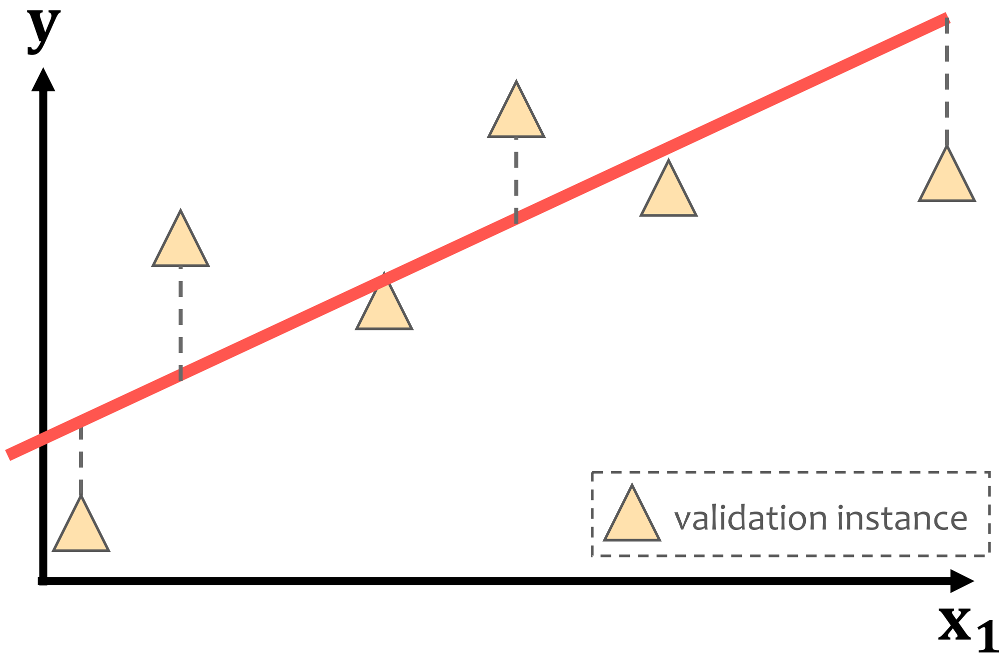


But the **error is similar** for different sets.



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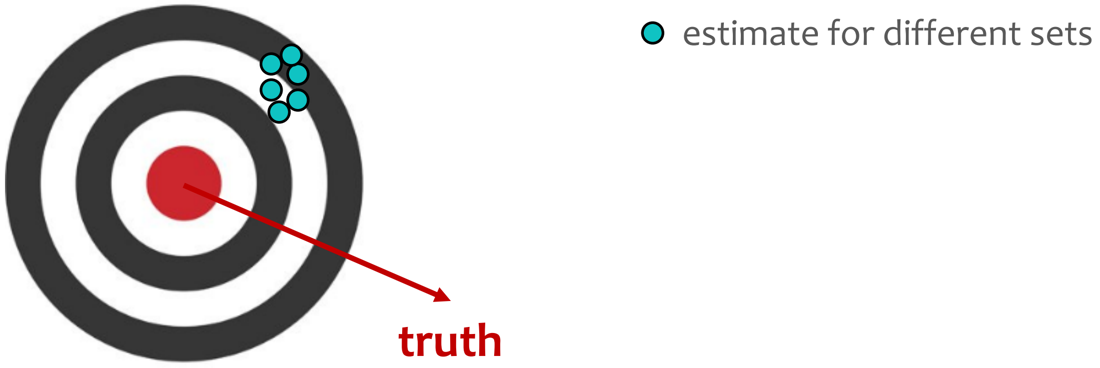
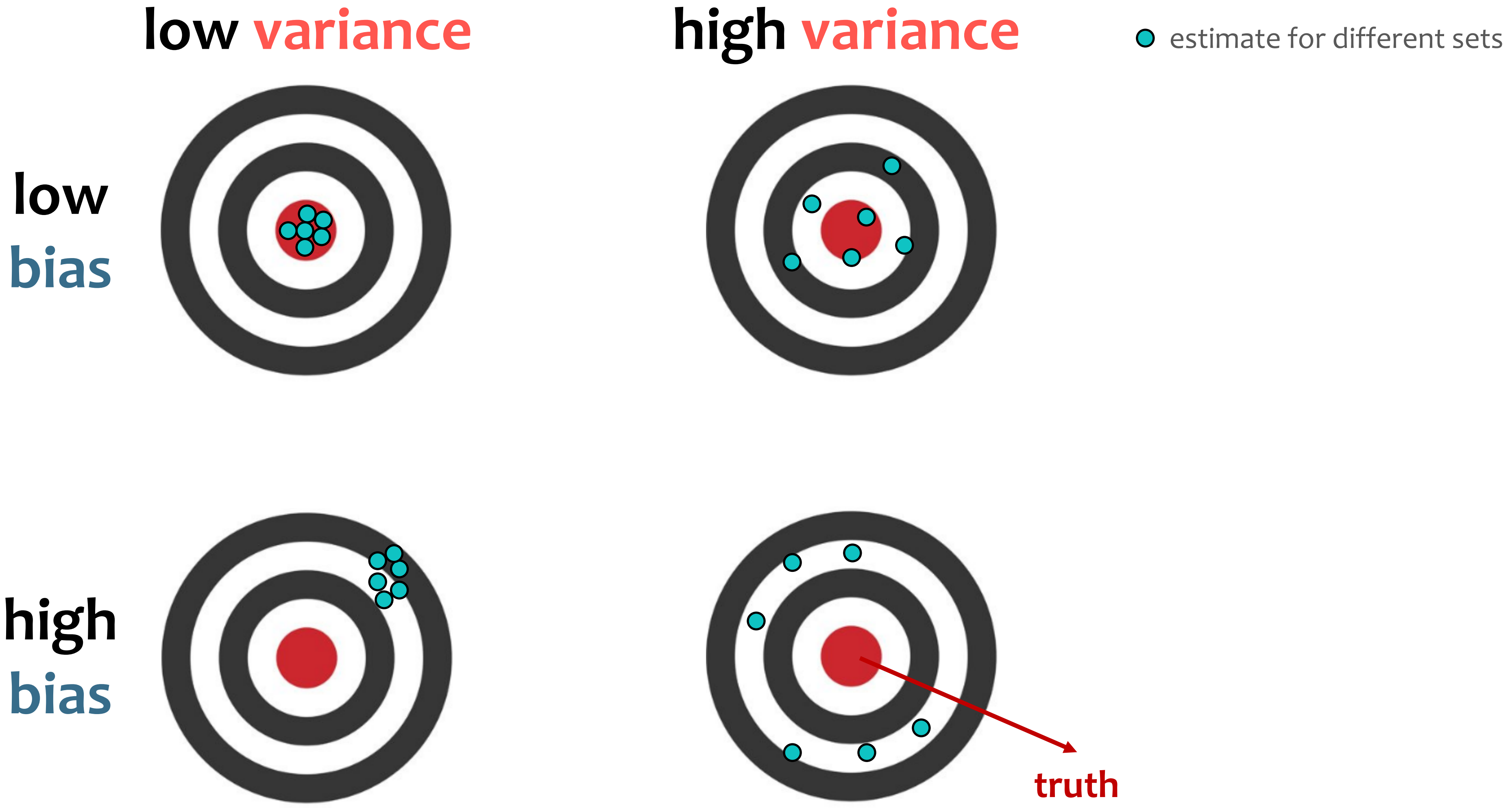
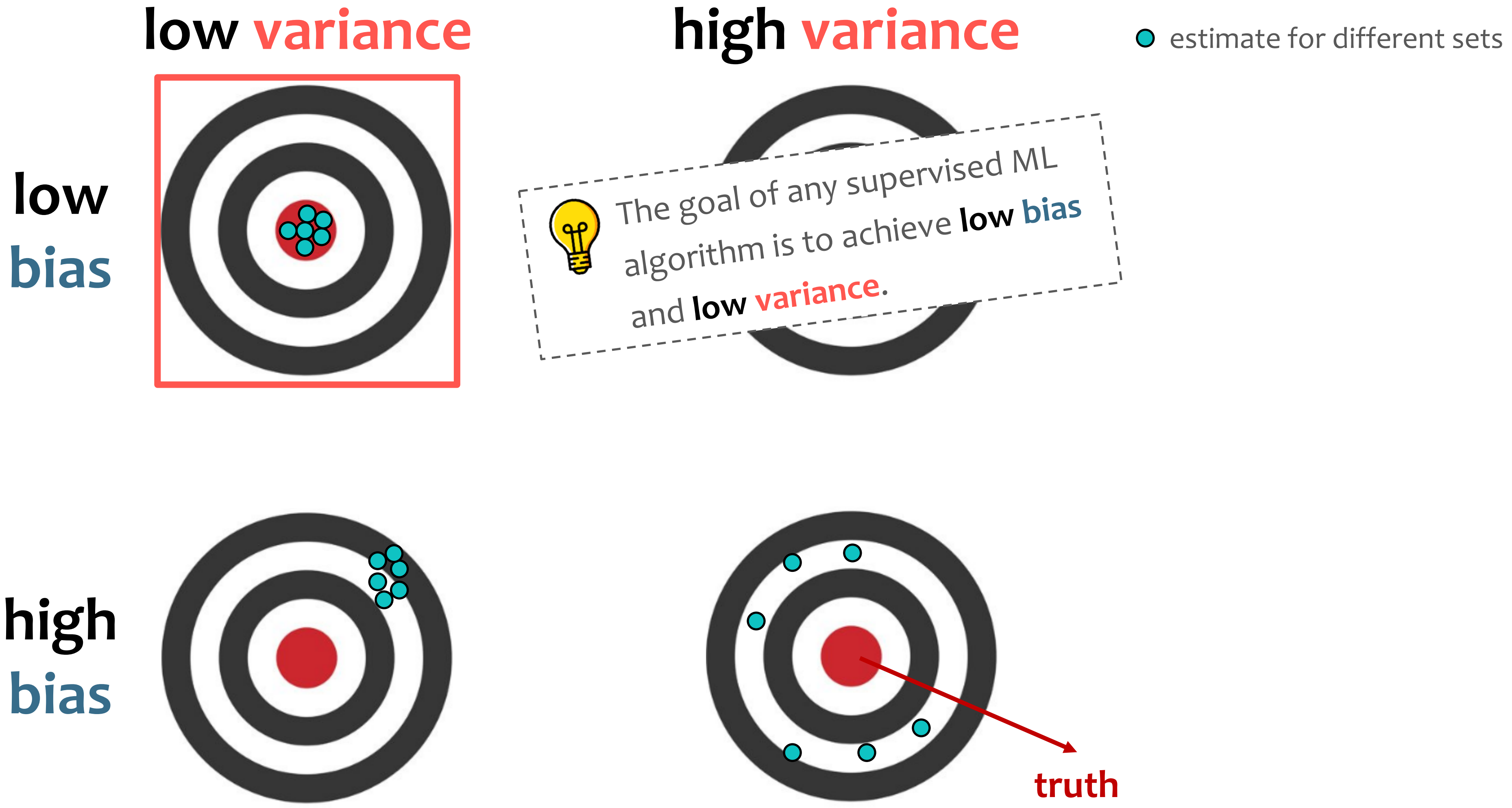



low variance
high variance
estimate for different sets
low
bias
high
bias
truth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high variance
estimate for different sets
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The goal of any supervised ML algorithm is to achieve low bias and low variance.
truth

The Bias-Variance Trade-off

- **Increasing ↑ a model's complexity** will typically:
  - increase ↑ its **variance**
  - reduce ↓ its **bias**.
- **Reducing ↓ a model's complexity** will:
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- Increasing ↑ **variance** reduces ↓ **bias**, and vice versa.
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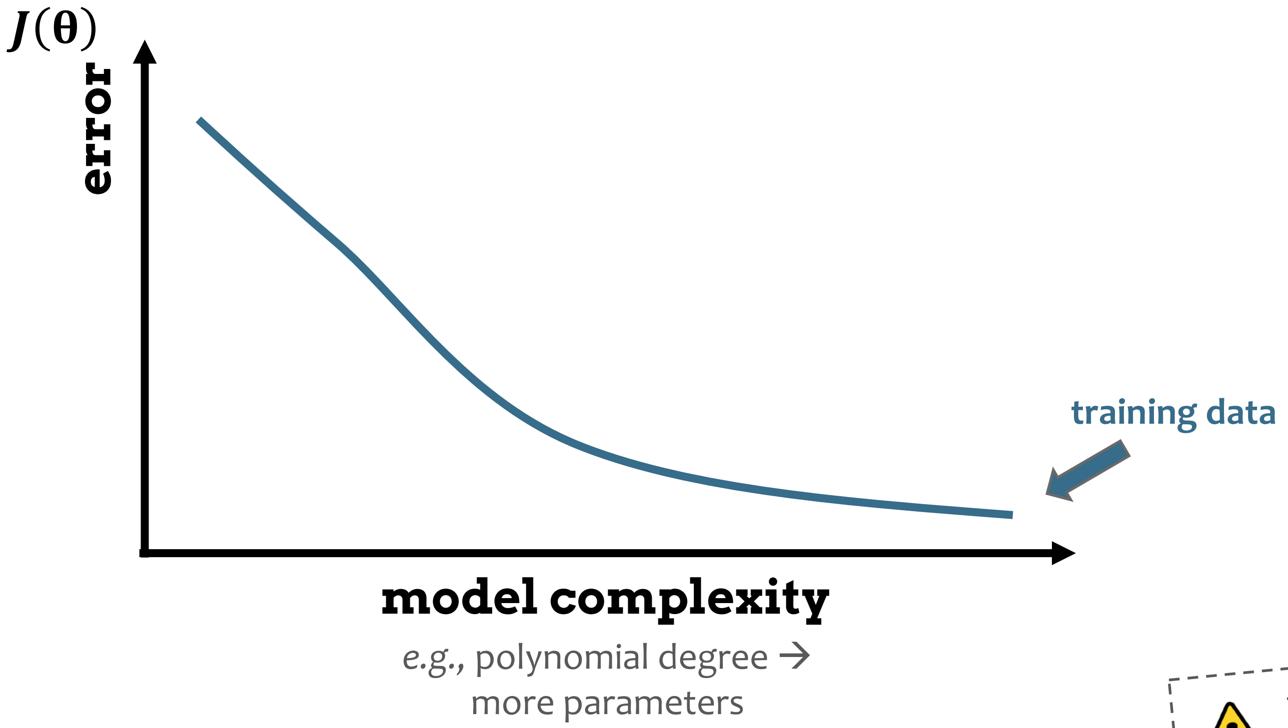
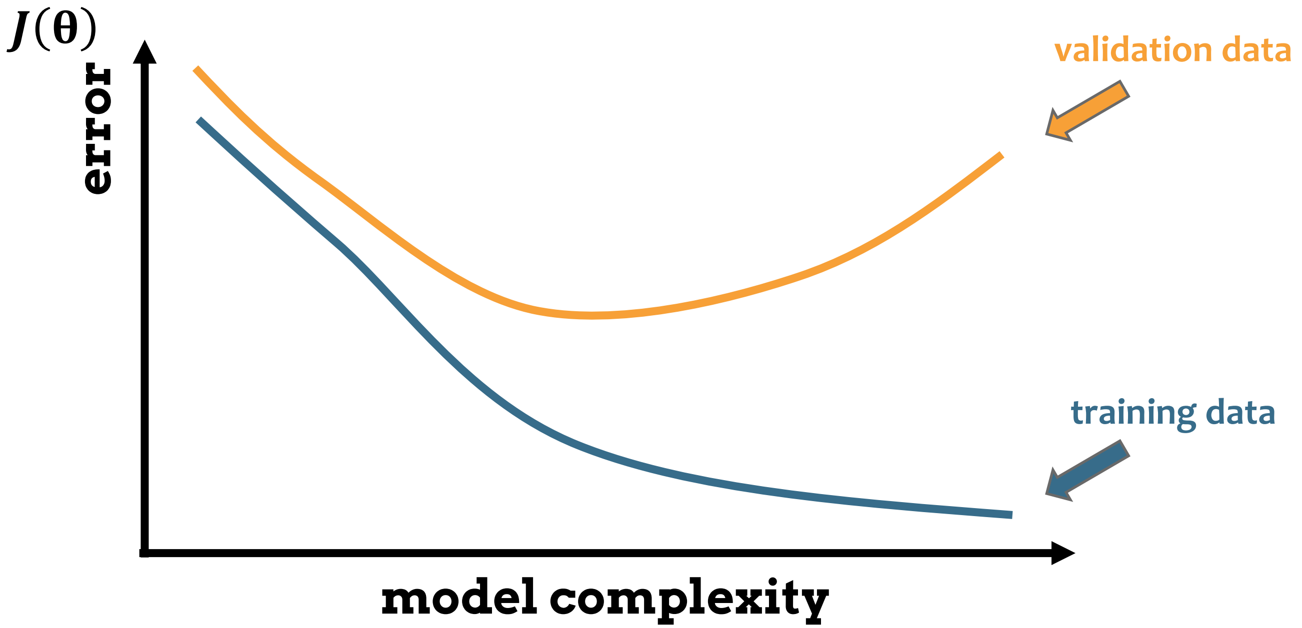
General trend:

- **Linear** ML algorithms often have a high **bias** but a low **variance**.
- **Nonlinear** ML algorithms often have a low **bias** but a high **variance**.

Diagnosing Bias vs Variance



These are hypothetical curves for hypothetical data.



e.g., polynomial degree → more parameters

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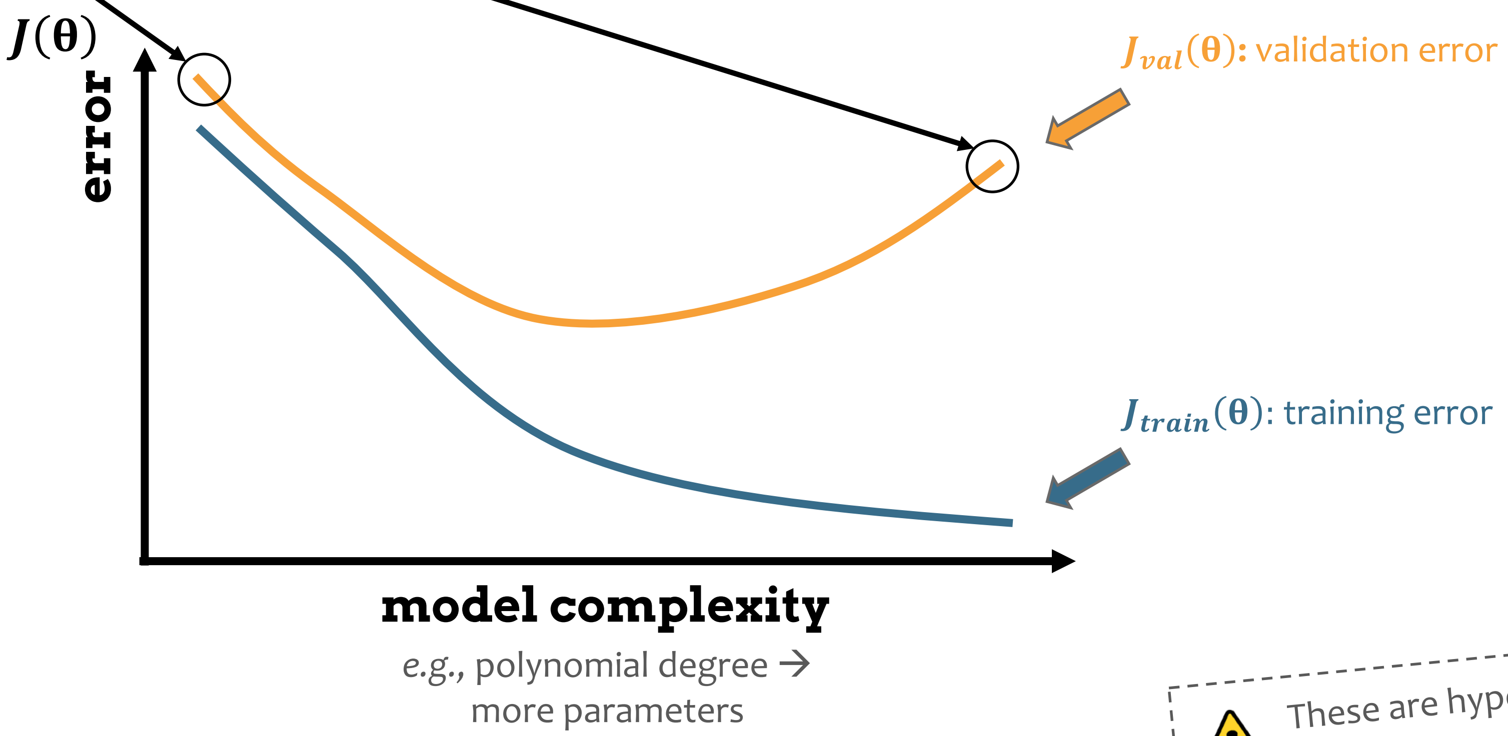
- Suppose your learning algorithm is performing less well than you were hoping.
- If $J_{val}(\theta)$ is **high**, is it a **bias** problem or a **variance** problem?



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$J_{train}(\theta) \gg J_{val}(\theta)$

Bias (underfit):

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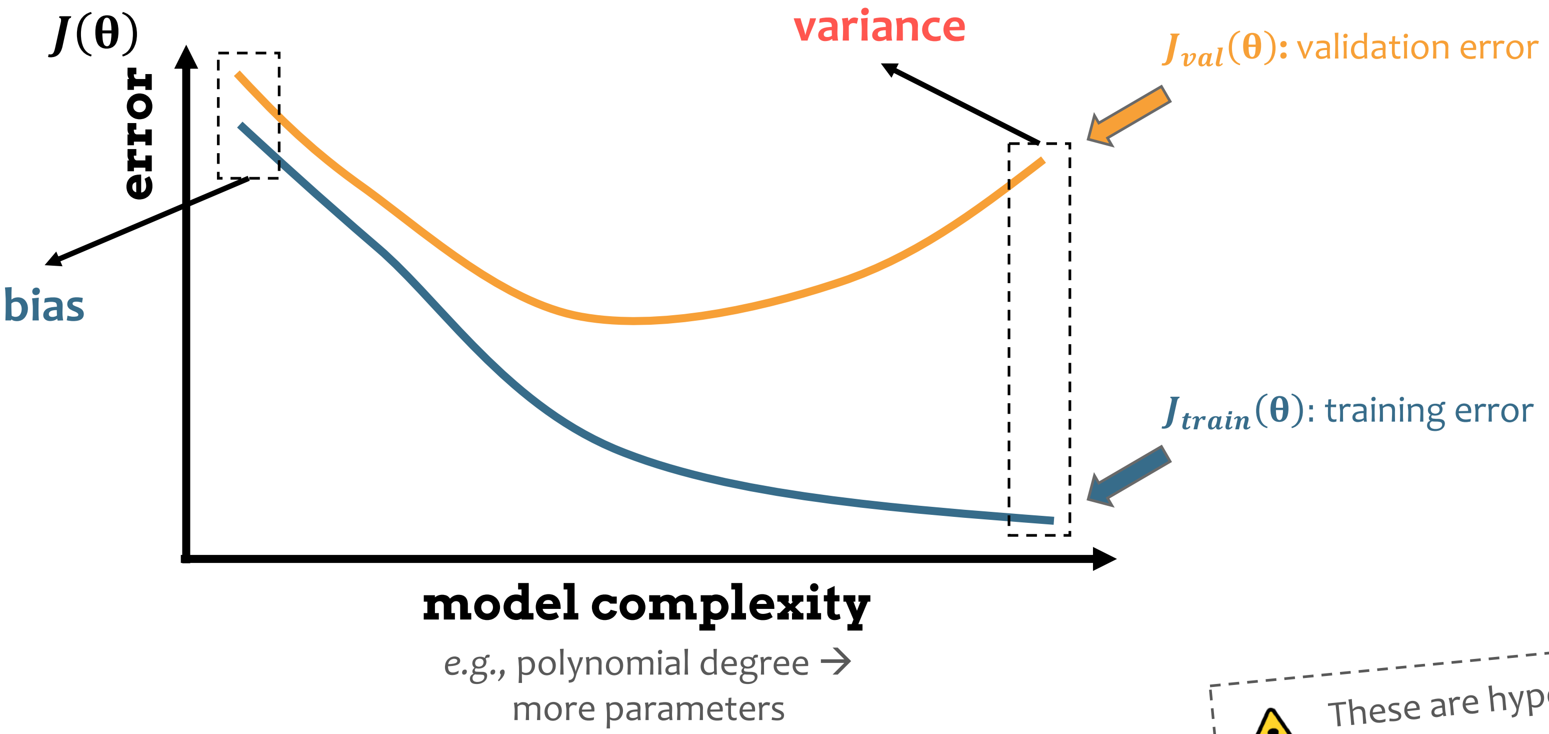

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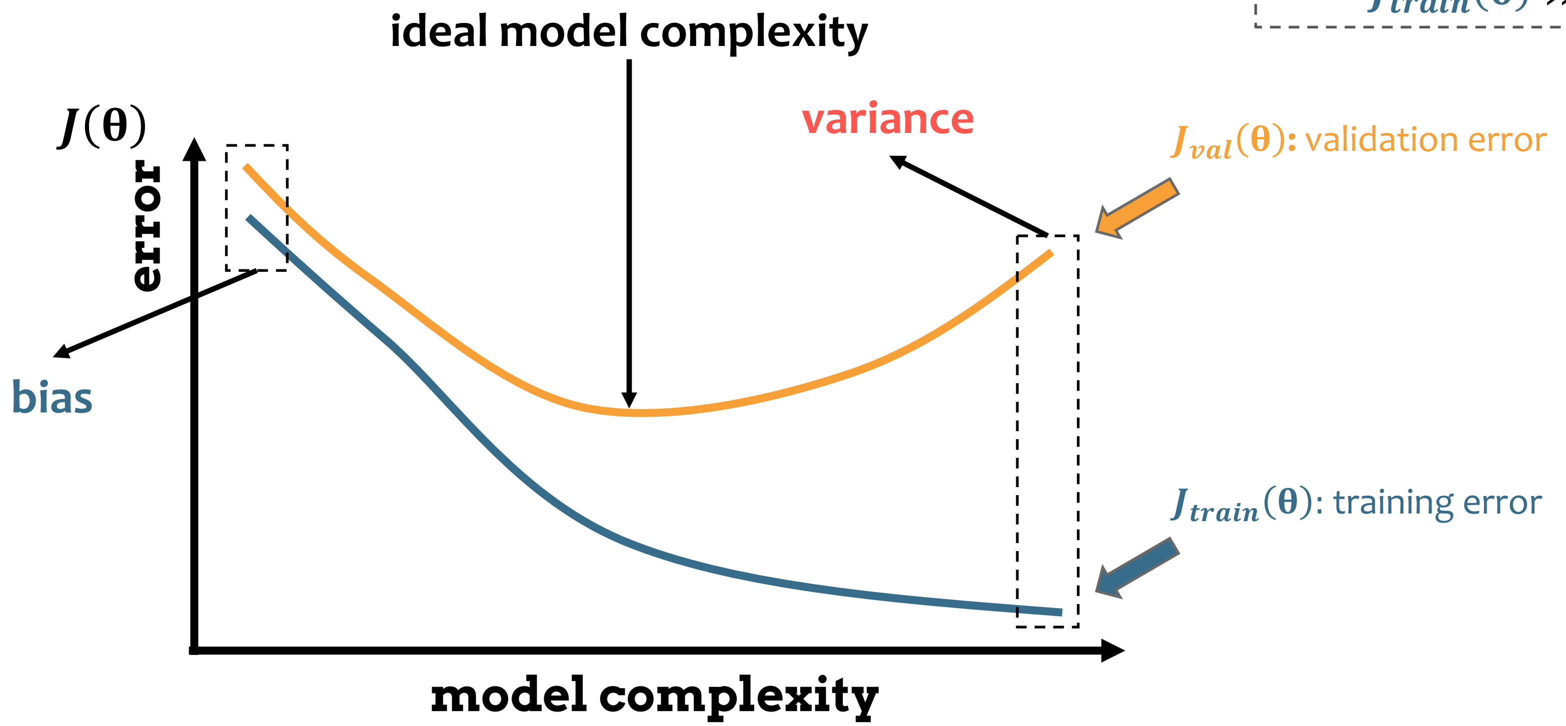

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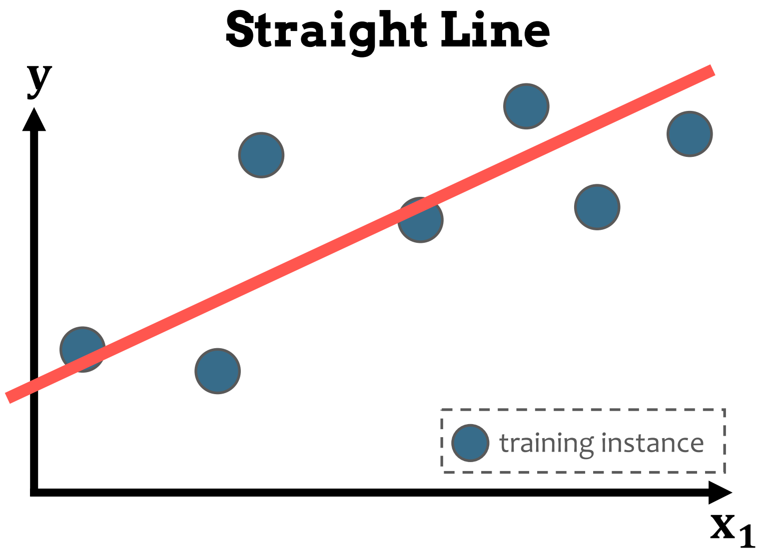
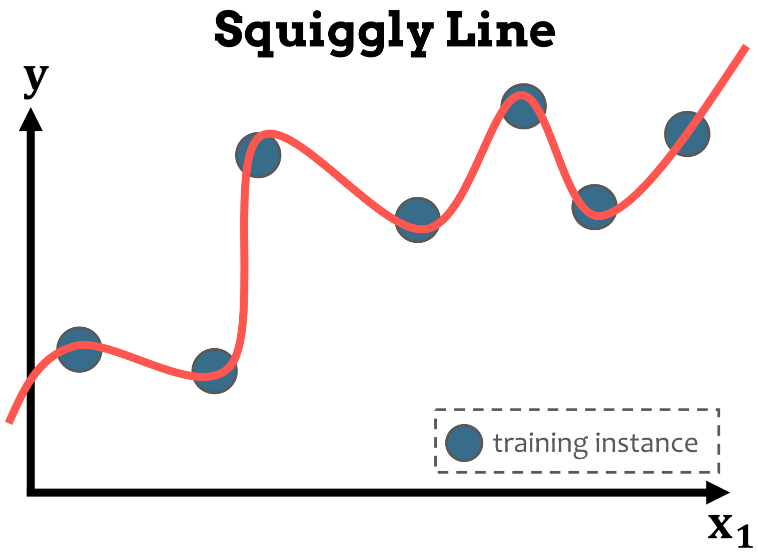
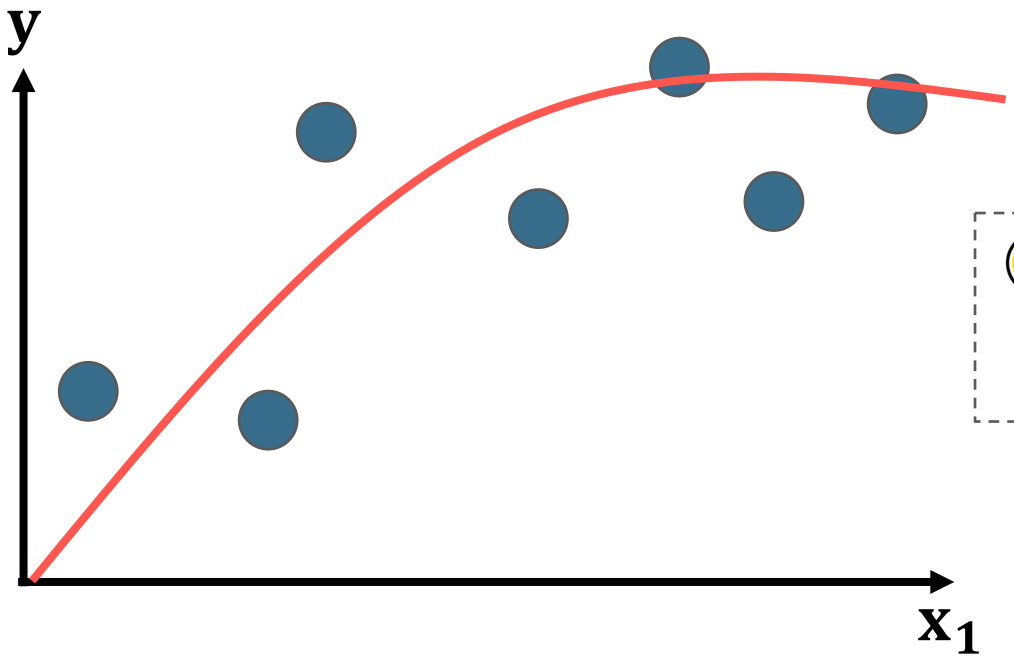
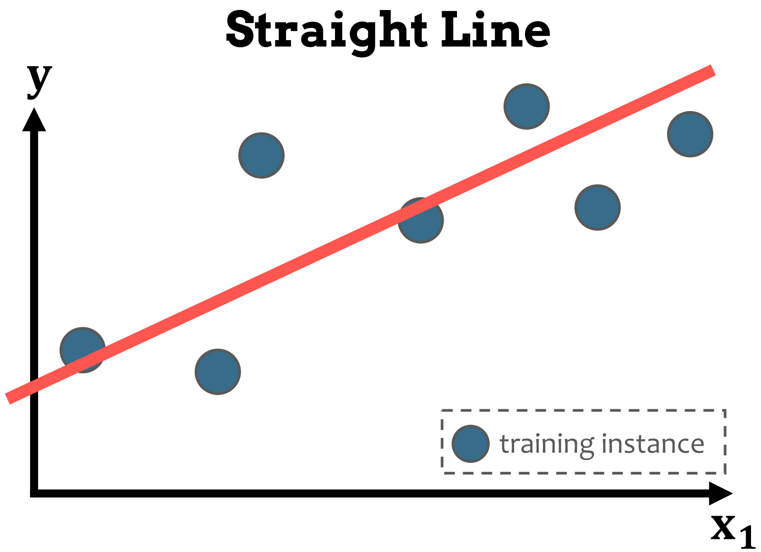


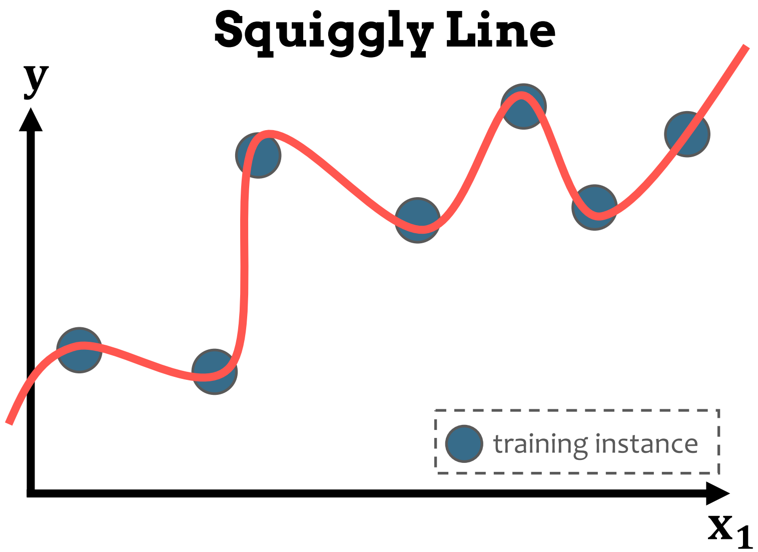




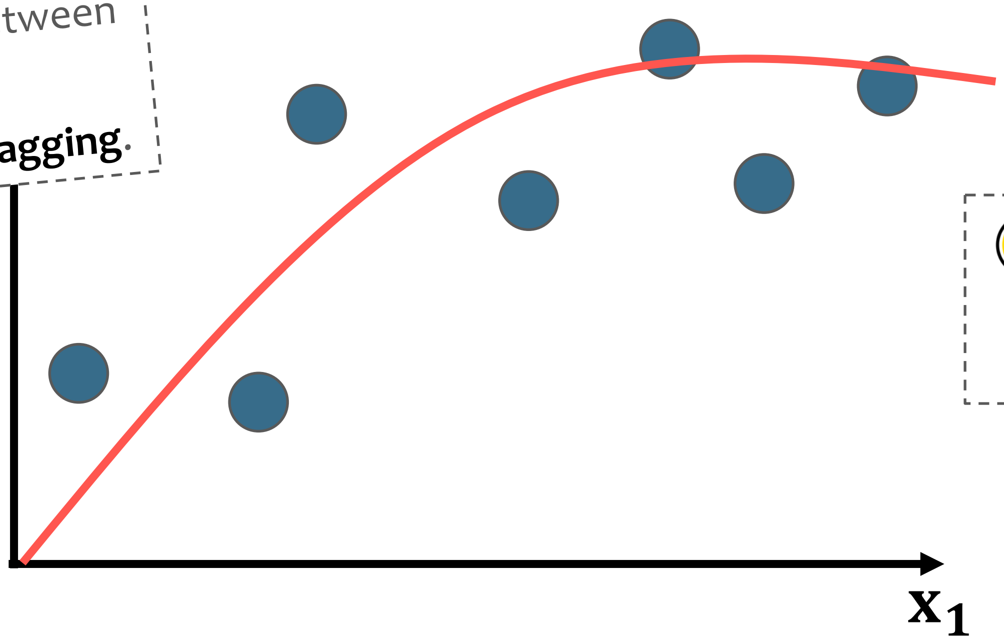
We want an **intermediate solution** between simple and overly complex one.

(relatively)
low bias
low variance





Three commonly strategies used to find the **intermediate model** between simple and complex are: **regularization, boosting** and **bagging**.



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