

CSE 417T

# Introduction to Machine Learning

Lecture 9

Instructor: Chien-Ju (CJ) Ho

# Logistics

- Homework 2 is due on **Feb 24 (Thursday)**
- Return of Homework
  - We plan to return each homework within 2 weeks after the deadline
  - Regrade requests
    - You will have up to 7 days to submit regrade requests
      - the regrade period might be shortened if there are schedule constraints
    - We might check the entire homework for each request, so the grades might go down as well if we find new mistakes
- Exam 1: **Mar 10 (Thursday)**
  - Content: LFD Chap 1 to 5 (The entire hardcopy of the textbook)
  - Covid-permitting
    - Timed exam (75 min) during lecture time in the classroom
    - Closed-book exam with 2 letter-size cheat sheets allowed (4 pages in total)
      - No format limitations (it can be typed, written, or a combination)

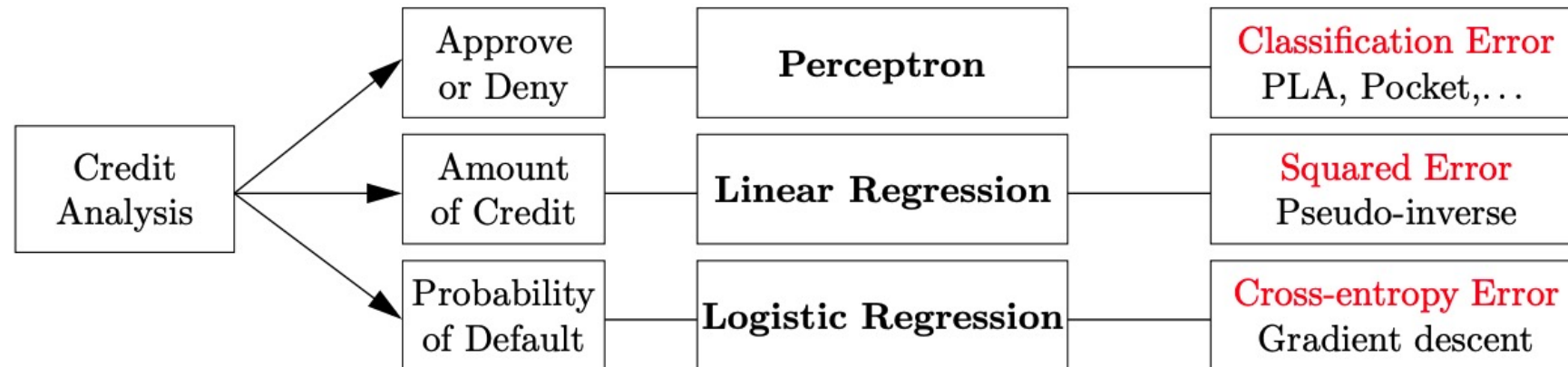
Recap

# Linear Models

This is why it's called linear models



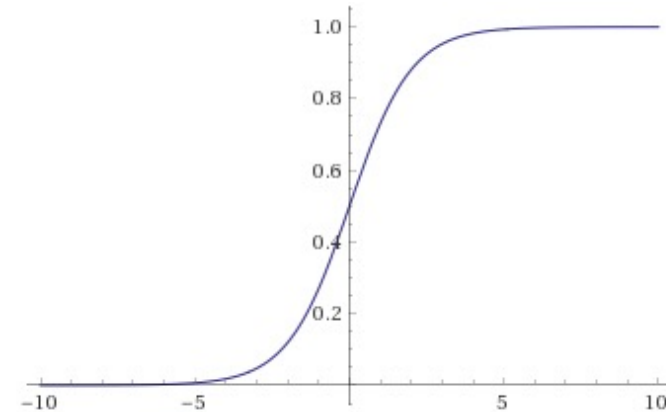
- $H$  contains hypothesis  $h(\vec{x})$  as **some function of  $\vec{w}^T \vec{x}$**



- Algorithm:
  - Focus on  $g = \operatorname{argmin}_{h \in H} E_{in}(h)$
  - **Gradient descent** is one of the common optimization algorithms

# Logistic Regression

- Predict a probability
  - Interpreting  $h(\vec{x}) \in [0,1]$  as the prob for  $y = +1$  given  $\vec{x}$
- Hypothesis set  $H = \{h(\vec{x}) = \theta(\vec{w}^T \vec{x})\}$ 
  - $\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$
- Algorithm
  - Find  $g = \operatorname{argmin}_{h \in H} E_{in}(h)$
- Two key questions
  - How to define  $E_{in}(h)$ ?
  - How to perform the optimization (minimizing  $E_{in}$ )?



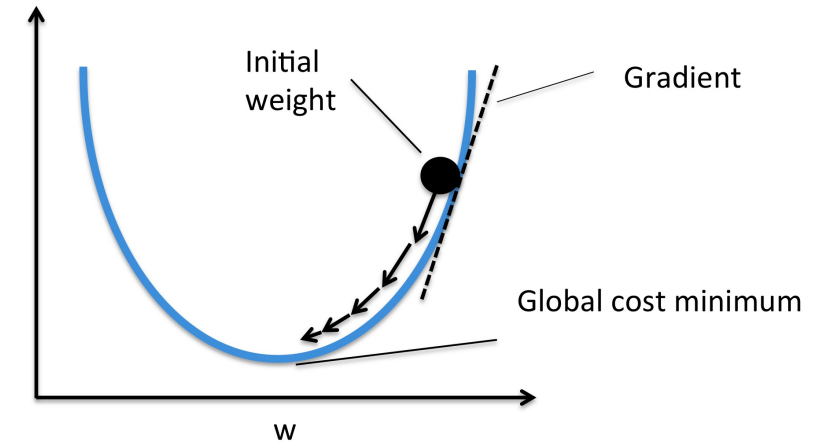
Define  $E_{in}(\vec{w})$ : Cross-Entropy Error

$$E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

- Minimizing cross entropy error is the same as maximizing likelihood
- Likelihood:  $\Pr(D|\vec{w})$ 
  - $\vec{w}^* = \operatorname{argmax}_{\vec{w}} \Pr(D|\vec{w})$  (maximizing likelihood)  
   $= \operatorname{argmin}_{\vec{w}} E_{in}(\vec{w})$  (minimizing cross-entropy error)

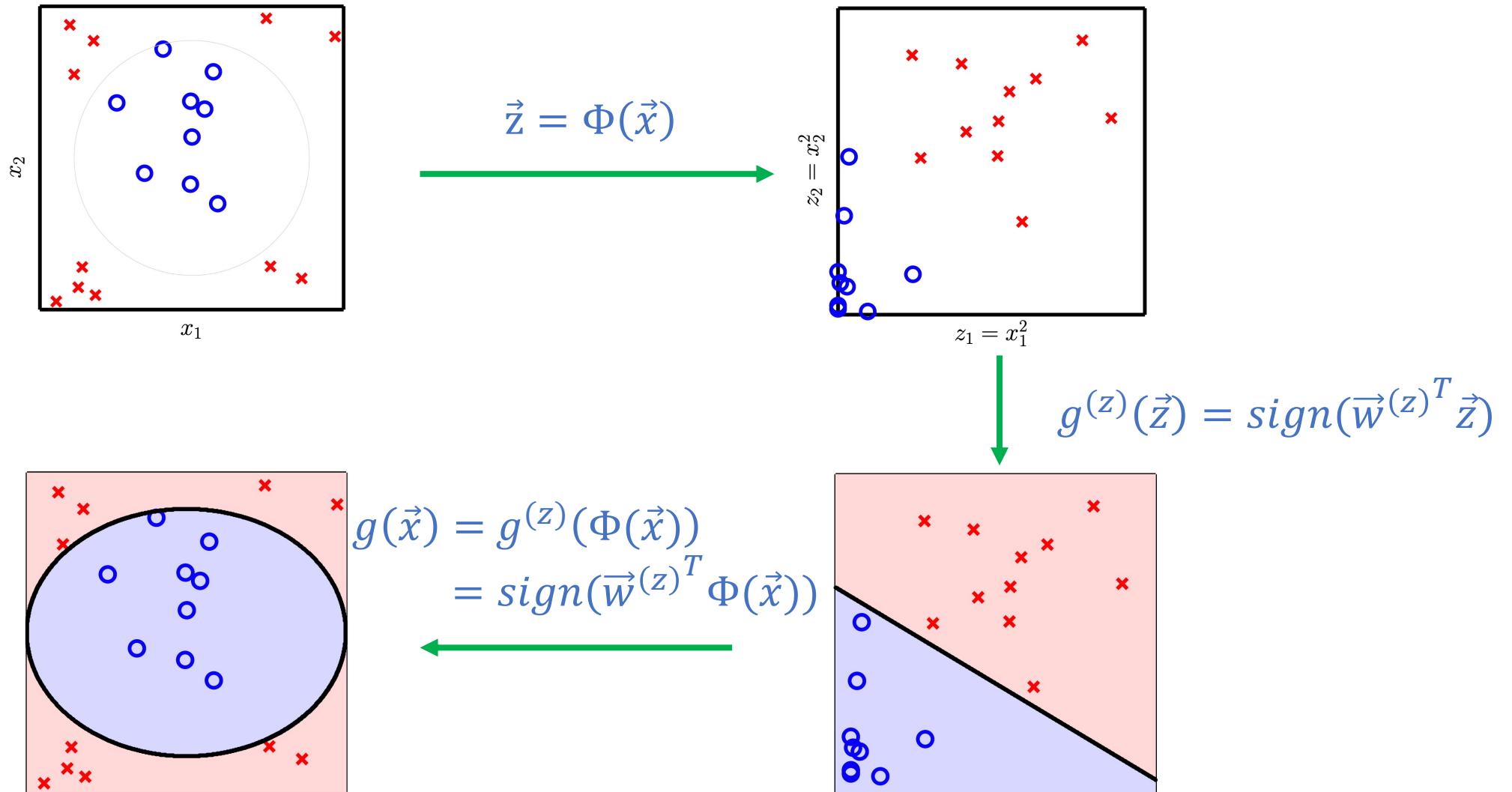
# Optimizing $E_{in}(\vec{w})$ : Gradient Descent

- Gradient descent algorithm
  - Initialize  $\vec{w}(0)$
  - For  $t = 0, \dots$ 
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}(\vec{w}(t))$
    - Terminate if the stop conditions are met
  - Return the final weights
- Stochastic gradient decent
  - Replace the update step:
    - Randomly choose  $n$  from  $\{1, \dots, N\}$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} e_n(\vec{w}(t))$



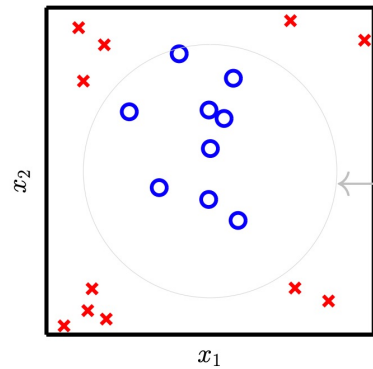
Works for functions where gradient exists everywhere

# Nonlinear Transformation

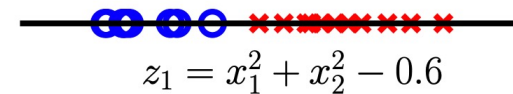
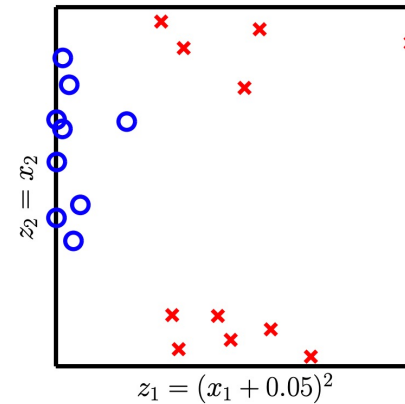
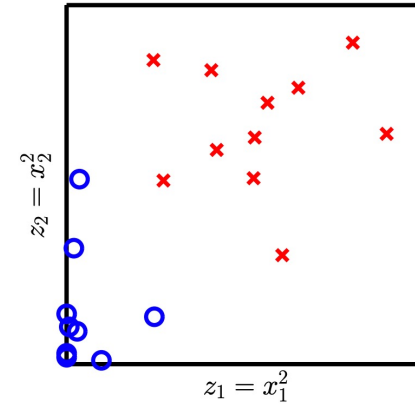




# How to Choose Feature Transform $\Phi$



$$x_1^2 + x_2^2 = 0.6$$



Something Seems Wrong!

Must choose  $\Phi$   
**BEFORE** looking at the data

Otherwise, you are doing “data snooping”

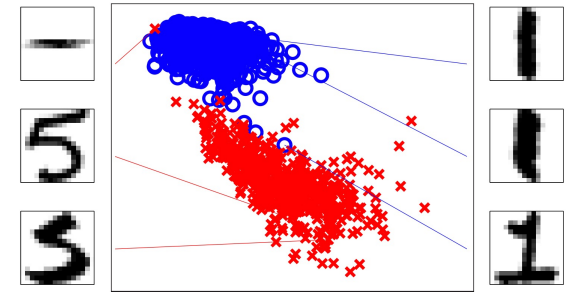
The hypothesis set  $H$  is as large as anything your brain can think of

# Today's Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.  
Let me know if you spot errors.

# Choose $\Phi$ Before Seeing Data

- Rely on domain knowledge (feature engineering)
  - Handwriting digit recognition example
- Use common sets of feature transformation
  - Polynomial transformation
  - 2nd order Polynomial transformation
    - $\vec{x} = (1, x_1, x_2)$
    - $\Phi_2(\vec{x}) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$
    - Pros: more powerful (contains circle, ellipse, hyperbola, etc)
    - Cons: 2-d  $\Rightarrow$  5-d
      - More computation/storage
      - Worse generalization error



The VC dimension of d-dim perceptron is  $d+1$

# Q-th Order Polynomial Transform

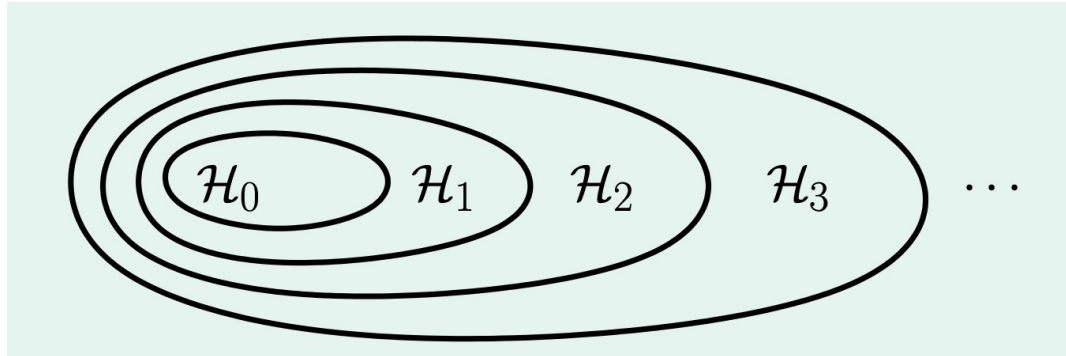
- $\vec{x} = (1, x_1, \dots, x_d)$
- From 1-st order to Q-th order polynomial transform:
  - $\Phi_1(\vec{x}) = \vec{x}$
  - $\Phi_2(\vec{x}) = (\Phi_1(\vec{x}), x_1^2, x_1x_2, x_1x_3, \dots, x_d^2)$
  - ...
  - $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1}x_2, \dots, x_d^Q)$
- Number of elements in  $\Phi_Q(\vec{x})$

# Q-th Order Polynomial Transform

- $\vec{x} = (1, x_1, \dots, x_d)$
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- Number of elements in  $\Phi_Q(\vec{x})$ 
  - $\binom{Q+d}{Q}$

# Structural Hypothesis Sets

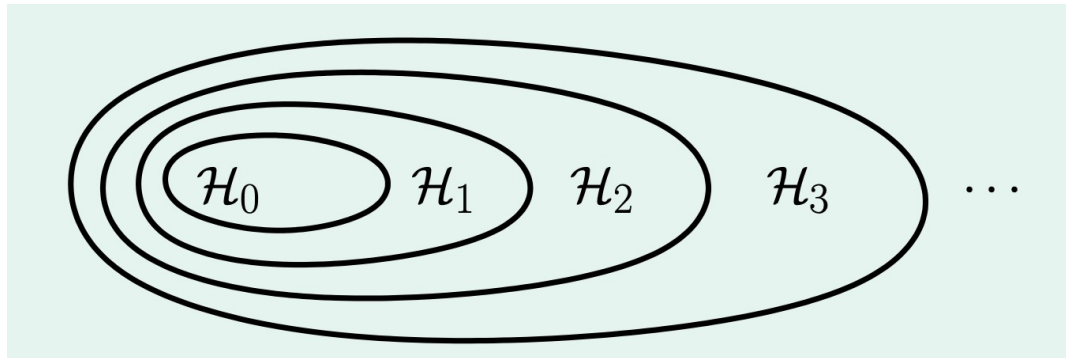
- Let  $H_Q$  be the linear model for the  $\Phi_Q(\vec{x})$  space



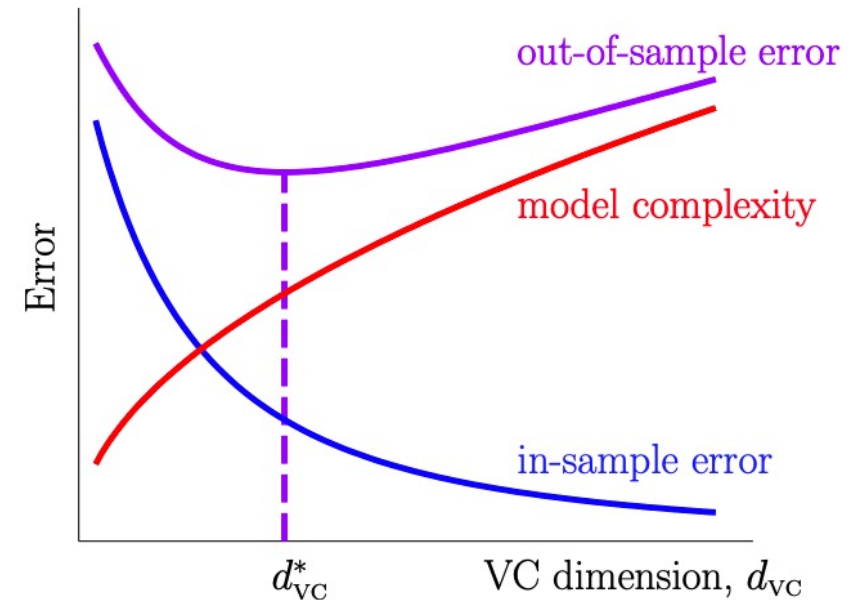
- Let  $g_Q = \operatorname{argmin}_{h \in H_Q} E_{in}(h)$ 
  - $H_0 \quad H_1 \quad H_2 \dots$
  - $d_{vc}(H_0) \quad d_{vc}(H_1) \quad d_{vc}(H_2) \dots$
  - $E_{in}(g_0) \quad E_{in}(g_1) \quad E_{in}(g_2) \dots$

# Structural Hypothesis Sets

- Let  $H_Q$  be the linear model for the  $\Phi_Q(\vec{x})$  space



- Let  $g_Q = \operatorname{argmin}_{h \in H_Q} E_{in}(h)$ 
  - $H_0 \subset H_1 \subset H_2 \dots$
  - $d_{vc}(H_0) \leq d_{vc}(H_1) \leq d_{vc}(H_2) \dots$
  - $E_{in}(g_0) \geq E_{in}(g_1) \geq E_{in}(g_2) \dots$





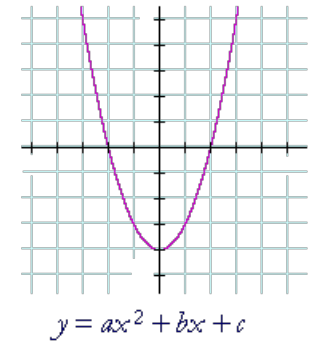
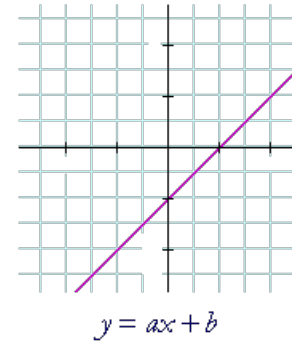
# Overfitting

[Adapted from the slides by Malik Magdon-Ismail]

# Setup of the Discussion

- Regression with polynomial transform

- Input: 1-dimensional  $x$
- $\Phi_Q(x) = (1, x, x^2, x^3, \dots, x^Q)$
- $H_Q = \{h(x) = w_0 + w_1x + w_2x^2 + \dots + w_Qx^Q\}$

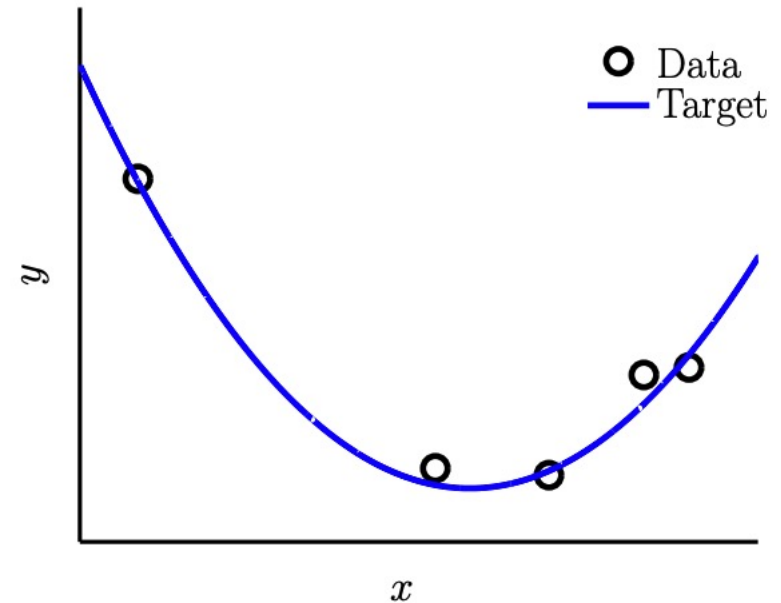


- $Q$ th-order polynomial fit

- Solve linear regression on the  $\Phi_Q(\vec{x})$  space using  $H_Q$
- Looking to minimize  $E_{in}$ :  $g_Q = \operatorname{argmin}_{h \in H_Q} E_{in}(h)$

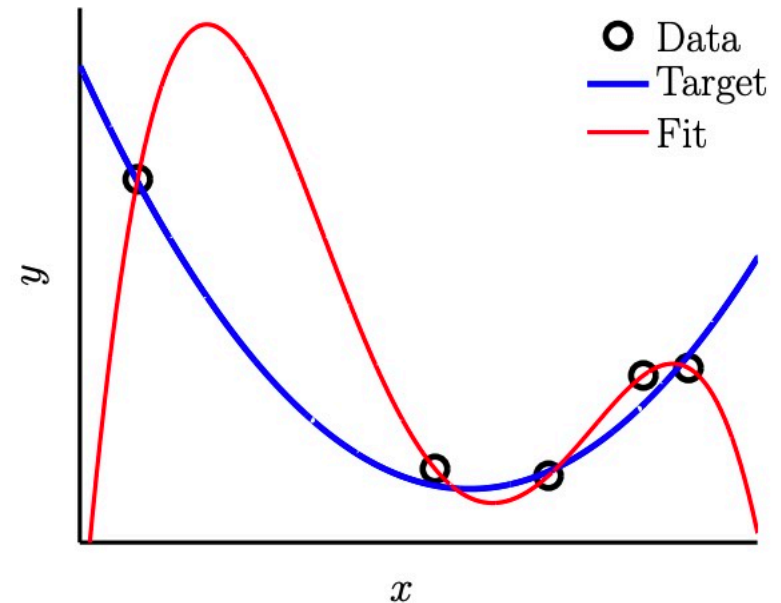
# A Simple Example

- Target  $f$ : 4<sup>th</sup> order function
- # data points:  $N = 5$
- Small noise:
  - $y = f(x) + \epsilon$  with small  $\epsilon$
- 4<sup>th</sup> order polynomial fit
  - $h(x) = w_0 + w_1x + w_2x^2 + w_3x^3 + w_4x^4$
  - Find  $g_4 = \operatorname{argmin}_h E_{in}(h)$



# A Simple Example

- Target  $f$ : 4<sup>th</sup> order function
- # data points:  $N = 5$
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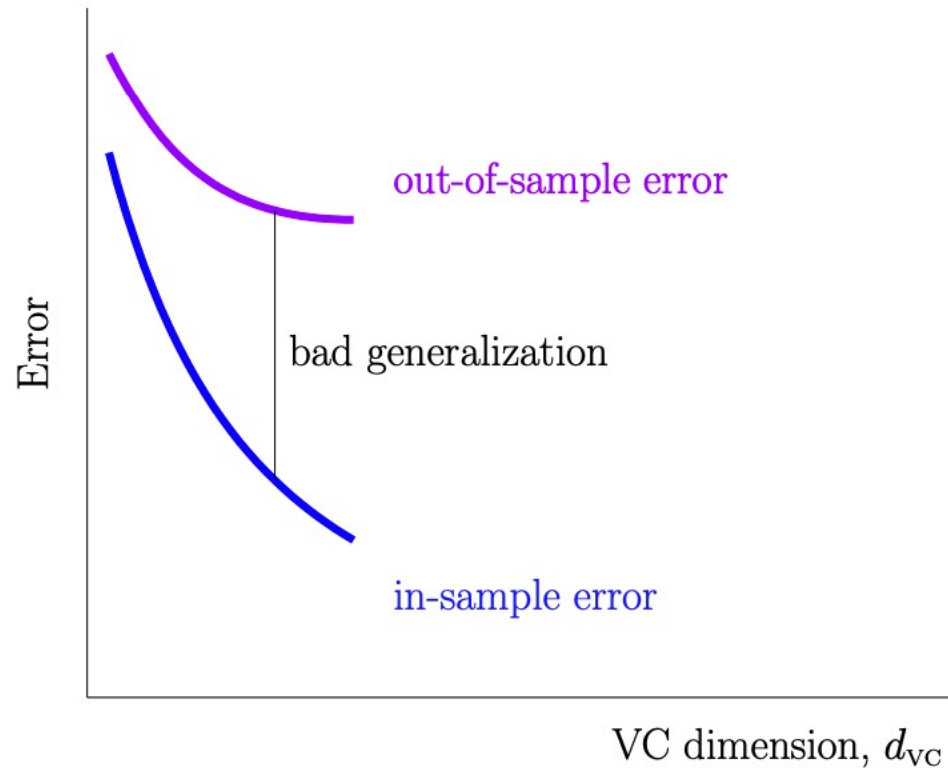
Classical overfitting:  $E_{in} = 0$ , but lead to a large  $E_{out}$

Fitting the **noise** instead of the target

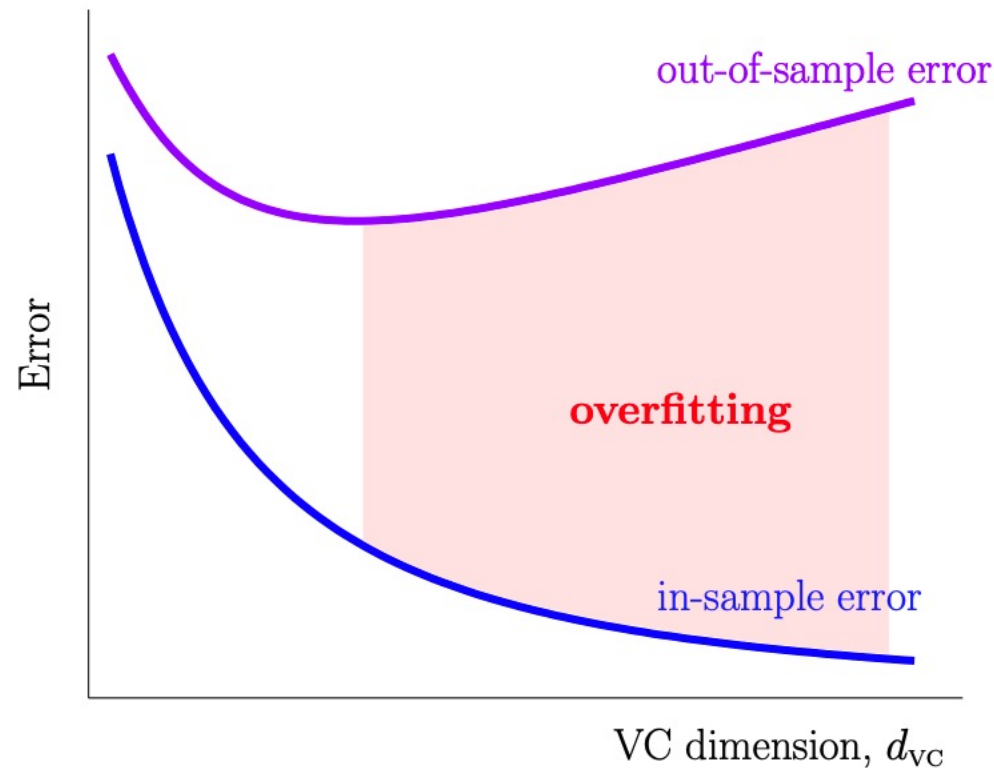
# What is Overfitting?

Fitting the data **more** than is **warranted**

# Overfitting is Not Just Bad Generalization



# Overfitting is Not Just Bad Generalization



Overfitting

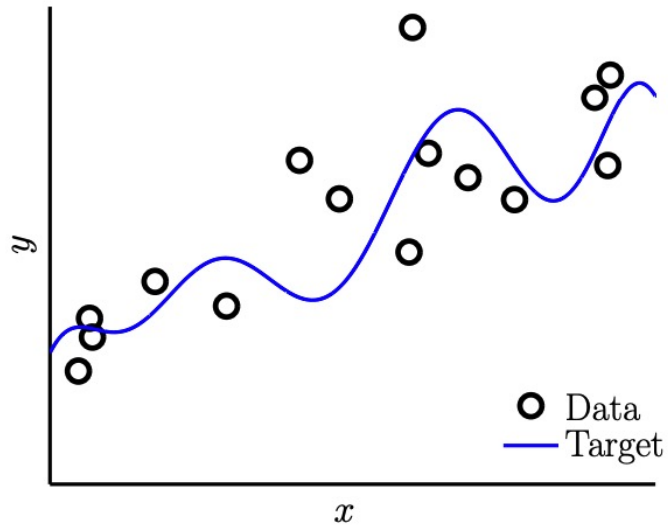
Going for **lower and lower**  $E_{in}$  results in **higher and higher**  $E_{out}$

# Case Study:

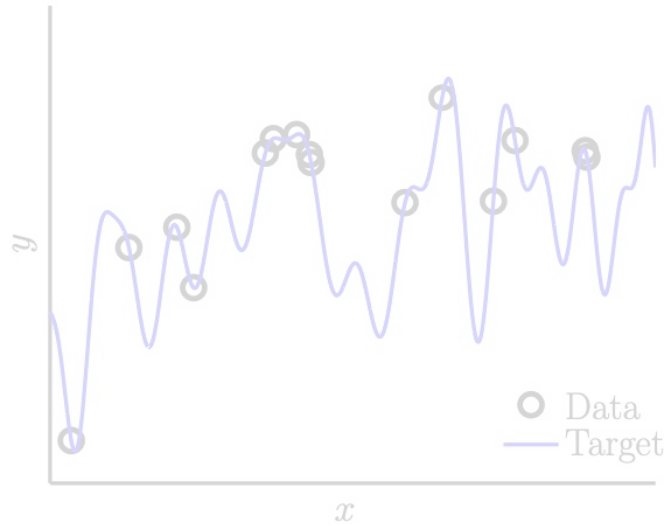
## $2^{\text{nd}}$ vs $10^{\text{th}}$ Order Polynomial Fit



N=15



10th order  $f$  with noise.



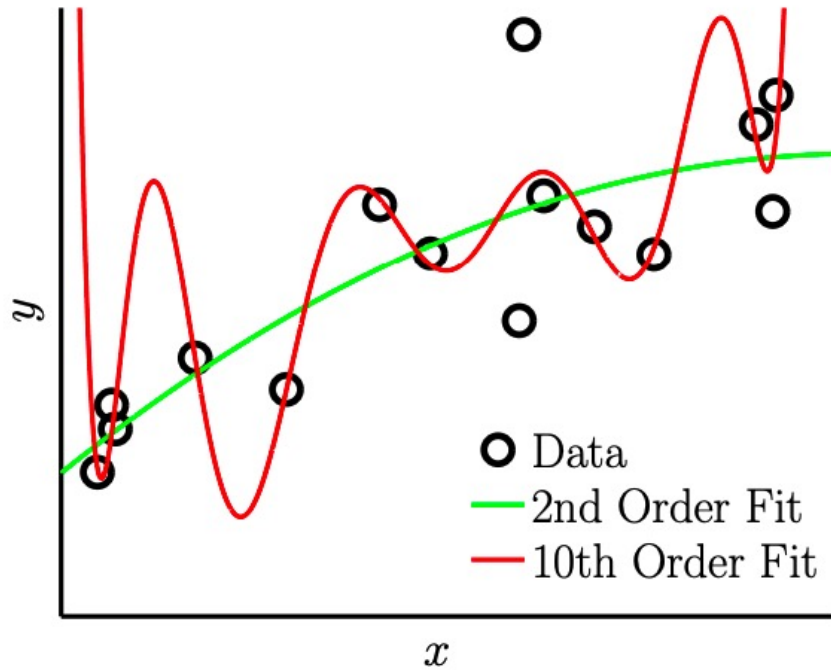
50th order  $f$  with no noise.

$H_2$ : 2<sup>nd</sup> order polynomial fit

$H_{10}$ : 10<sup>th</sup> order polynomial fit

**Which model would you choose for the left problem and why?**

# Target Function: 10<sup>th</sup> Order $f$ with Noise



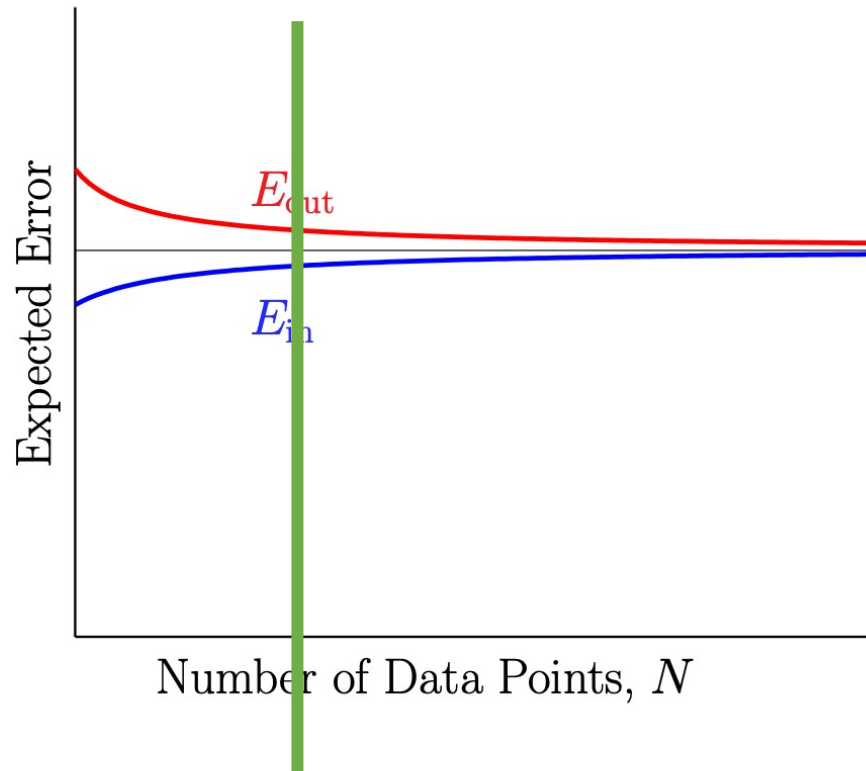
simple noisy target

	2nd Order	10th Order
$E_{\text{in}}$	0.050	0.034
$E_{\text{out}}$	0.127	9.00

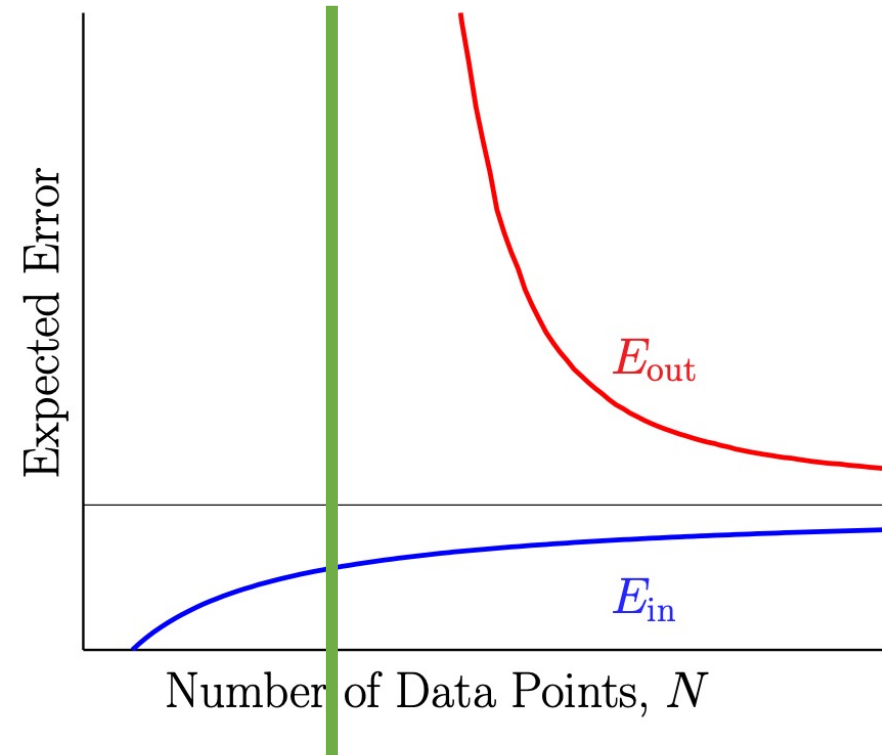
- Irony of two learners **Red** and **Green**
- Both know the target is 10<sup>th</sup> order
- **Red** chooses  $H_{10}$
- **Green** chooses  $H_2$
- **Green** outperforms **Red**

# Why is $H_2$ Better than $H_{10}$ ?

Learning curve for  $H_2$

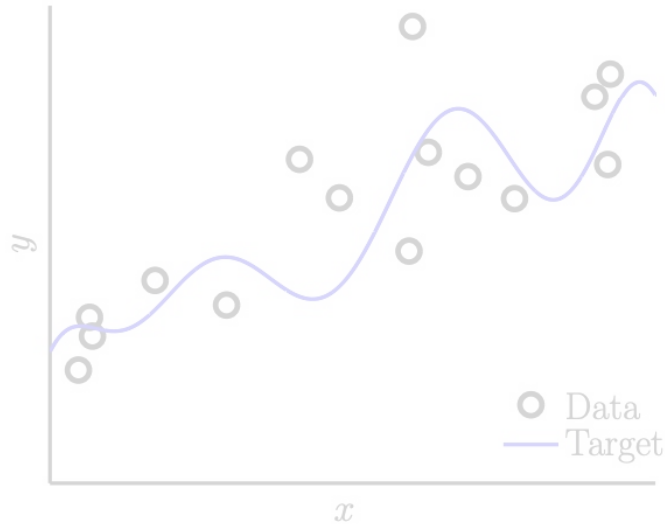


Learning curve for  $H_{10}$

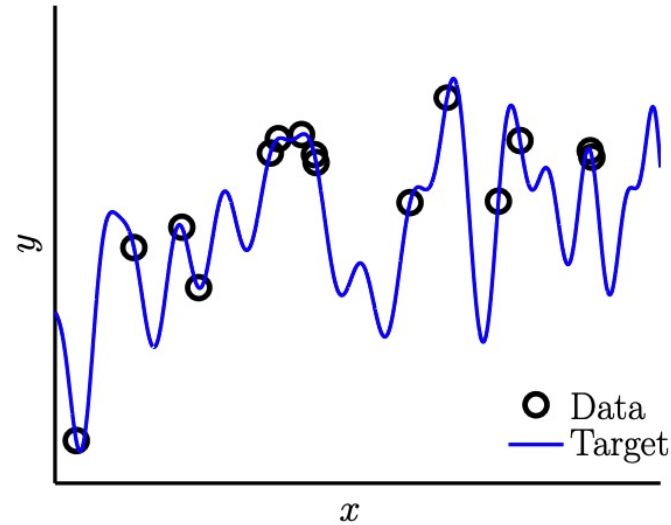


When  $N$  is small,  $E_{out}(g_{10}) \geq E_{out}(g_2)$

N=15



10th order  $f$  with noise.



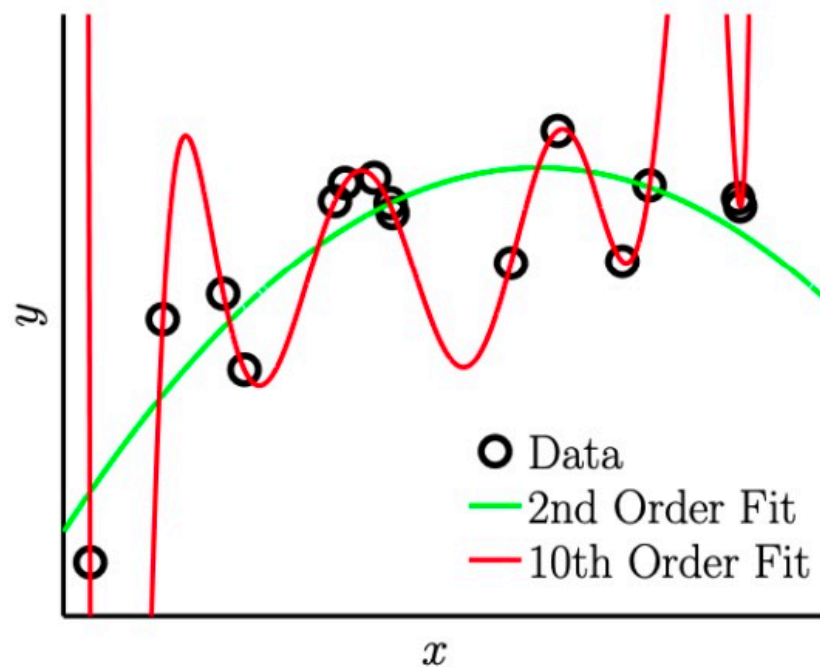
50th order  $f$  with no noise.

$H_2$ : 2<sup>nd</sup> order polynomial fit

$H_{10}$ : 10<sup>th</sup> order polynomial fit

**Which model do you choose for the right problem and why?**

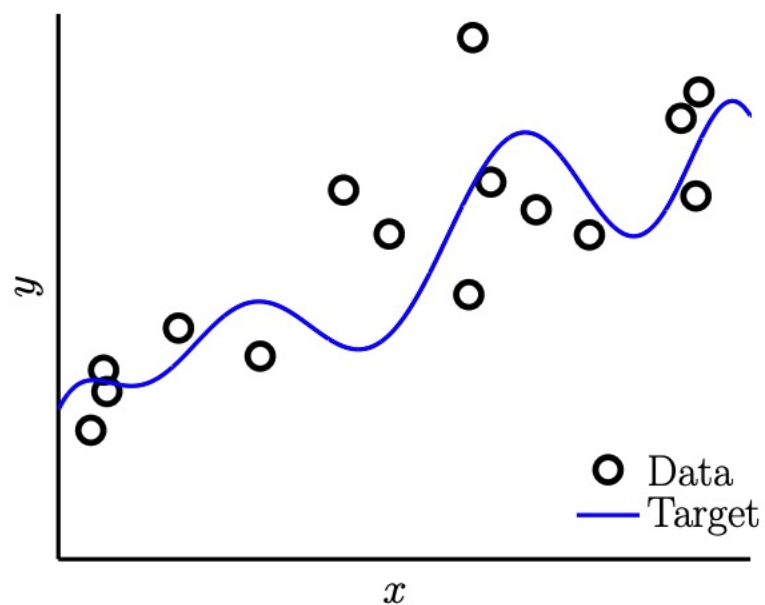
Simpler  $H$  is better even for complex target with **no noise**



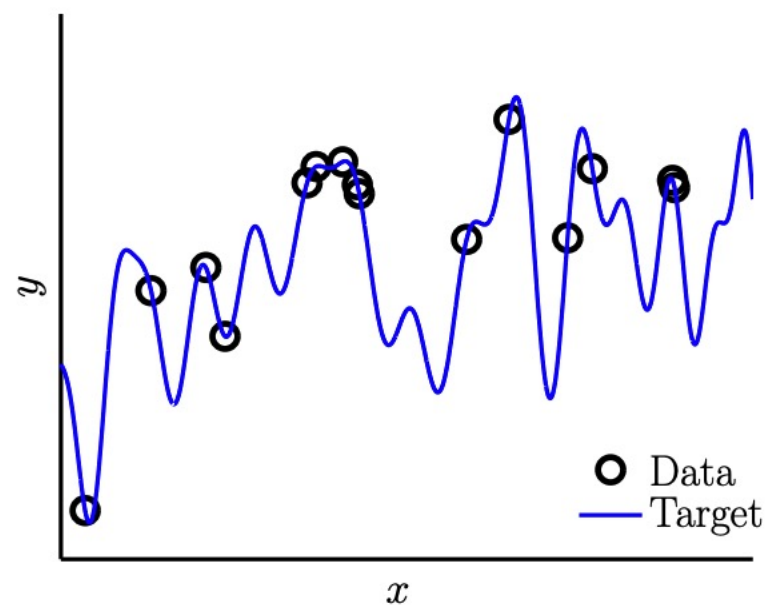
complex noiseless target

	2nd Order	10th Order
$E_{\text{in}}$	0.029	$10^{-5}$
$E_{\text{out}}$	0.120	<b>7680</b>

# Is There Really “No Noise”?

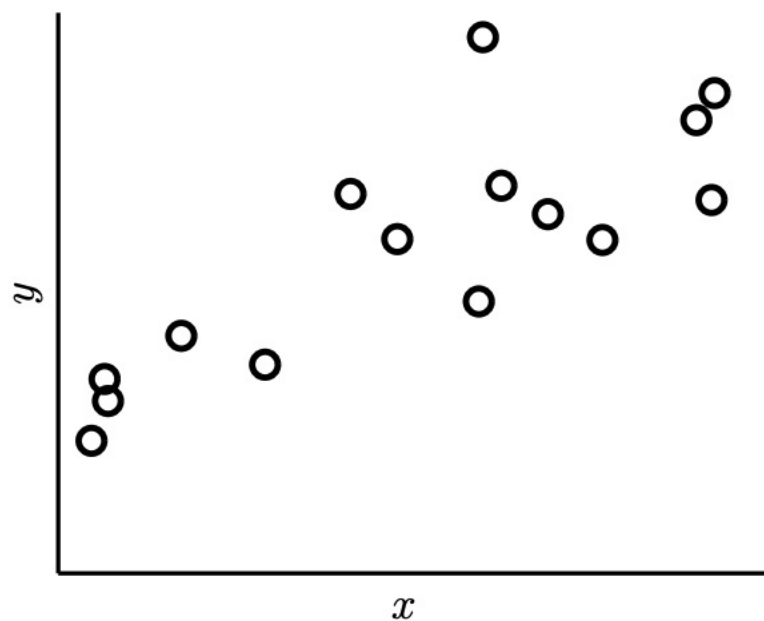


Simple  $f$  with noise.

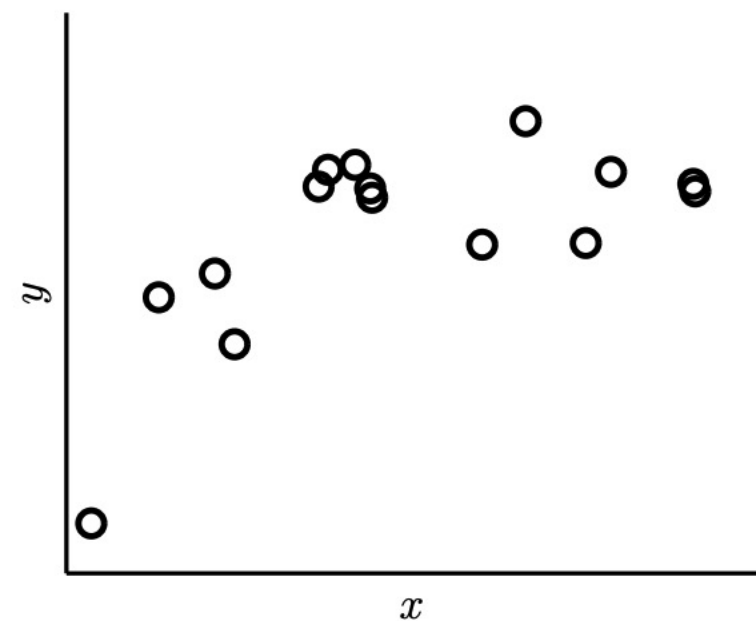


Complex  $f$  with no noise.

# Is There Really “No Noise”?



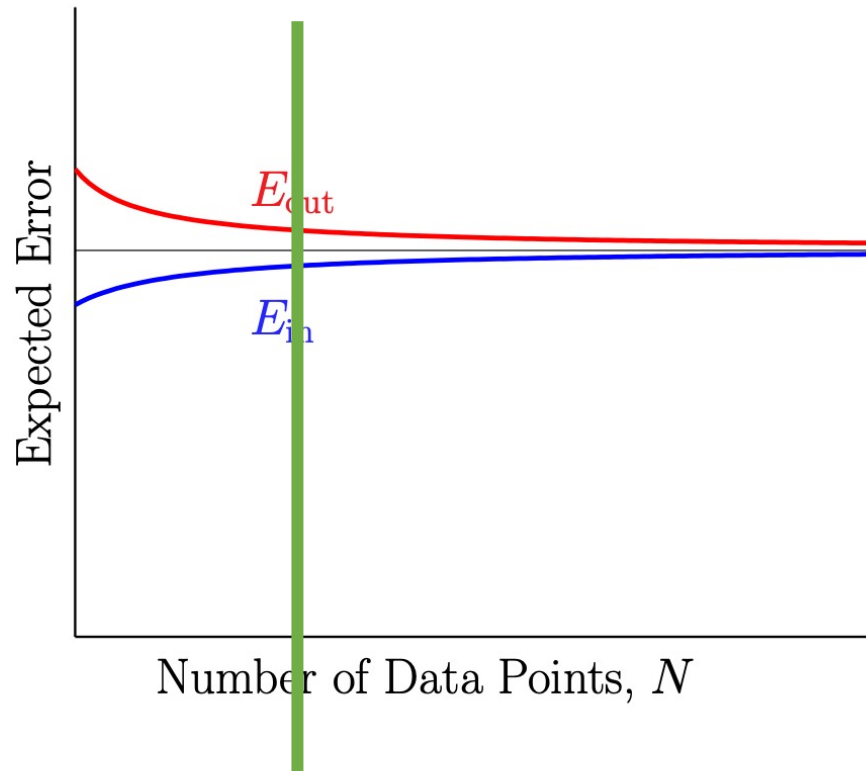
Simple  $f$  with noise.



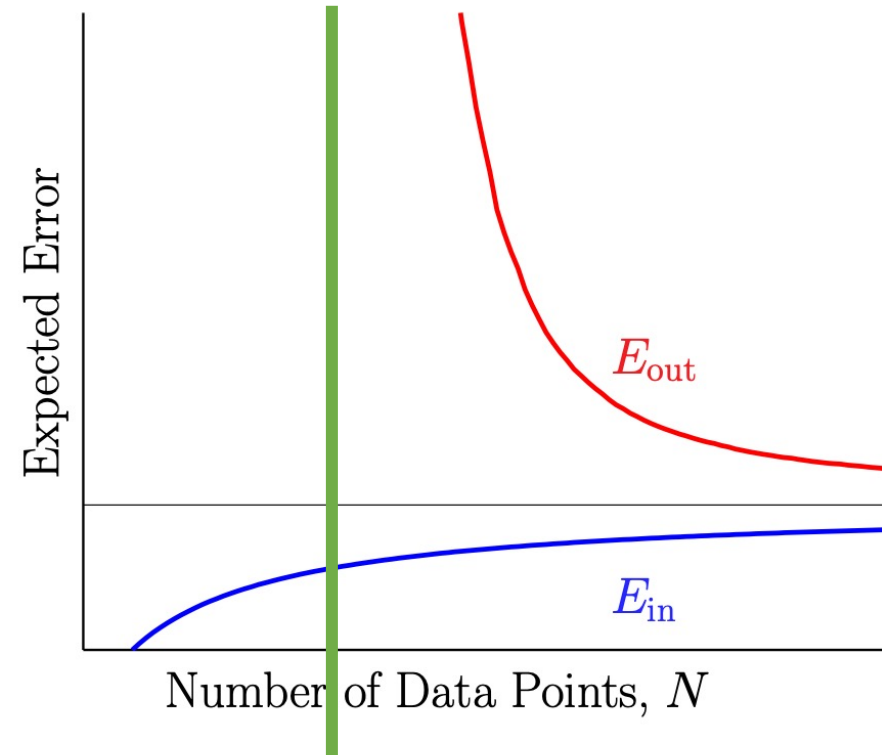
Complex  $f$  with no noise.

# Why is $H_2$ Better than $H_{10}$ ?

Learning curve for  $H_2$



Learning curve for  $H_{10}$



When  $N$  is small,  $E_{out}(g_{10}) \geq E_{out}(g_2)$



# A Detailed Experiment

Study the **level of noise** and **target complexity**, and **# data points  $N$**

$$y = f(x) + \epsilon(x) = \sum_{q=0}^{Q_f} \alpha_q x^q + \epsilon(x)$$

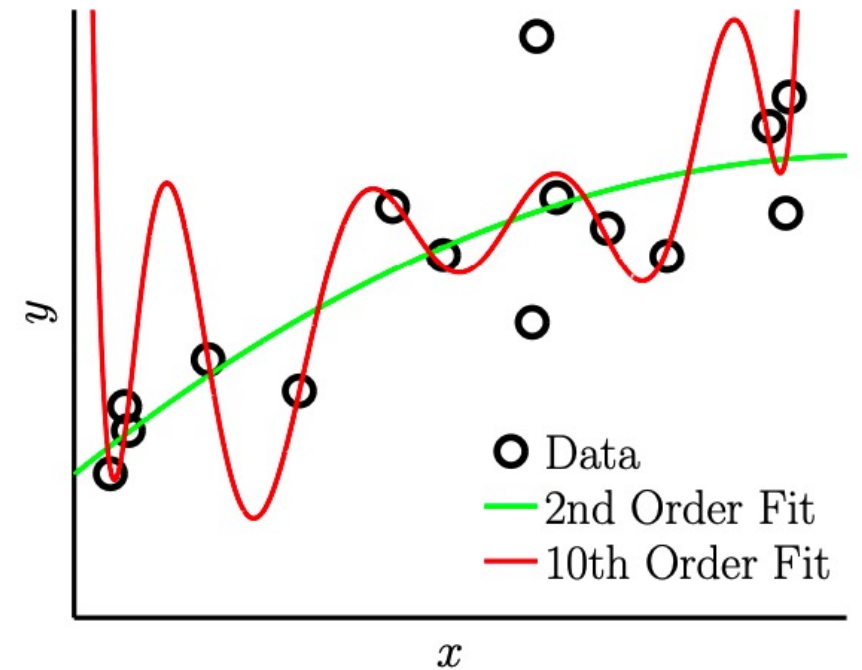
Noise level: variance  $\sigma^2$  of  $\epsilon(x)$

Target complexity:  $Q_f$

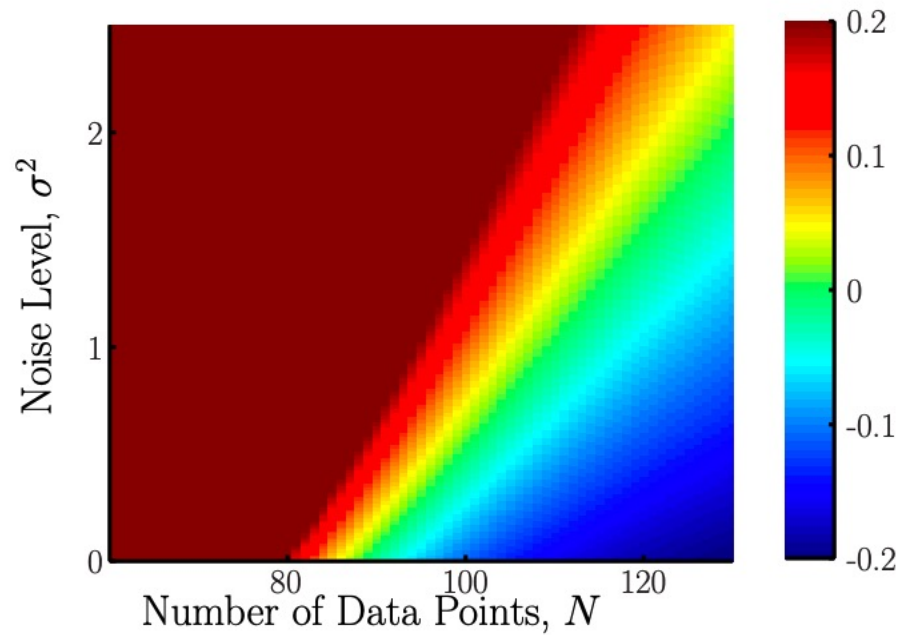
Data set size:  $N$

# The Overfit Measure

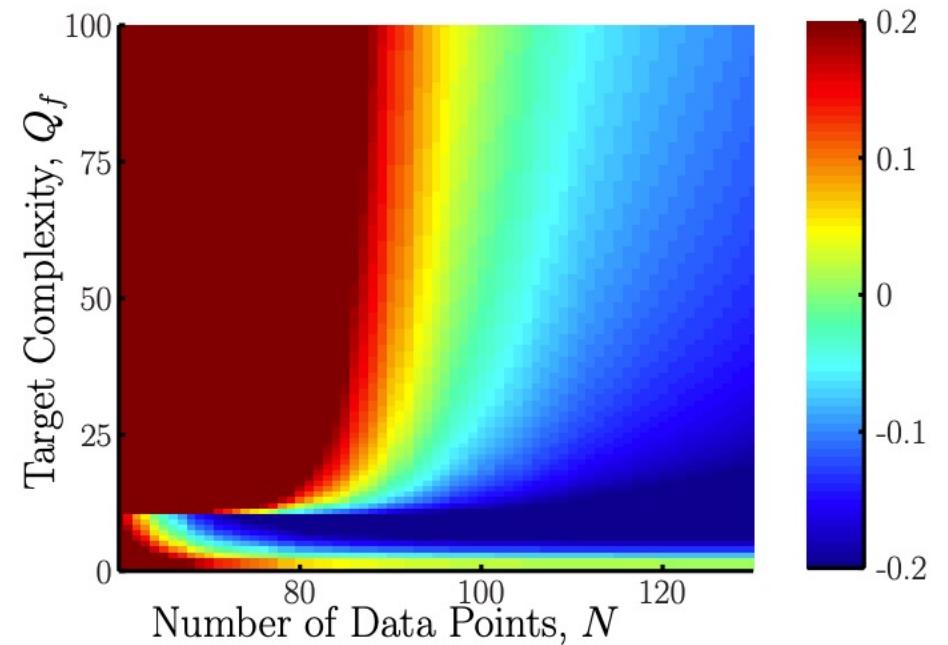
- Fit the data set using  $H_2$  and  $H_{10}$ 
  - Let  $g_2$  and  $g_{10}$  be the learned hypothesis
- Overfit measure
  - $E_{out}(g_{10}) - E_{out}(g_2)$
  - This value is large is overfitting happens



Overfit Measure:  $E_{out}(g_{10}) - E_{out}(g_2)$



Stochastic noise



deterministic noise

Number of data points $\uparrow$	Overfitting $\downarrow$
Noise $\uparrow$	Overfitting $\uparrow$
Target complexity $\uparrow$	Overfitting $\uparrow$

Noise:

The part of  $y$  we cannot model

# Stochastic Noise

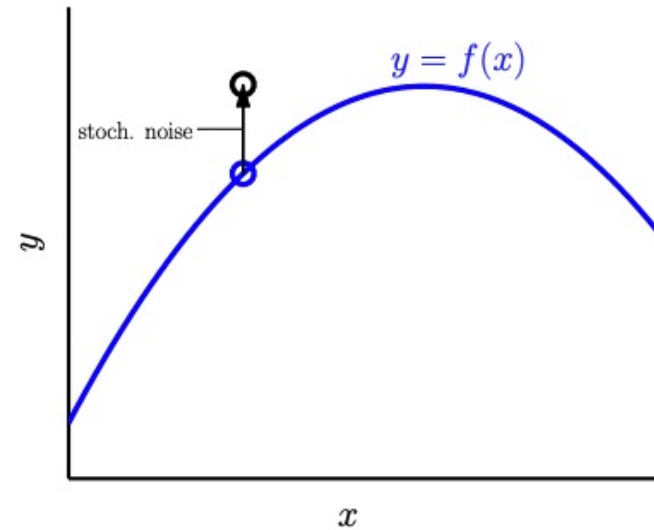
We would like to learn from ○:

$$y_n = f(x_n)$$

Unfortunately, we only observe ●:

$$y_n = f(x_n) + \text{'stochastic noise'}$$

↑  
no one can model this



**Stochastic Noise:** fluctuations/measurement errors we cannot model.

# Stochastic Noise

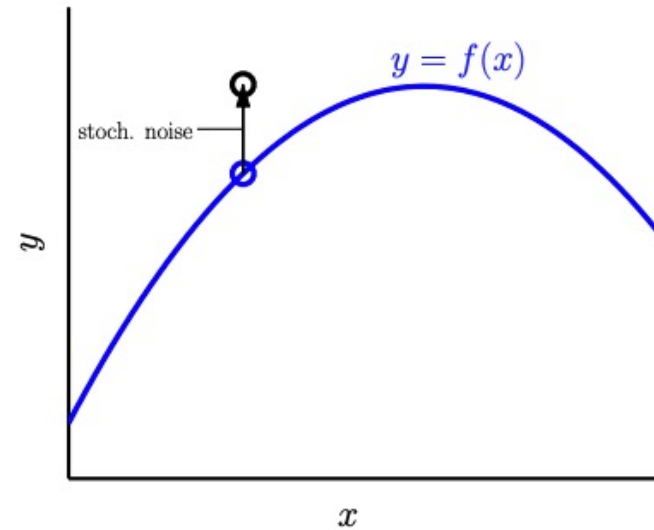
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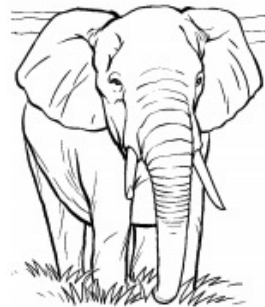
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**Stochastic Noise:** fluctuations/measurement errors we cannot model.



# Deterministic Noise

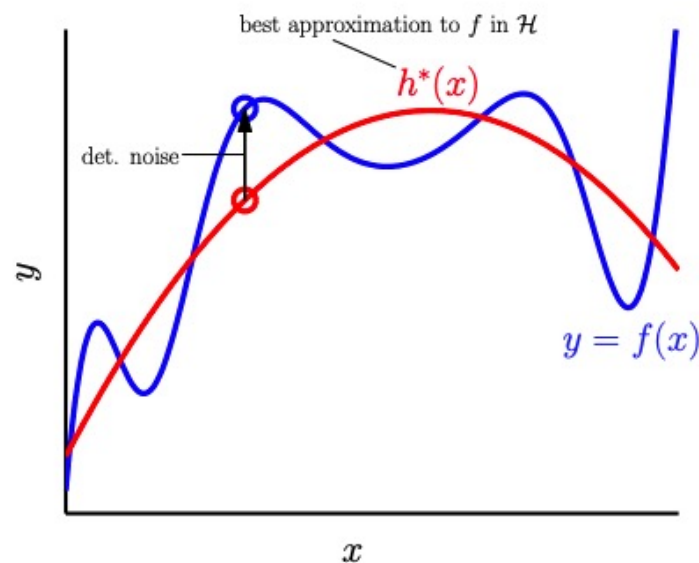
We would like to learn from  $\circ$ :

$$y_n = h^*(x_n)$$

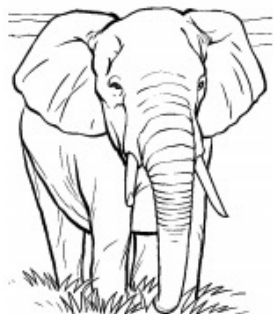
Unfortunately, we only observe  $\circ$ :

$$\begin{aligned} y_n &= f(x_n) \\ &= h^*(x_n) + \text{'deterministic noise'} \end{aligned}$$

↑  
 $\mathcal{H}$  cannot model this



**Deterministic Noise:** the part of  $f$  we cannot model.



# Deterministic Noise

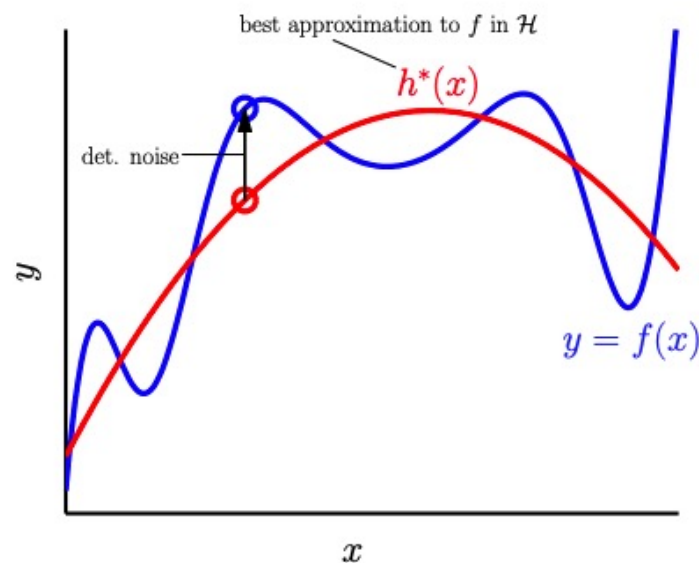
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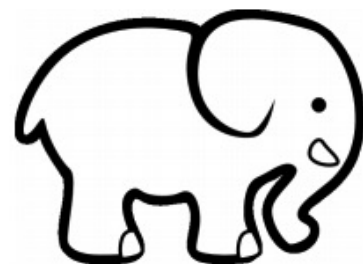
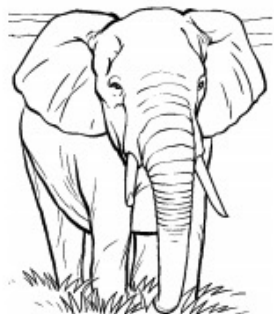
Unfortunately, we only observe  $\circ$ :

$$\begin{aligned} y_n &= f(x_n) \\ &= h^*(x_n) + \text{'deterministic noise'} \end{aligned}$$

↑  
 $\mathcal{H}$  cannot model this



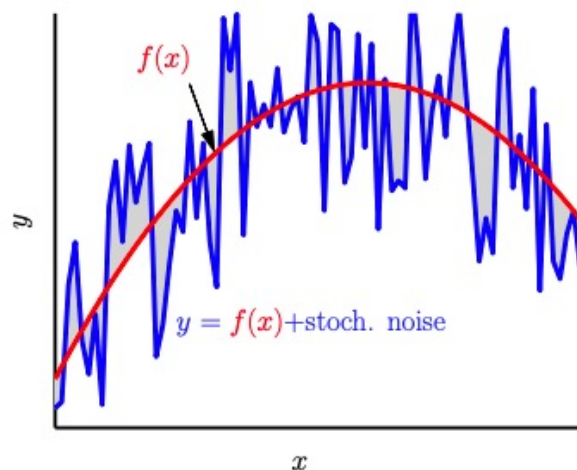
**Deterministic Noise:** the part of  $f$  we cannot model.





# Both sources of noises hurt learning

Stochastic Noise



**source:** random measurement errors

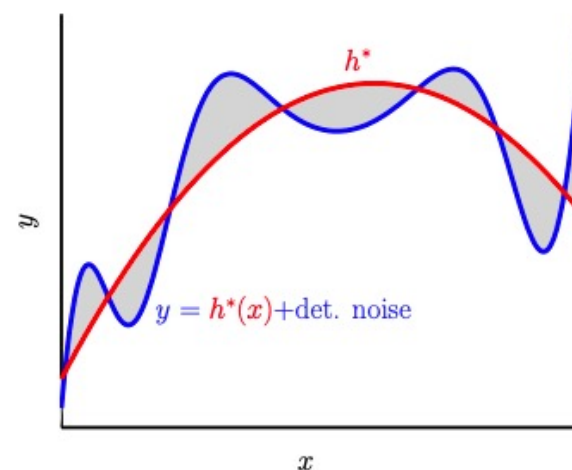
re-measure  $y_n$

stochastic noise changes.

change  $\mathcal{H}$

stochastic noise the same.

Deterministic Noise



**source:** learner's  $\mathcal{H}$  cannot model  $f$

re-measure  $y_n$

deterministic noise the same.

change  $\mathcal{H}$

deterministic noise changes.

**We have single  $\mathcal{D}$  and fixed  $\mathcal{H}$  so we cannot distinguish**

# Noise and Bias-Variance Decomposition

$$y = f(\vec{x}) + \epsilon$$

$$\mathbb{E}[E_{out}(\vec{x})] = \sigma^2 + \text{bias} + \text{variance}$$



Stochastic Noise



Deterministic noise

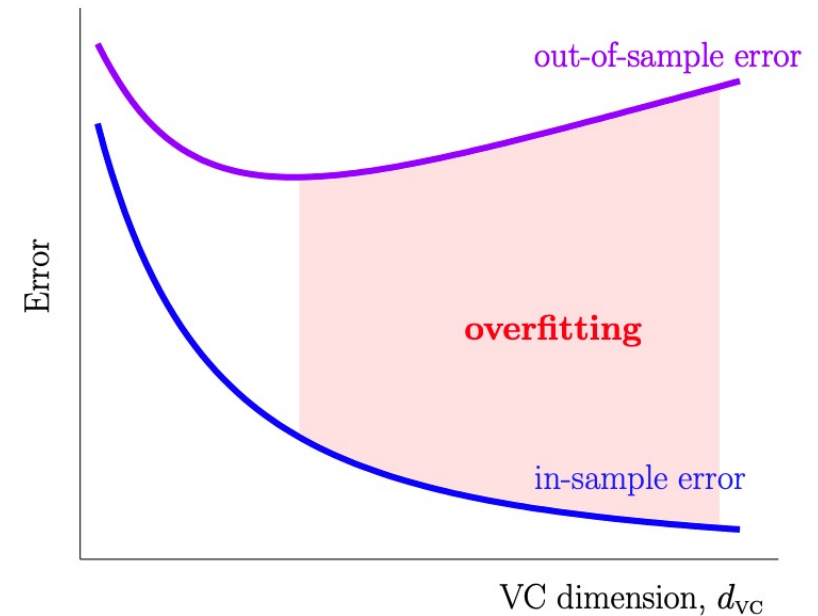
# How to Fight Overfitting

- VC Bound

$$E_{out}(g) \leq E_{in}(g) + O\left(\sqrt{d_{vc} \frac{\ln N}{N}}\right)$$

- Fighting overfitting

- Regularization
- Validation
- (The focus of the next two lectures)



VC Dimension of  $d$ -dim Perceptron

# Recall the Definitions

- Shatter

- $H$  **shatters**  $(\vec{x}_1, \dots, \vec{x}_N)$  if  $|H(\vec{x}_1, \dots, \vec{x}_N)| = 2^N$
- $H$  can induce all label combinations for  $(\vec{x}_1, \dots, \vec{x}_N)$

- Break point

- $k$  is a **break point** for  $H$  if no data set of size  $k$  can be shattered by  $H$
- $k$  is a break point for  $H \leftrightarrow m_H(k) < 2^k$

- VC Dimension:  $d_{vc}(H)$  or  $d_{vc}$

- The VC dimension of  $H$  is the largest  $N$  such that  $m_H(N) = 2^N$
- Equivalently, if  $k^*$  is the smallest break point for  $H$ ,  $d_{vc}(H) = k^* - 1$

# VC Dimension of d-dimension Perceptron

- Claim:
  - The VC Dimension of d-dim perceptron is  $d + 1$
- How to prove it?
  1. Show that the VC dimension of d-dim perceptron  $\geq d + 1$
  2. Show that the VC dimension of d-dim perceptron  $\leq d + 1$

- To prove  $d_{vc}(H) \geq d + 1$ , what do we need to prove?
  - A. There is a set of  $d + 1$  points that can be shattered by  $H$
  - B. There is a set of  $d + 1$  points that cannot be shattered by  $H$
  - C. Every set of  $d + 1$  points can be shattered by  $H$
  - D. Every set of  $d + 1$  points cannot be shattered by  $H$

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- To prove  $d_{vc}(H) \leq d + 1$ , what do we need to prove?
  - A. There is a set of  $d + 1$  points that can be shattered by  $H$
  - B. There is a set of  $d + 2$  points that cannot be shattered by  $H$
  - C. Every set of  $d + 2$  points can be shattered by  $H$
  - D. Every set of  $d + 1$  points cannot be shattered by  $H$
  - E. Every set of  $d + 2$  points cannot be shattered by  $H$

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  - E. Every set of  $d + 2$  points cannot be shattered by  $H$

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Every set of  $d + 2$  points cannot be shattered by  $H$

- To prove  $d_{vc}(H) \geq d + 1$ , what do we need to prove?  
**There is a set of  $d + 1$  points that can be shattered by  $H$**

Proof Sketch:

1. Let's construct a dataset of  $d + 1$  points:  $X = \begin{bmatrix} \vec{x}_1^T \\ \vdots \\ \vec{x}_{d+1}^T \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & \dots & 1 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 1 & 1 & 0 & \dots & 0 & 0 \end{bmatrix}$ ; It's easy to check that  $X^{-1}$  exist
2. For any possible dichotomy  $\vec{y}$ , there exists a  $\vec{w}$  such that  $X\vec{w} = \vec{y}$ , i.e.,  $\vec{w} = X^{-1}\vec{y}$
3. Therefore, d-dim perceptron can shatter  $X$

- To prove  $d_{vc}(H) \leq d + 1$ , what do we need to prove?  
**Every set of  $d + 2$  points cannot be shattered by  $H$**

Proof Sketch:

1. For every set of  $d + 2$  points (in  $d+1$  dimensions), there exists a point that can be written as linear combinations of the others.
2. Denote the point  $\vec{x}_{d+2}$ , we have  $\vec{x}_{d+2} = \sum_{i=1}^{d+1} a_i \vec{x}_i$
3. Consider the dichotomy  $(y_1, \dots, y_{d+2}) = (\text{sign}(a_1), \dots, \text{sign}(a_{d+1}), -1)$ , we can show that no linear separator can generate this dichotomy (think about why).
4. Therefore, for every set of  $d + 2$  points, there exist at least one dichotomy that  $H$  cannot induce.