CSE 417T
Introduction to Machine Learning

Lecture 10

Instructor: Chien-Ju (CJ) Ho

Logistics

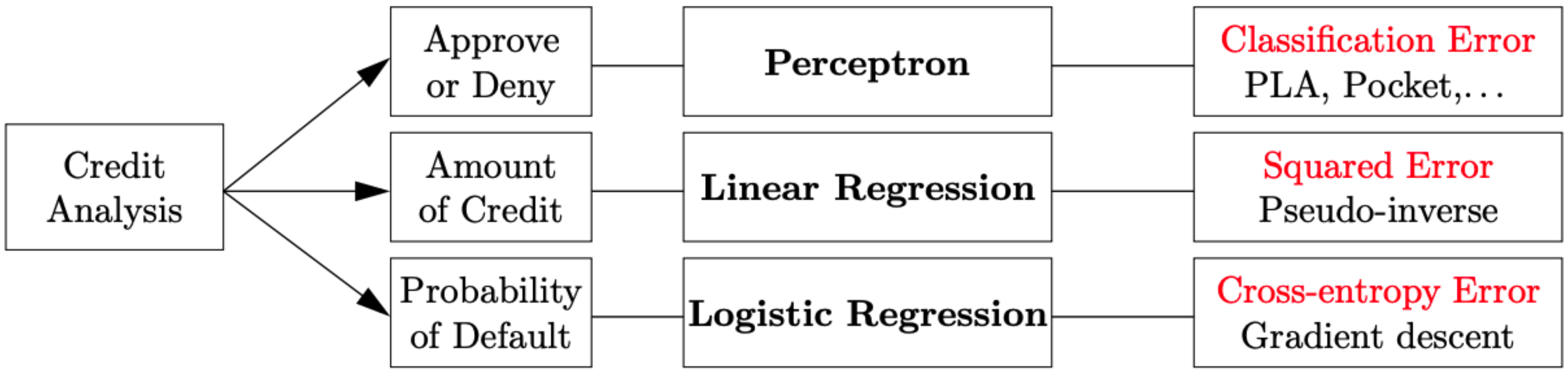
- Homework 2: due on **Mar 8, Monday**
- Exam 1: **Mar 23 (Tuesday)**
- No class next Tuesday (Wellness day)

Recap

Linear Models

This is why it's called linear models

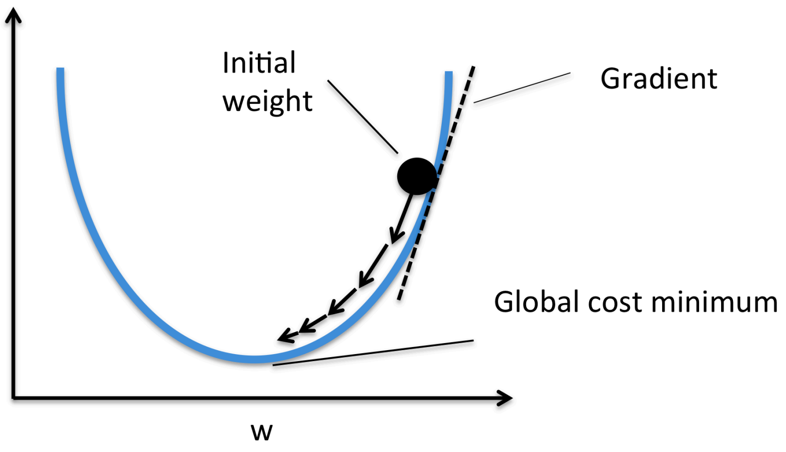
- H contains hypothesis $h(\vec{x})$ as **some function of $\vec{w}^T\vec{x}$**



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

Gradient Descent

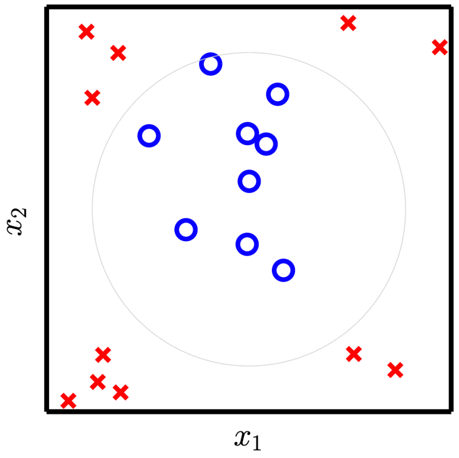
- Gradient descent algorithm
  - Initialize $\vec{w}(0)$
  - For $t = 0, \ldots$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}\left(\vec{w}(t)\right)$
    - Terminate if the stop conditions are met
  - Return the final weights



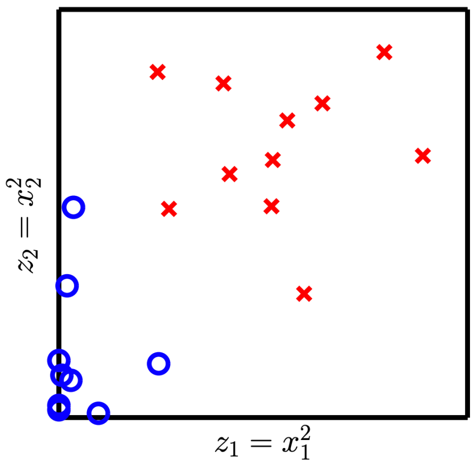
Works for functions where gradient exists everywhere

- Stochastic gradient decent
  - Replace the update step:
    - Randomly choose n from $\{1, \ldots, N\}$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} e_n(\vec{w}(t))$

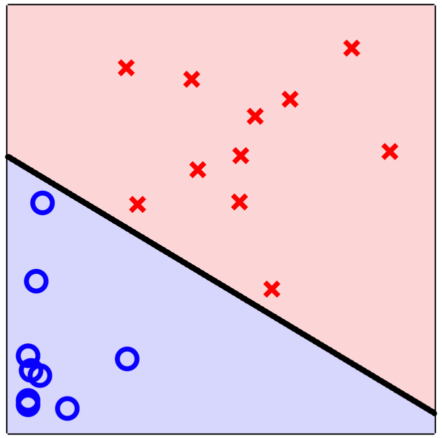
Nonlinear Transformation



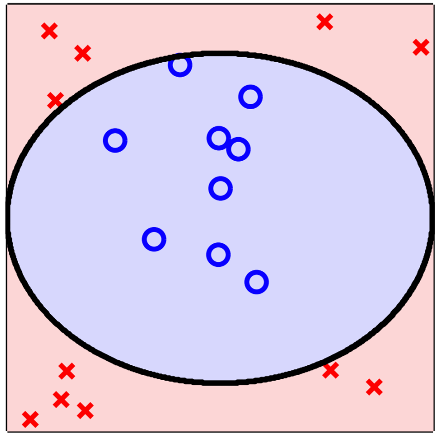
$$\vec{z} = \Phi(\vec{x})$$



$$g^{(z)}(\vec{z}) = sign(\overrightarrow{w}^{(z)^T}\vec{z})$$



$$g(\vec{x}) = g^{(z)}(\Phi(\vec{x}))$$
$$= sign(\overrightarrow{w}^{(z)^T}\Phi(\vec{x}))$$



Must Choose Φ BEFORE Looking at the Data

- Rely on domain knowledge (feature engineering)
  - Handwriting digit recognition example

- Use common sets of feature transformation
  - Polynomial transformation
  - E.g., 2nd order Polynomial transformation
    - $\vec{x} = (1, x_1, x_2),\ \Phi_2(\vec{x}) = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$
    - Plus: more powerful (contains circle, ellipse, hyperbola, etc)
    - Minus:
      - More computation/storage
      - Worse generalization error

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

Q-th Order Polynomial Transform

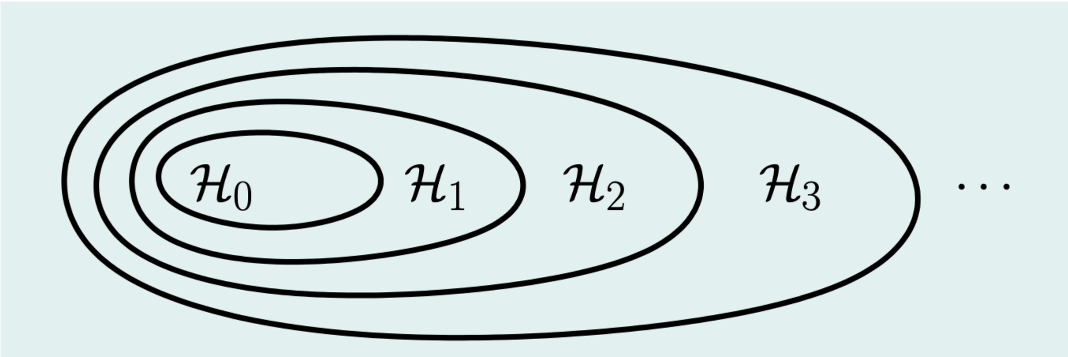
- Q-th Order Polynomial Transform
  - $\Phi_1(\vec{x}) = \vec{x}$
  - $\Phi_2(\vec{x}) = (\Phi_1(\vec{x}), x_1^2, x_1 x_2, x_1 x_3, \dots, x_d^2)$
  - …
  - $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1} x_2, \dots, x_d^Q)$

- Each element in $\Phi_Q(\vec{x})$ is in the form of $\prod_{i=1}^{d} x_i^{a_i}$
  - where $\sum_{i=1}^{d} a_i \leq Q$, and a_i is a non-negative integer

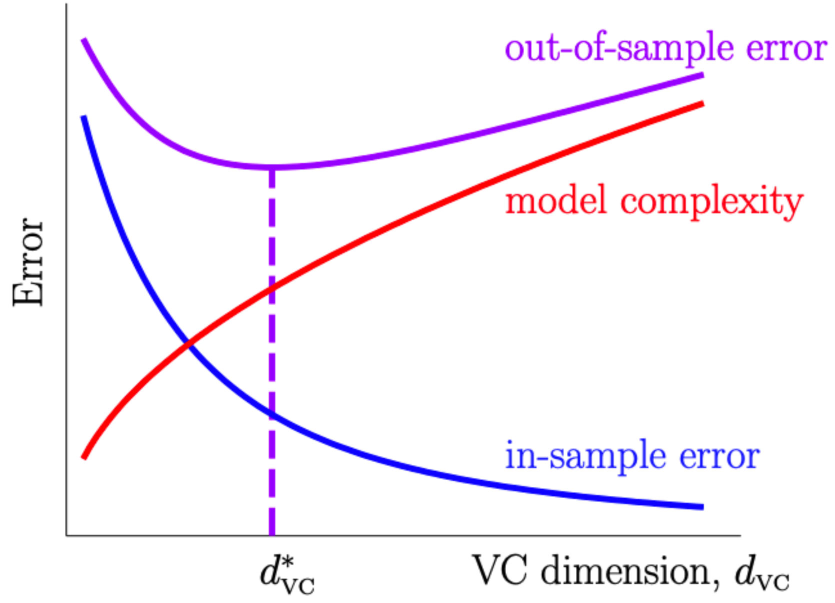
- Number of elements in $\Phi_Q(\vec{x})$: $\binom{Q+d}{Q}$ (including the initial 1)

Structural Hypothesis Sets

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



- Let $g_Q = argmin_{h \in H_Q} E_{in}(h)$
  - $H_1 \subseteq H_2 \subseteq H_3 \subseteq \cdots$
  - $d_{vc}(H_1) \leq d_{vc}(H_2) \leq \cdots$
  - $E_{in}(g_1) \geq E_{in}(g_2) \geq \cdots$



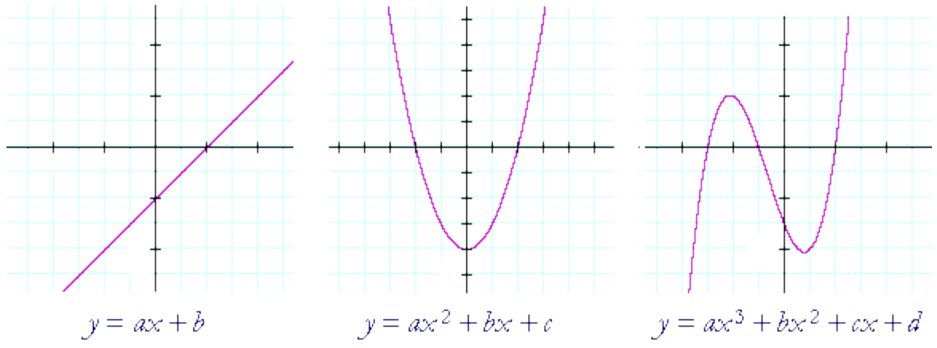
Today’s Lecture

Overfitting

[Adapted from the slides by Malik Magdon-Ismail]

Setup of the Discussion

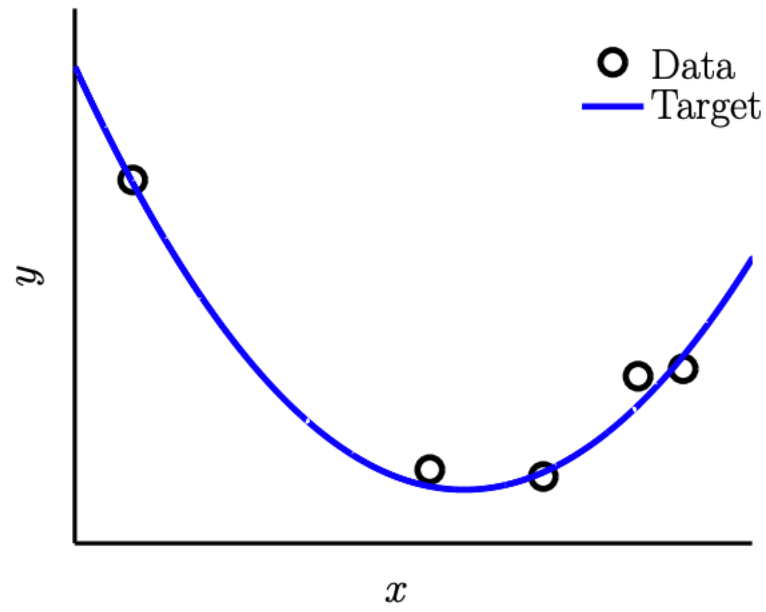
- Regression with polynomial transform
  - Input: 1-dimensional x
  - $\Phi_Q(x) = (1, x, x^2, x^3, \dots, x^Q)$
  - $H_Q = \{h(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_Q x^Q\}$



- Qth-order polynomial fit
  - Solve linear regression on the $\Phi_Q(\vec{x})$ space using H_Q
  - Looking to minimize E_{in}: $g_Q = argmin_{h \in H_Q} E_{in}(h)$

A Simple Example

- Target f: 4th order function
- # data points: $N = 5$
- Small noise:
    - $y = f(x) + \epsilon$ with small ϵ
- 4th order polynomial fit
    - $h(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4$
    - Find $g_4 = argmin_h E_{in}(h)$



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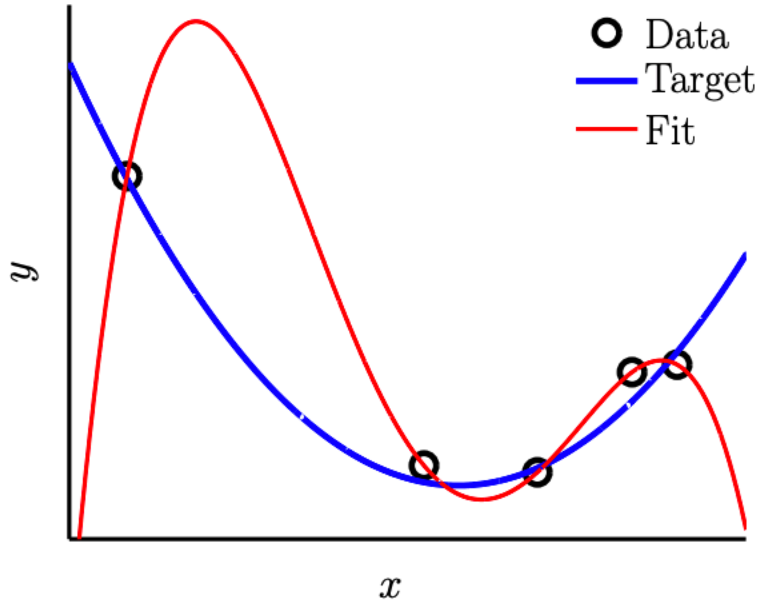


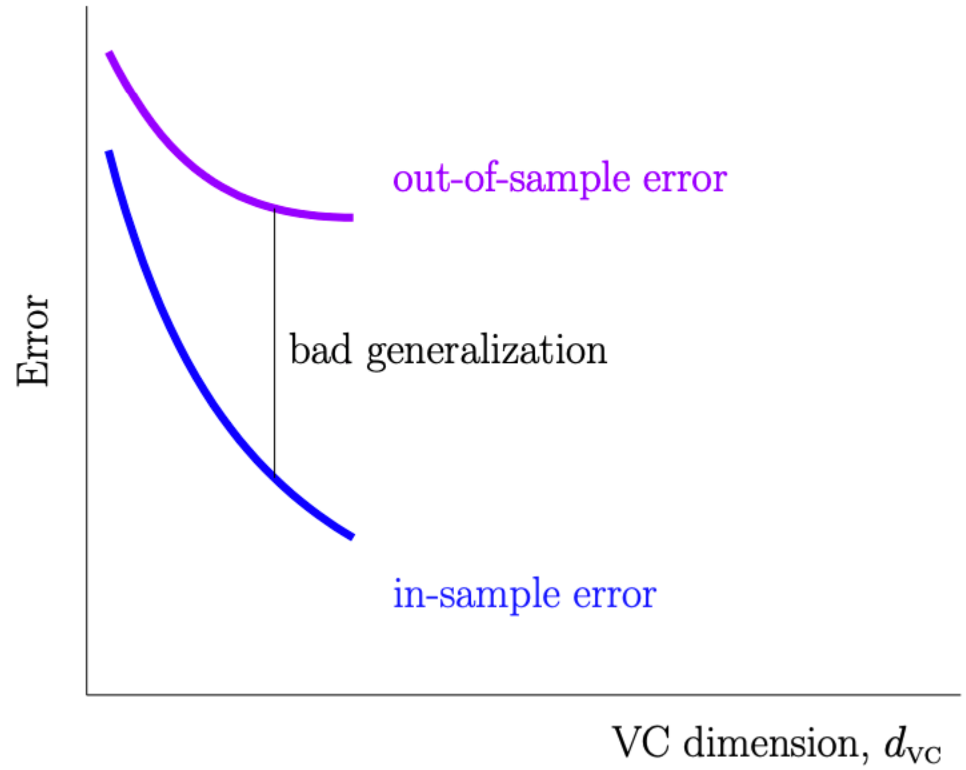
Classical overfitting: $E_{in} = 0$, but lead to a large E_{out}

Fitting the **noise** instead of the target

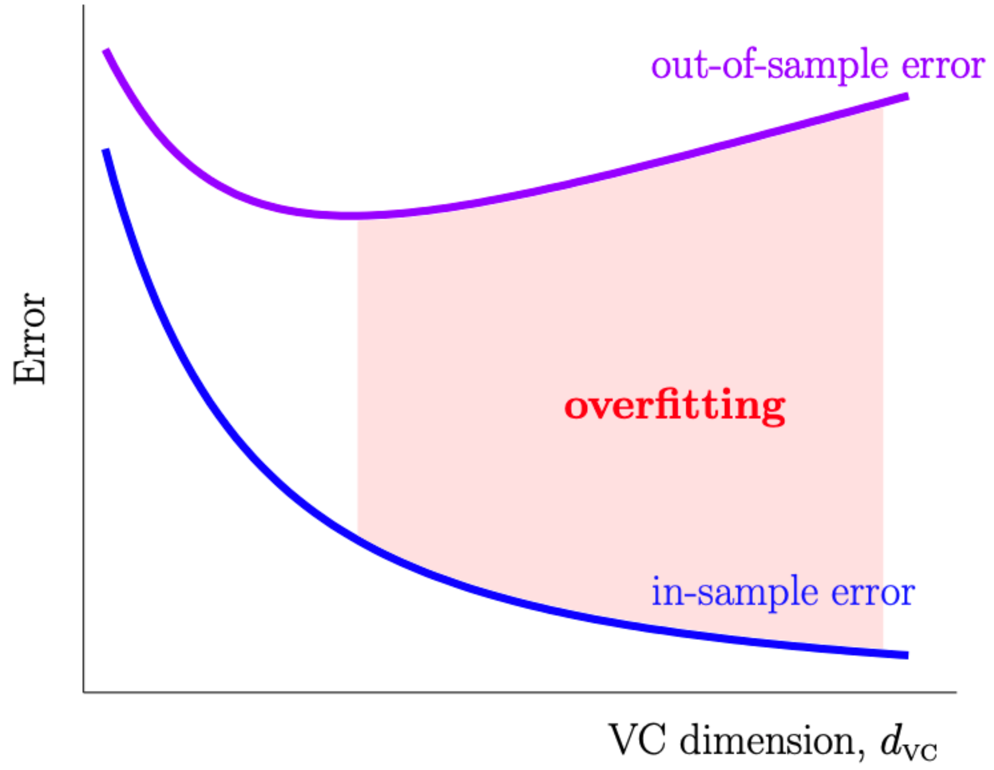
What is Overfitting?

Fitting the data more than is warranted

Overfitting is Not Just Bad Generalization



Overfitting is Not Just Bad Generalization

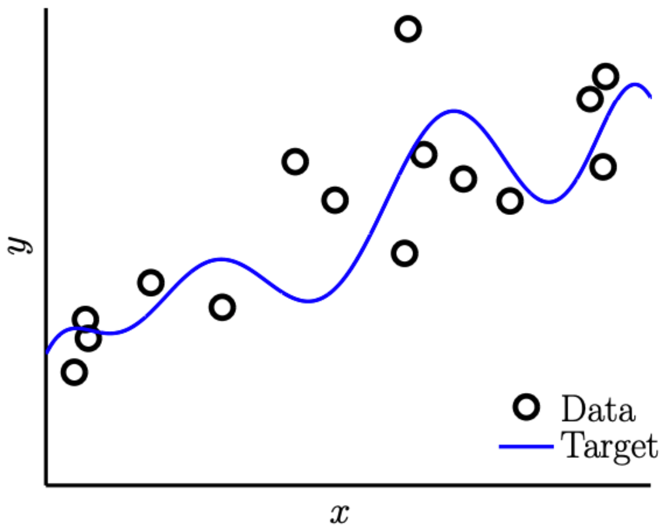


Overfitting

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

Case Study:
2^{nd} vs 10^{th} Order Polynomial Fit

N=15



10th order f with noise.

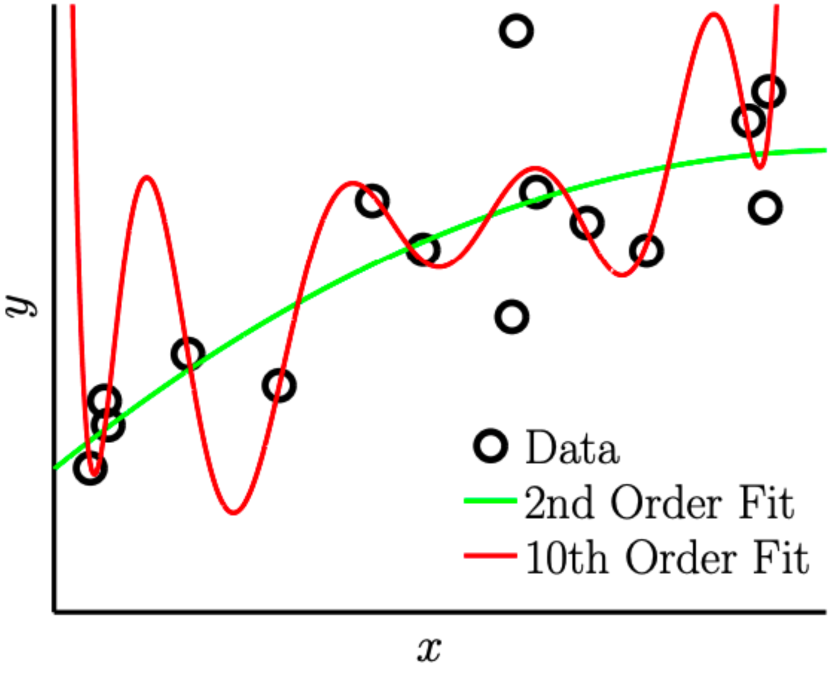
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

Which model do you choose for the left problem and why?

Target Function: 10^{th} Order f with Noise



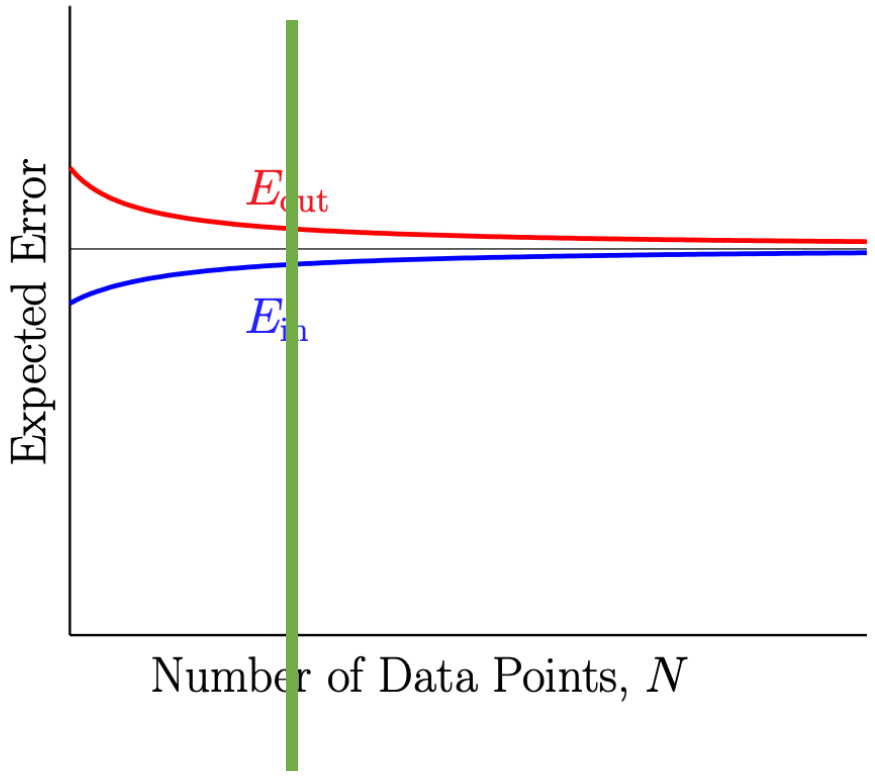
simple noisy target

	2nd Order	10th Order
E_{in}	0.050	0.034
E_{out}	0.127	**9.00**

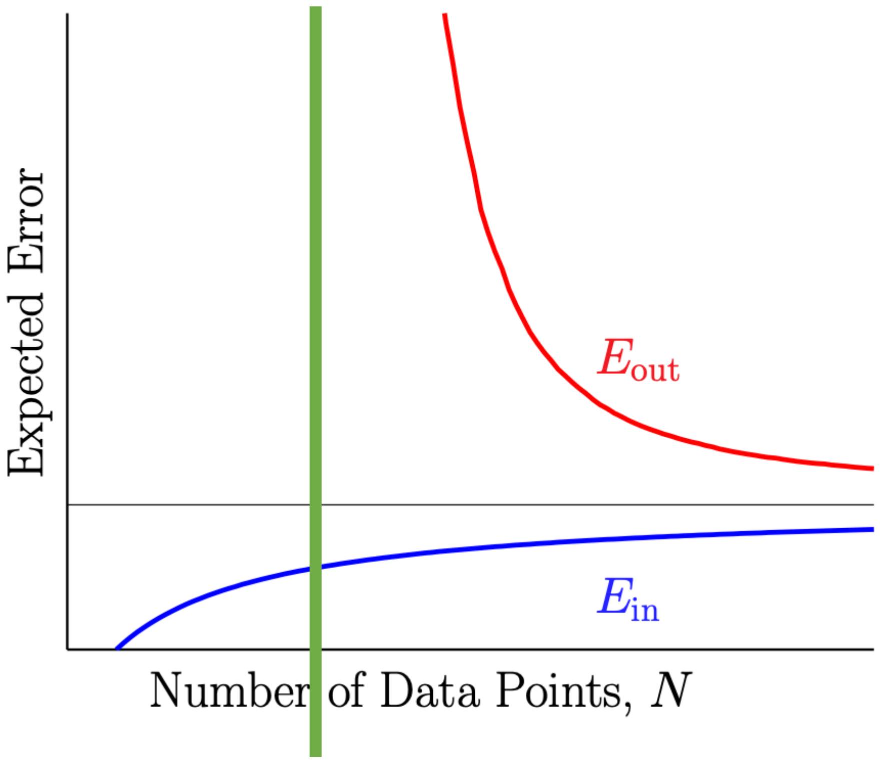
- Irony of two learners Red and Green
- Both **know** the target is 10^{th} order
- Red chooses H_{10}
- Green chooses H_2
- Green outperforms Red

Why is H_2 Better than H_{10}?

Learning curve for H_2



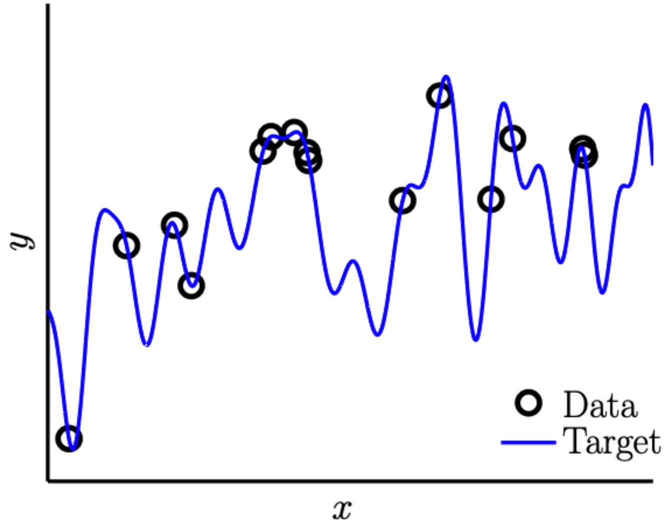
Learning curve for H_{10}



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

N=15

10th order f with noise.



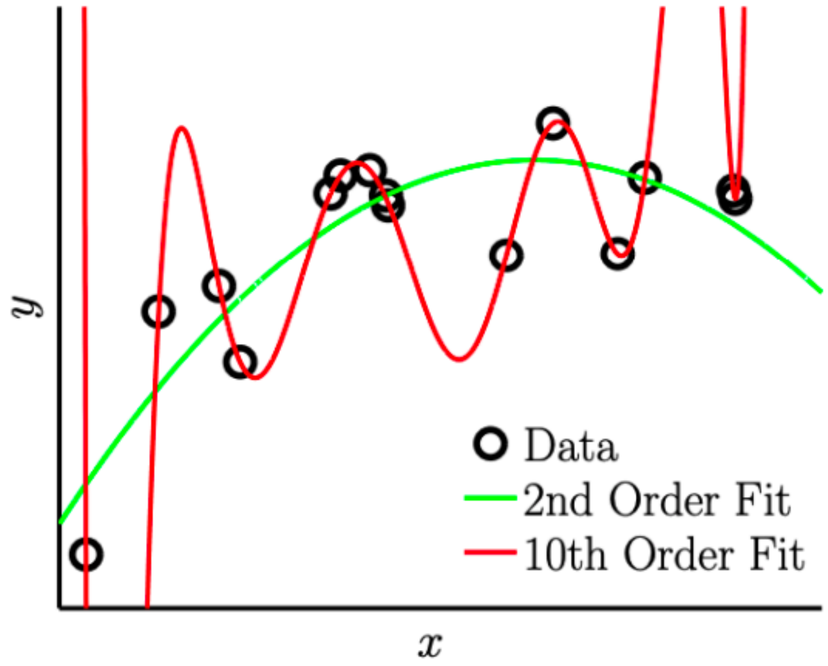
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

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

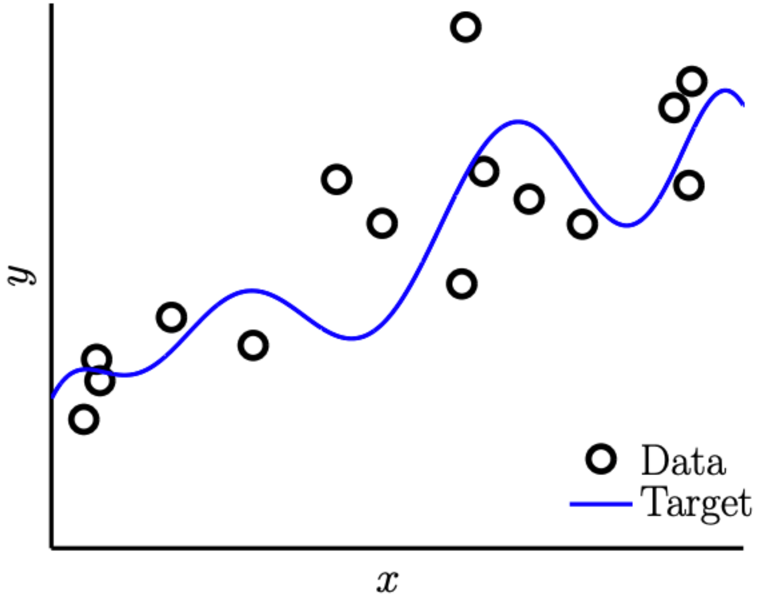
Simpler H is better even for complex target with no noise



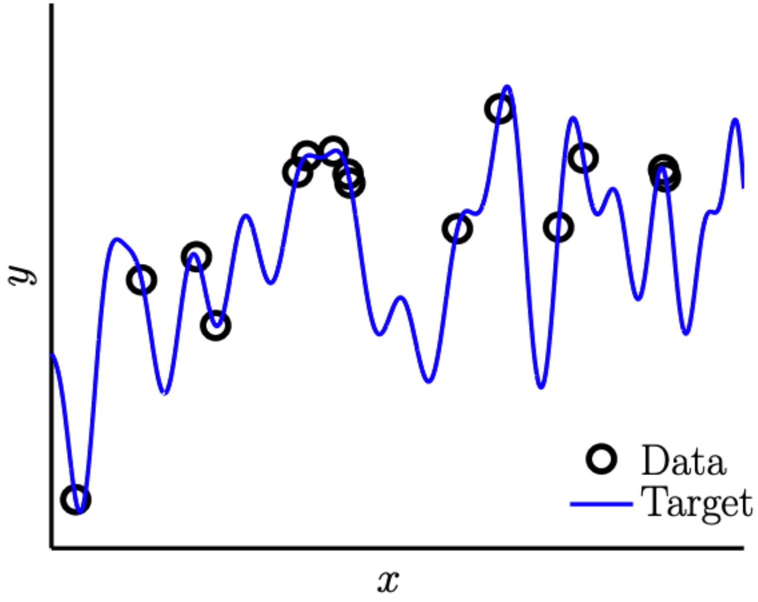
complex noiseless target

	2nd Order	10th Order
E_{in}	0.029	10^{-5}
E_{out}	0.120	**7680**

Is There Really "No Noise"?

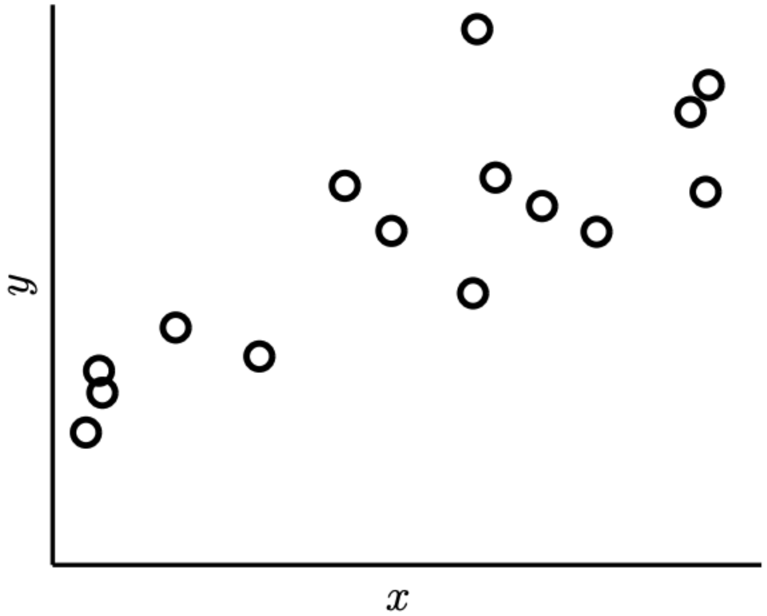


Simple f with noise.

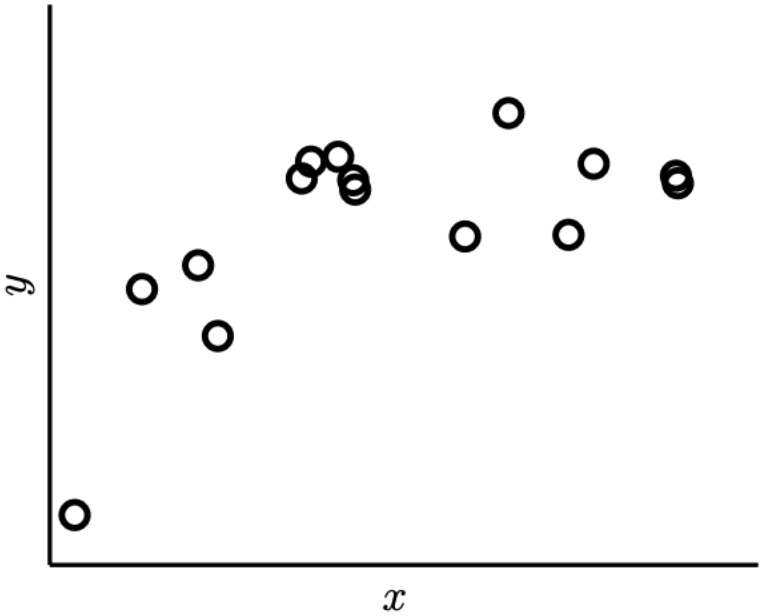


Complex f with no noise.

Is There Really “No Noise”?



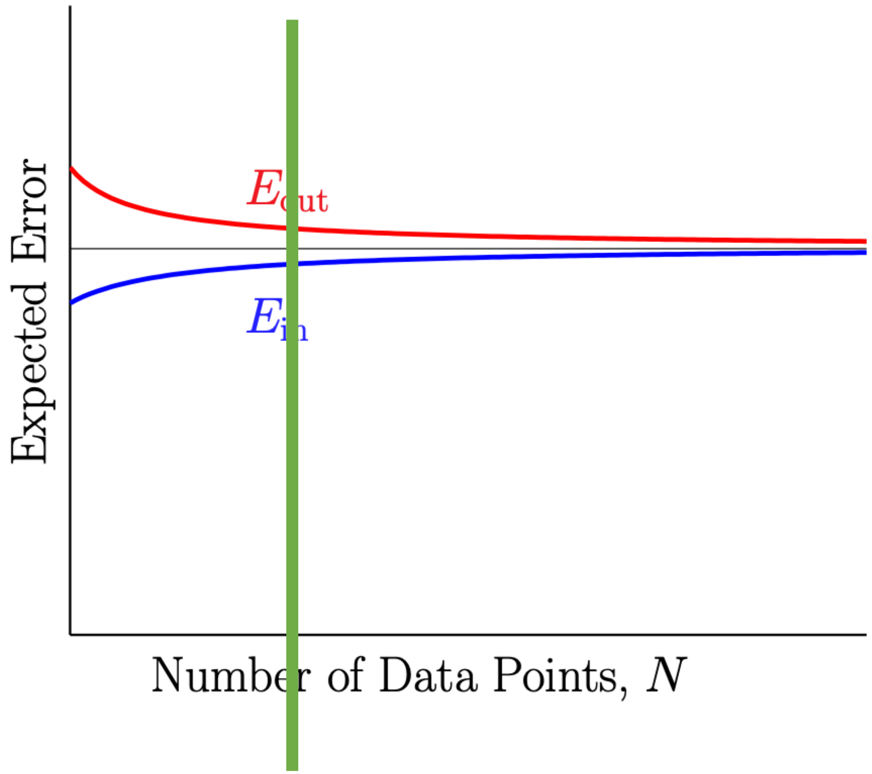
Simple f with noise.



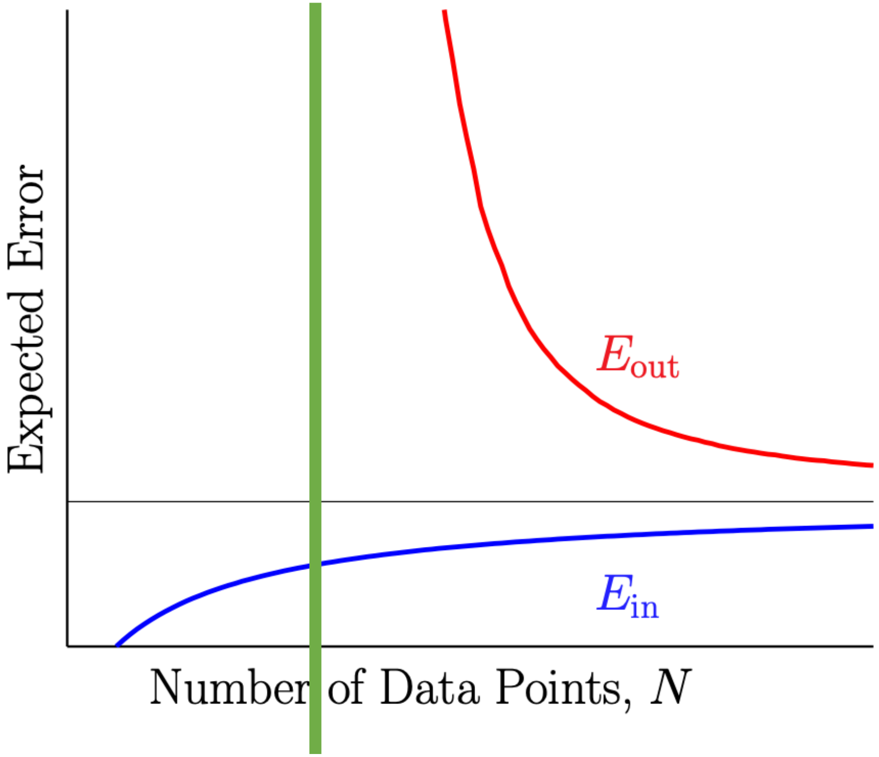
Complex f with no noise.

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 σ^2 of $\epsilon(x)$

Target complexity: Q_f

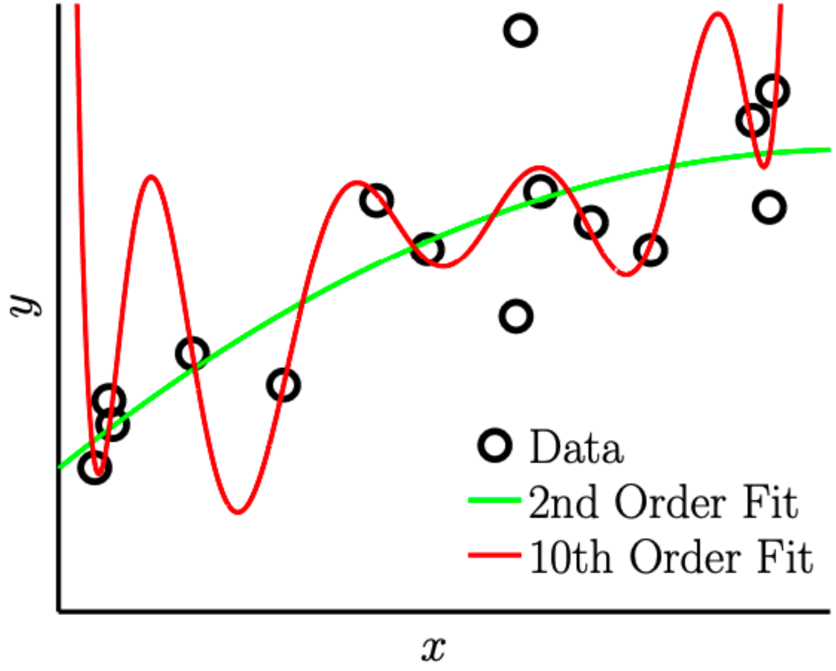
Data set size: N

The Overfit Measure

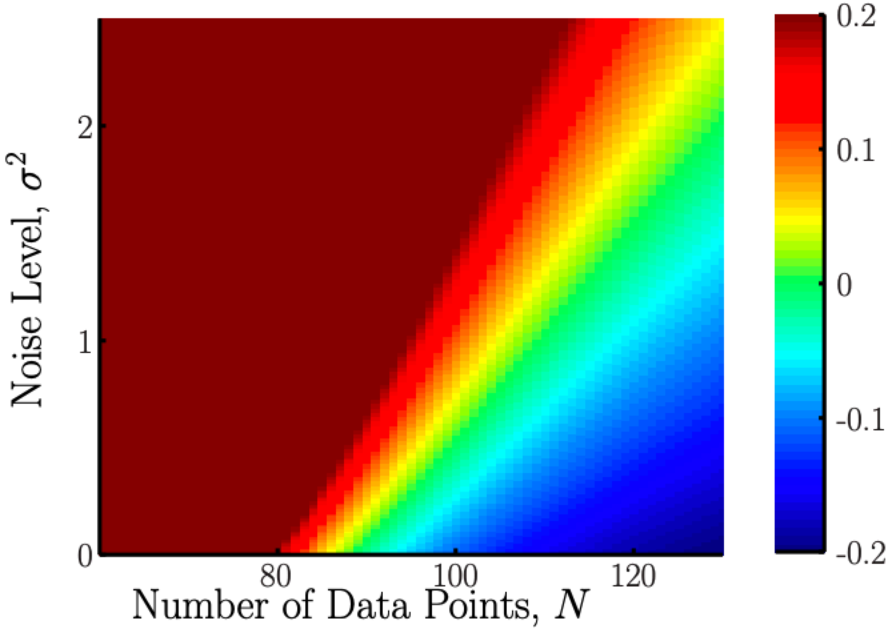
- Fit the data set using H_2 and H_{10}
  - Let g_2 and g_{10} be the learned hypothesis

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

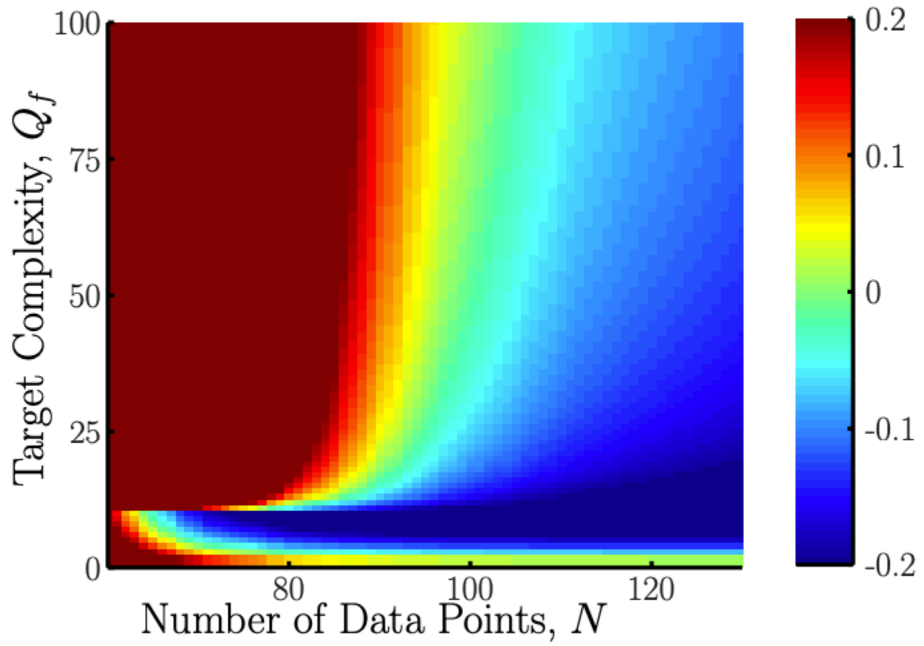
  - This value is large is overfit happens



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



Stochastic noise



deterministic noise

Number of data points ↑	Overfitting ↓
Noise ↑	Overfitting ↑
Target complexity ↑	Overfitting ↑

Noise:
The part of y we cannot model

Stochastic Noise

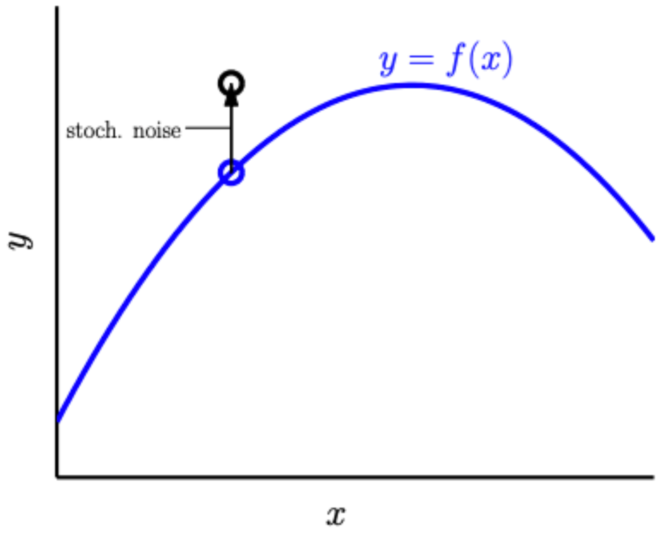
We would like to learn from ○:

$$y_n = f(x_n)$$

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.**

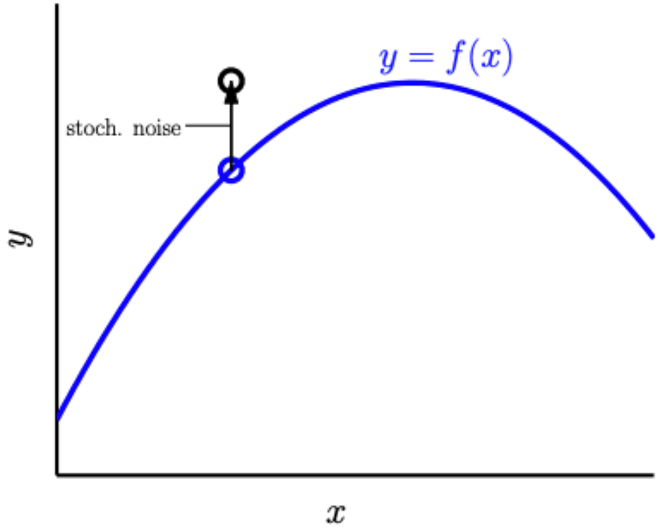
Stochastic Noise

We would like to learn from ○:

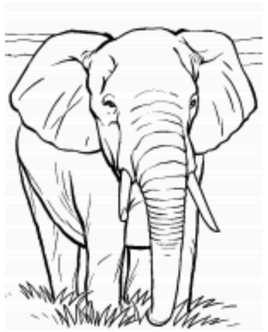
$$y_n = f(x_n)$$

Unfortunately, we only observe ○:

$$y_n = f(x_n) + \underset{\substack{\uparrow \\ \text{no one can model this}}}{\text{'stochastic noise'}}$$



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



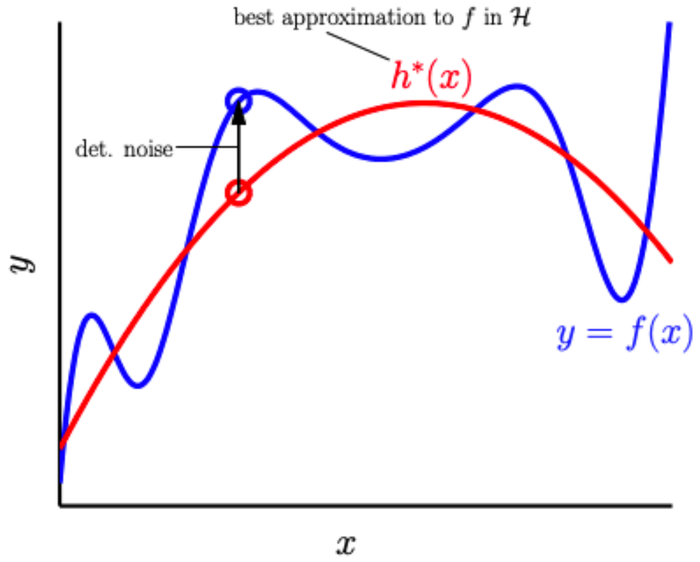
Deterministic Noise

We would like to learn from $\color{red}{\bigcirc}$:

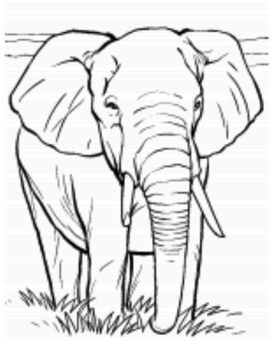
$$y_n = \color{red}{h^*(x_n)}$$

Unfortunately, we only observe $\color{blue}{\bigcirc}$:

$$\begin{aligned} y_n &= \color{blue}{f(x_n)} \\ &= \color{red}{h^*(x_n)} + \underbrace{\text{‘deterministic noise’}}_{\uparrow\ \mathcal{H} \text{ cannot model this}} \end{aligned}$$



Deterministic Noise: the part of f we cannot model.



Deterministic Noise

We would like to learn from ○:

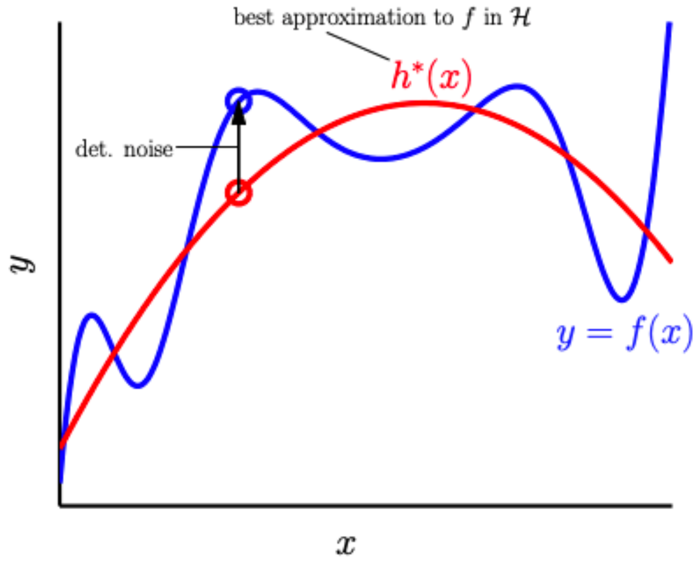
$$y_n = h^*(x_n)$$

Unfortunately, we only observe ○:

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

$\uparrow$

$\mathcal{H}$ cannot model this



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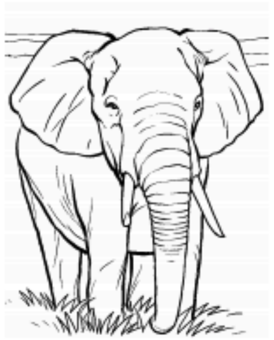
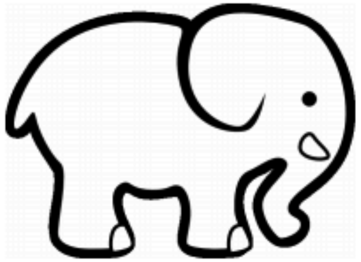
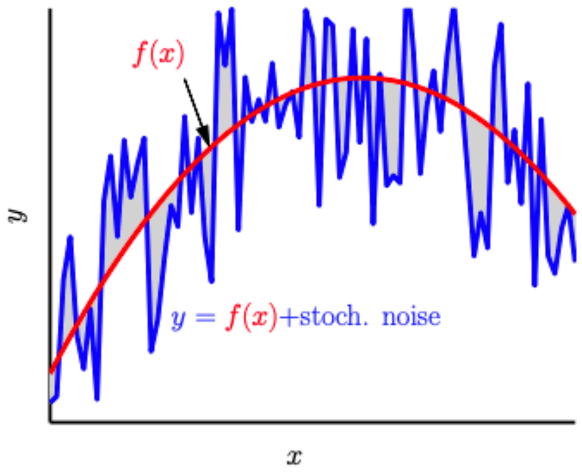




Both sources of noises hurt learning

<u>Stochastic Noise</u>

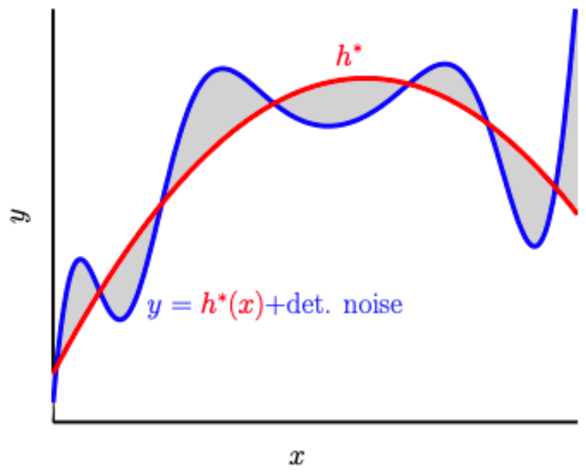


source: random measurement errors

re-measure y_n
stochastic noise changes.

change $\mathcal{H}$
stochastic noise the same.

<u>Deterministic Noise</u>



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

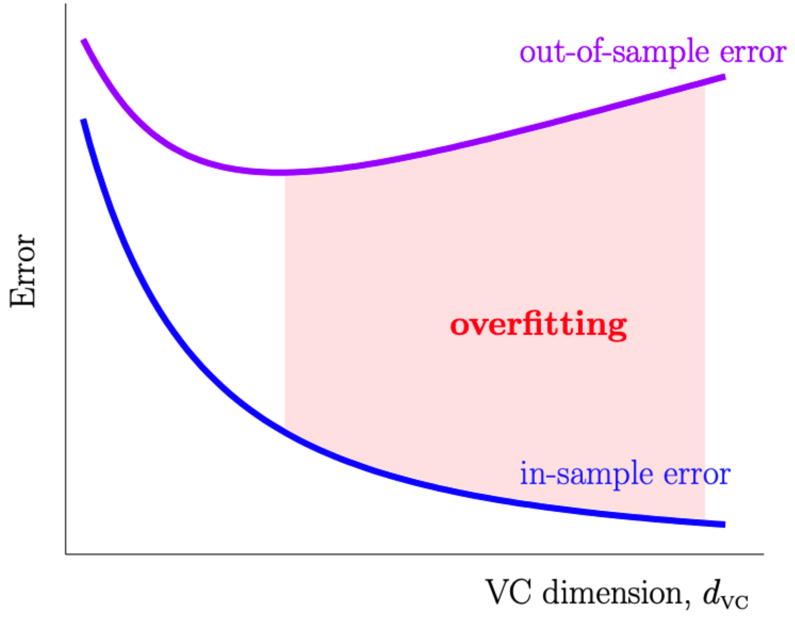
Deterministic noise

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

- To prove $d_{vc}(H) \geq d+1$, what do we need to prove?

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- 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

- 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