CSE 417T
Introduction to Machine Learning

Lecture 9
Instructor: Chien-Ju (CJ) Ho

Logistics

- Homework 2 is due on **October 7(Friday)**

- Return of homework
  - We plan to return each homework within 1.5~2 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

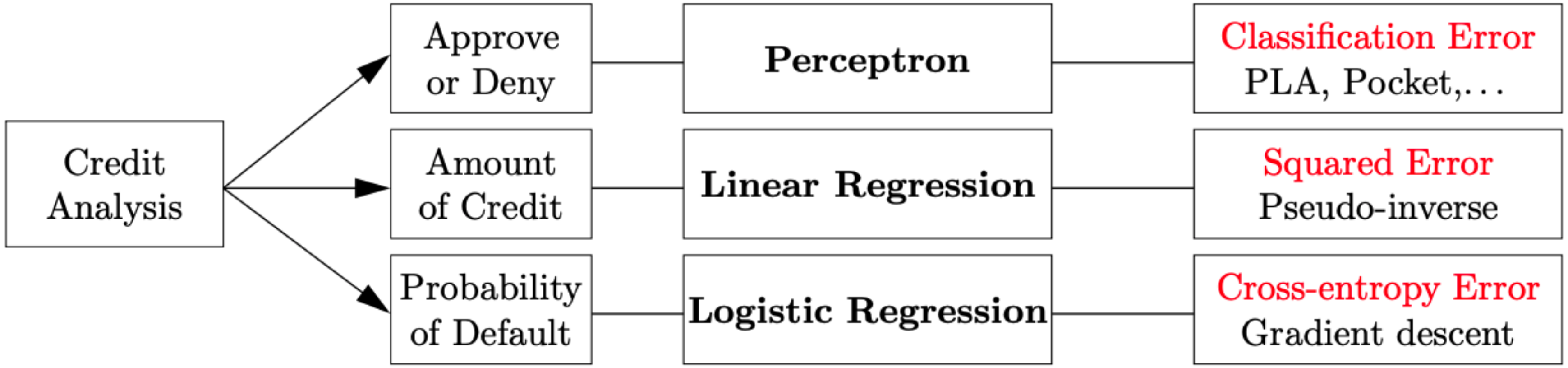
- Exam 1: **October 27 (Thursday)**
  - Content: LFD Chap 1 to 5 (The entire hardcopy of the textbook)
  - Timed exam (75 min) during lecture time (location TBD)
  - Closed-book exam with 2 letter-size cheat sheets allowed (4 pages in total)
    - No format limitations (it can be typed, written, or a combination)

Recap

Linear Models

This is why it's called linear models

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

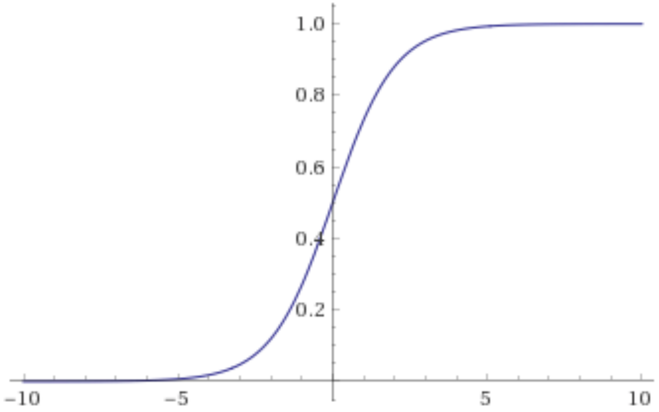


- Algorithm:
  - Focus on $g = argmin_{h \in H} E_{in}(h)$
  - Gradient descent is one of the common optimization algorithms

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 $g = argmin_{h\in H} E_{in}(h)$

- 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

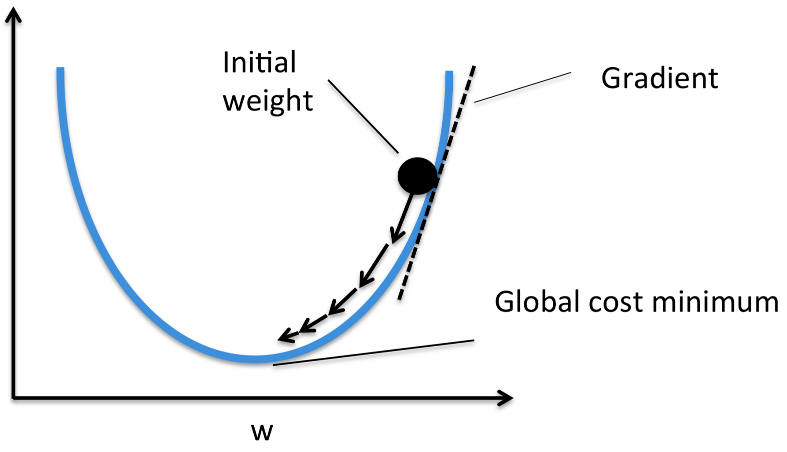
$$E_{in}(\vec{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

- Minimizing cross entropy error is the same as maximizing likelihood

- Likelihood: $\Pr(D|\vec{w})$
  - $\vec{w}^* = argmax_{\vec{w}} \Pr(D|\vec{w})$ (maximizing likelihood)
    $= argmin_{\vec{w}} E_{in}(\vec{w})$ (minimizing cross-entropy error)

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

- Gradient descent algorithm
  - Initialize $\vec{w}(0)$
  - For $t = 0, \ldots$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}\big(\vec{w}(t)\big)$
    - 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 $\{1, \ldots, N\}$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} e_n(\vec{w}(t))$

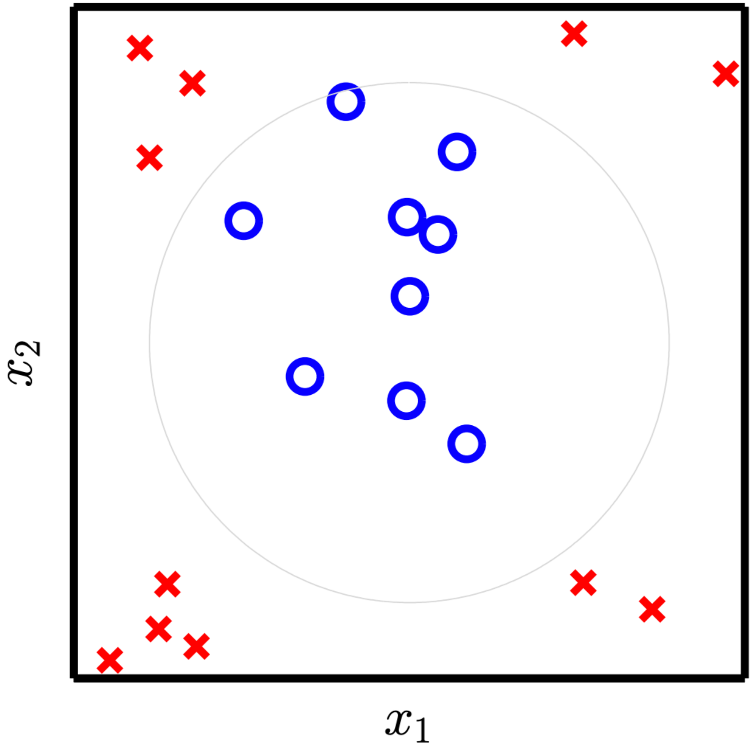
Today’s Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

Let me know if you spot errors.

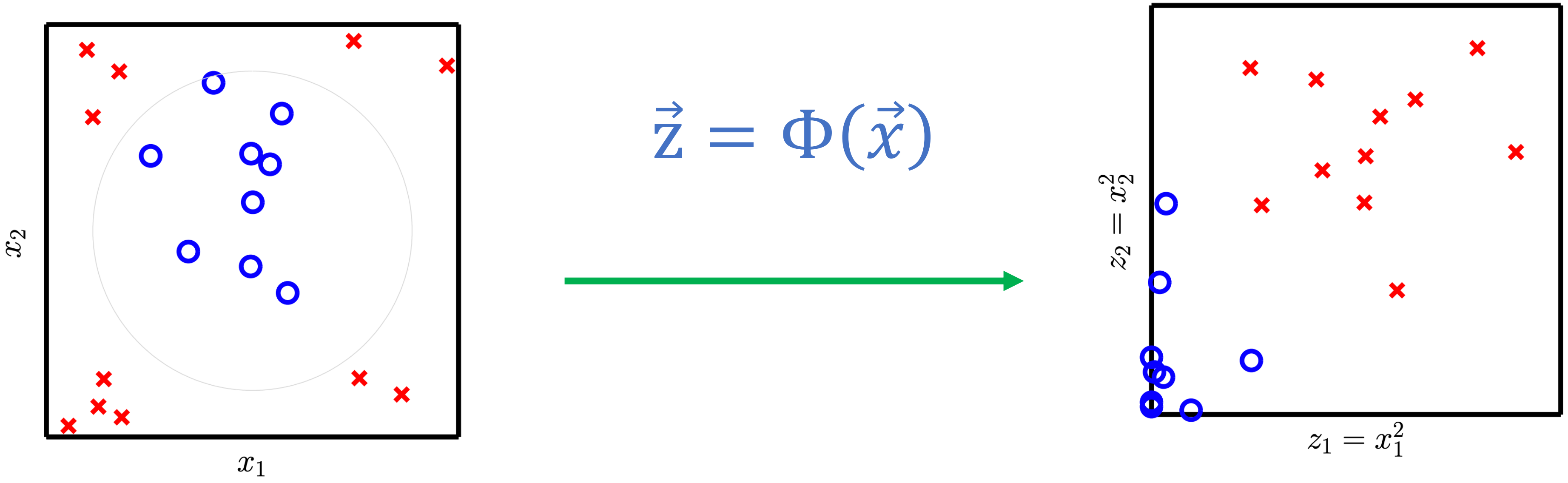
Non-Linear Transformation

Limitations of Linear Models



Using Non-Linear Transformations

- Find a feature transform Φ that maps data from $\vec{x}$ space to $\vec{z}$ space



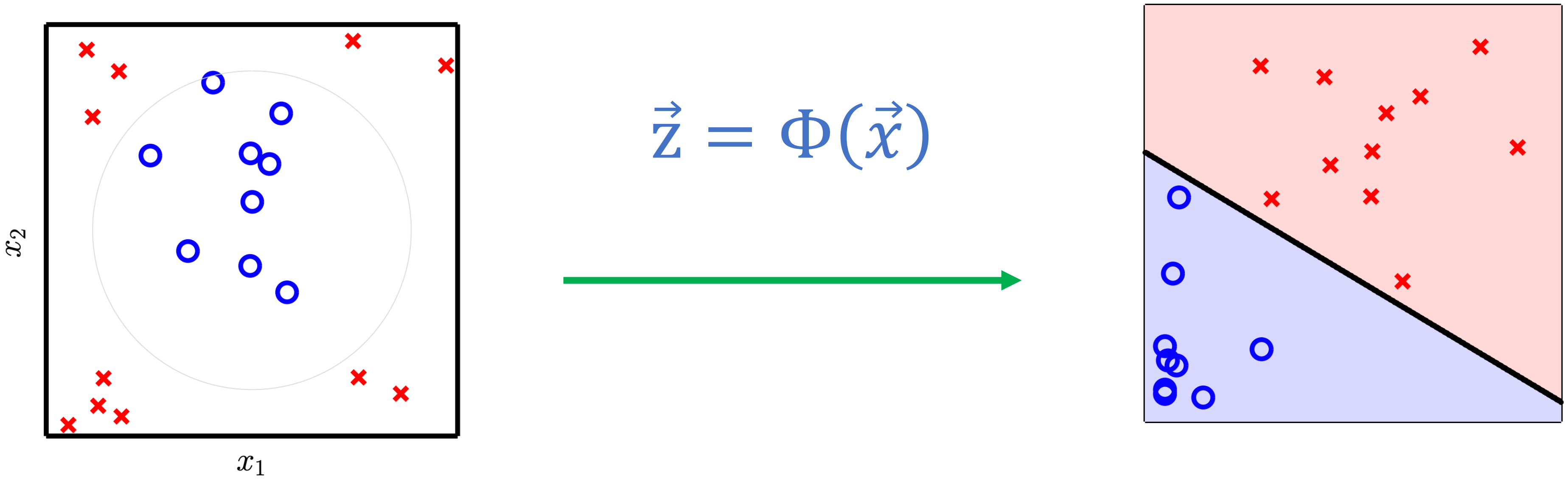
$$\vec{z} = \Phi(\vec{x})$$

$$\vec{x} = (1, x_1, x_2)$$

$$\vec{z} = (1, x_1^2, x_2^2)$$

Using Non-Linear Transformations

- Learn a linear classifier in $\vec{z}$ space: $g^{(z)}(\vec{z}) = sign\left(\overrightarrow{w}^{(z)^T}\vec{z}\right)$



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

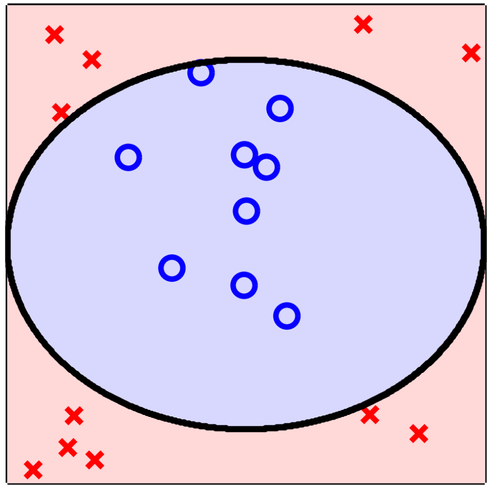
$\vec{x} = (1, x_1, x_2)$

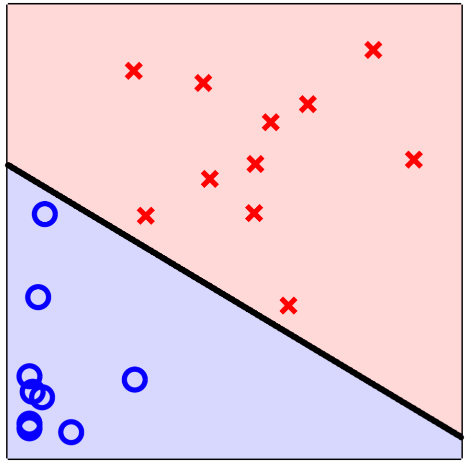
$\vec{z} = (1, x_1^2, x_2^2)$

$g^{(z)}(\vec{z}) = sign(-0.6 + z_1 + z_2)$

Using Non-Linear Transformations

- Transform the learned hypothesis back to $\vec{x}$ space
  - $g(\vec{x}) = g^{(z)}(\Phi(\vec{x})) = sign\left(\vec{w}^{(z)^T}\Phi(\vec{x})\right)$





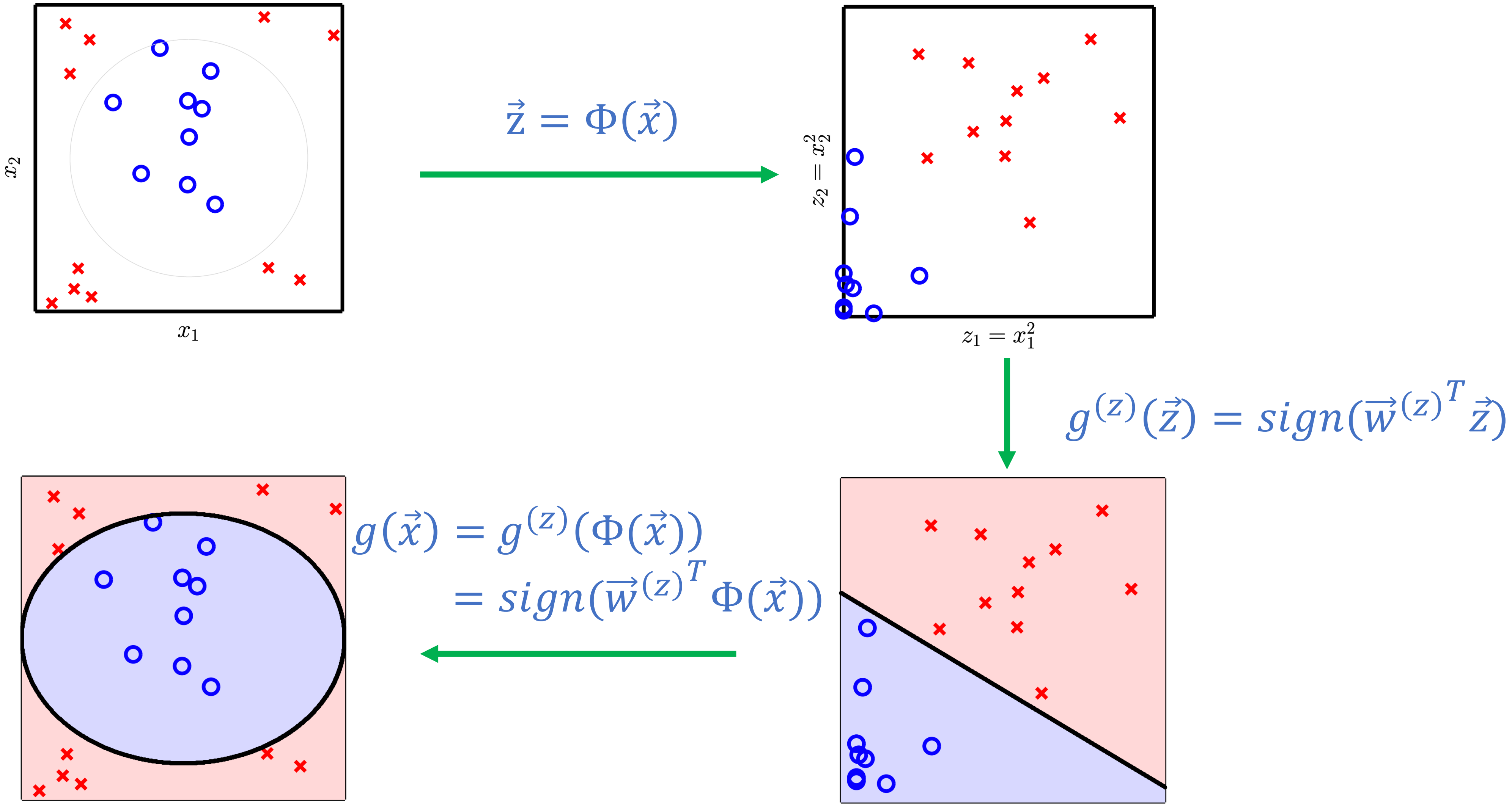
$\vec{x} = (1, x_1, x_2)$

$\vec{z} = (1, x_1^2, x_2^2)$

$g(\vec{x}) = sign(-0.6 + x_1^2 + x_2^2)$

$g^{(z)}(\vec{z}) = sign(-0.6 + z_1 + z_2)$

Nonlinear Transformation



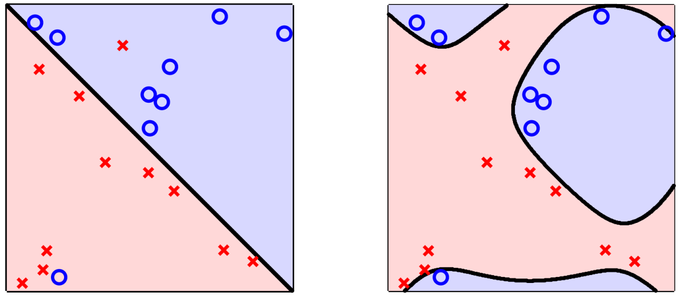
$$\vec{z} = \Phi(\vec{x})$$

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

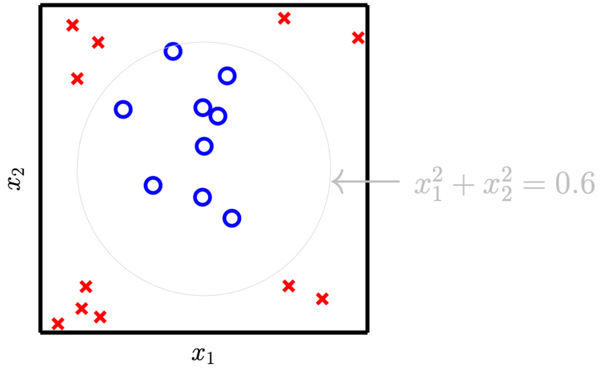
$$\begin{aligned} g(\vec{x}) &= g^{(z)}(\Phi(\vec{x})) \\ &= sign(\vec{w}^{(z)^T}\Phi(\vec{x})) \end{aligned}$$

Generalization of Nonlinear Transformation

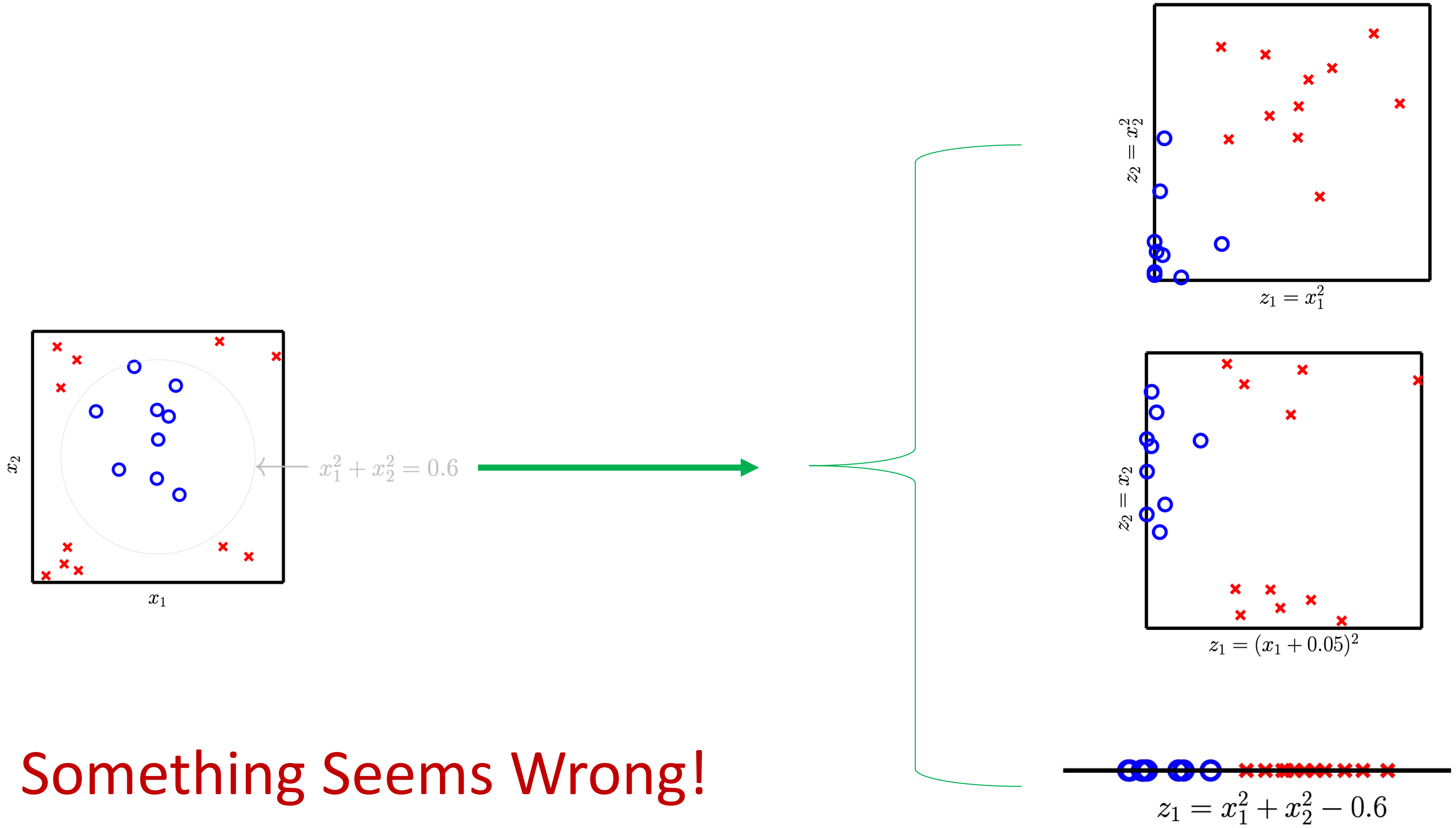
- Fact (We'll prove this later)
  - The VC Dimension of d-dim perceptron is $d + 1$
- VC dimension of perceptron on input space $\vec{x} = (x_0, .., x_d)$
  - d+1
- VC dimension of perceptron on input space $\vec{z} = (z_0, .., z_{d'})$
  - $\leq d' + 1$ (usually treated as $\approx d' + 1$)
- Careful: Non-linear transform might lead to ”nonsense” behavior



How to Choose Feature Transform Φ



How to Choose Feature Transform Φ



Something Seems Wrong!

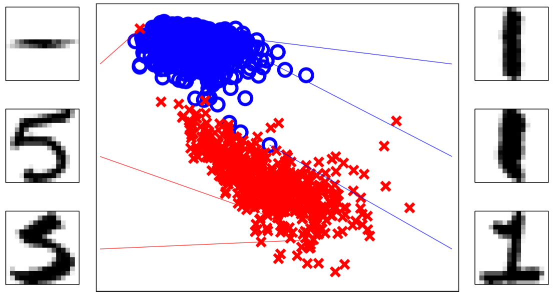
Must choose Φ BEFORE looking at the data

Otherwise, you are doing “data snooping”

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

Choose Φ 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
    - $\vec{x} = (1, x_1, x_2)$
    - $\Phi_2(\vec{x}) = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$
    - Pros: more powerful (contains circle, ellipse, hyperbola, etc)
    - Cons: 2-d => 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:
  - $\Phi_1(\vec{x}) = \vec{x}$
  - $\Phi_2(\vec{x}) = (\Phi_1(\vec{x}), x_1^2, x_1 x_2, x_1 x_3, \dots, x_d^2)$
  - …
  - $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1} x_2, \dots, x_d^Q)$

- Number of elements in $\Phi_Q(\vec{x})$

Q-th Order Polynomial Transform

- $\vec{x} = (1, x_1, \dots, x_d)$
- From 1-st order to Q-th order polynomial transform:
  - $\Phi_1(\vec{x}) = \vec{x}$
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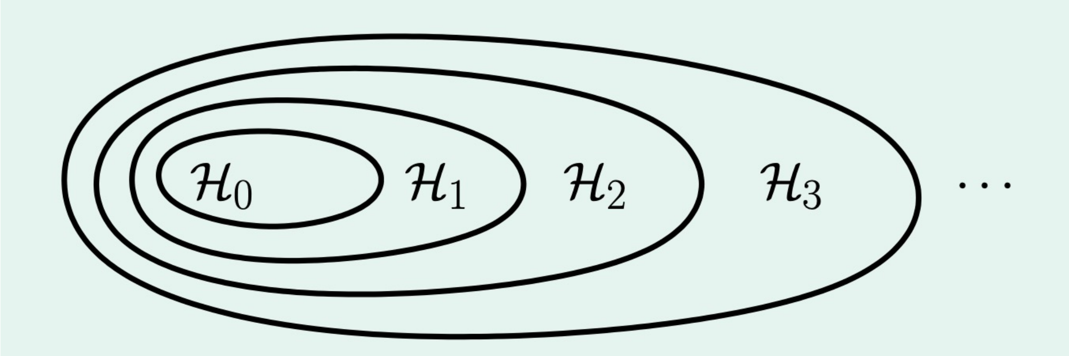
  - …
  - $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1} x_2, \dots, x_d^Q)$

- Number of elements in $\Phi_Q(\vec{x})$
  - $\binom{Q+d}{Q}$

Structural Hypothesis Sets

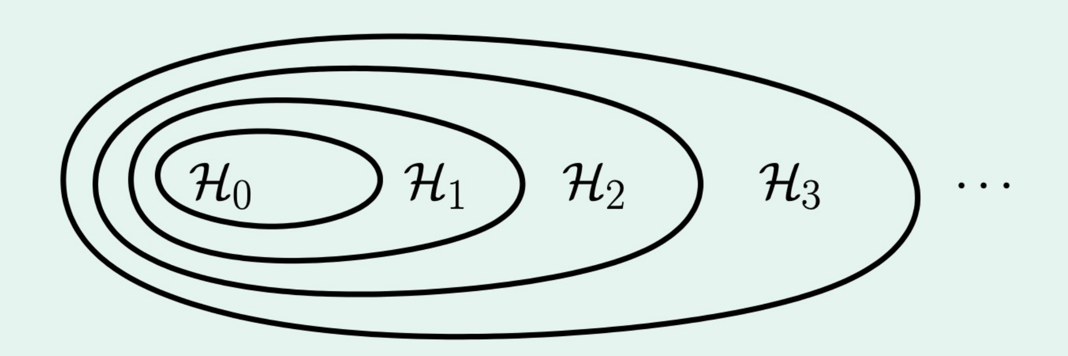
- Let H_Q be the linear model for the $\Phi_Q(\vec{x})$ space



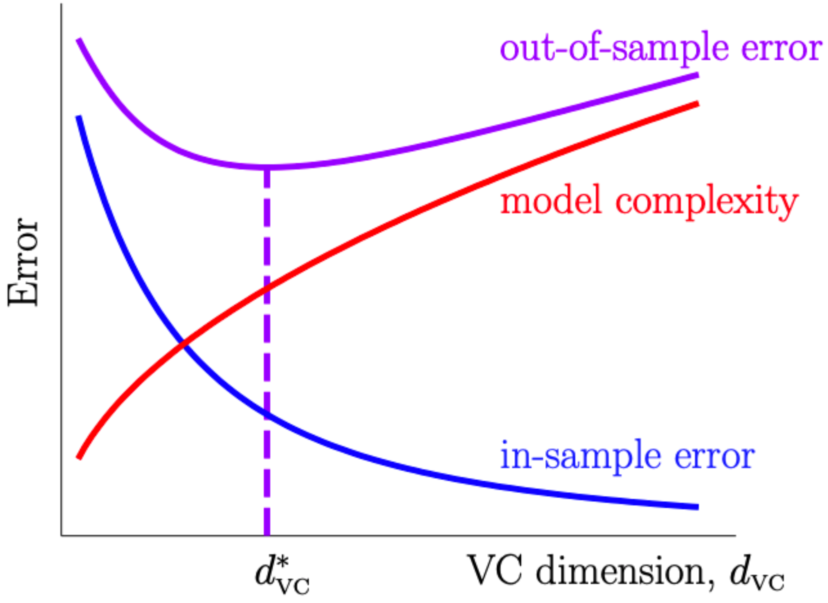
- Let $g_Q = argmin_{h \in H_Q} E_{in}(h)$
  - $H_0 \quad H_1 \quad H_2$ …
  - $d_{vc}(H_0) \quad d_{vc}(H_1) \quad d_{vc}(H_2)$ …
  - $E_{in}(g_0) \quad E_{in}(g_1) \quad E_{in}(g_2)$ …

Structural Hypothesis Sets

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



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

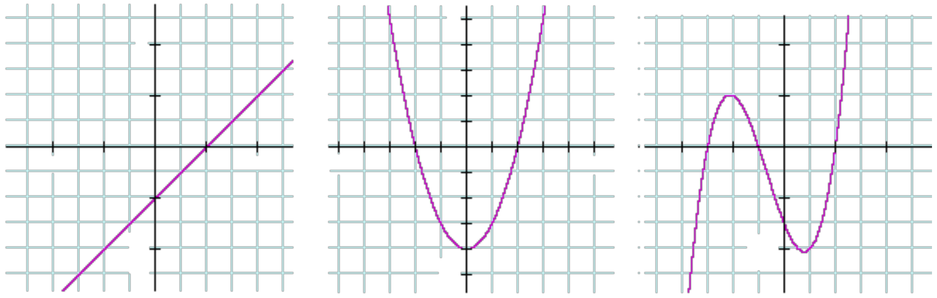


Overfitting

[Adapted from the slides by Malik Magdon-Ismail]

Setup of the Discussion

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



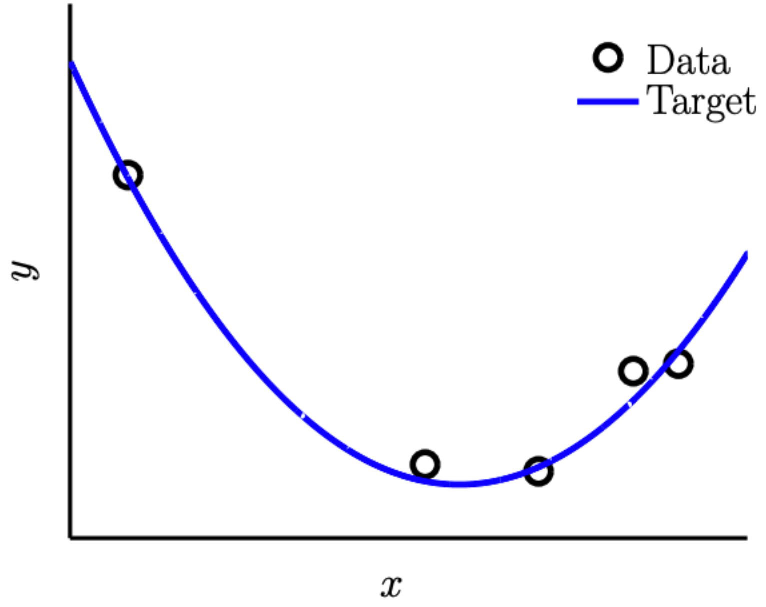
$y = ax + b$ $y = ax^2 + bx + c$ $y = ax^3 + bx^2 + cx + d$

- Qth-order polynomial fit
  - Solve linear regression on the $\Phi_\mathrm{Q}(\vec{x})$ 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 $g_4 = argmin_h E_{in}(h)$



A Simple Example

- Target f: 4th order function
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- 4th order polynomial fit
  - $h(x) = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4$
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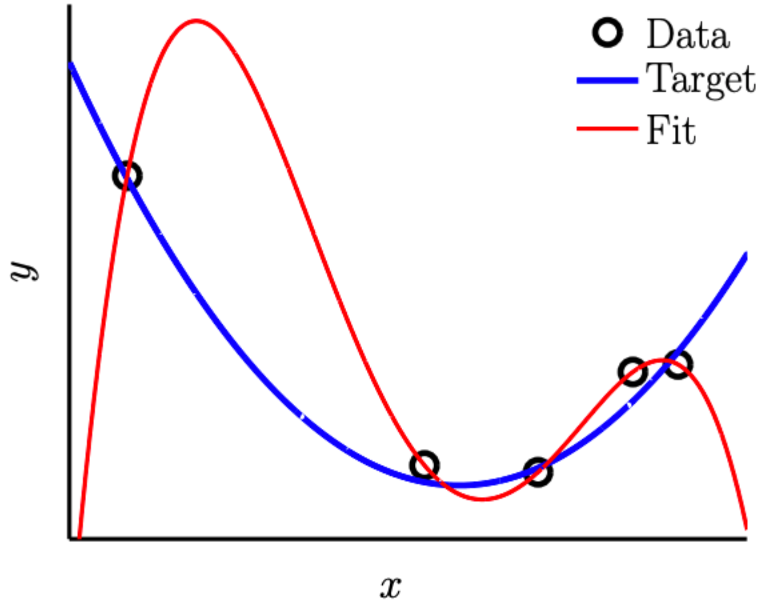


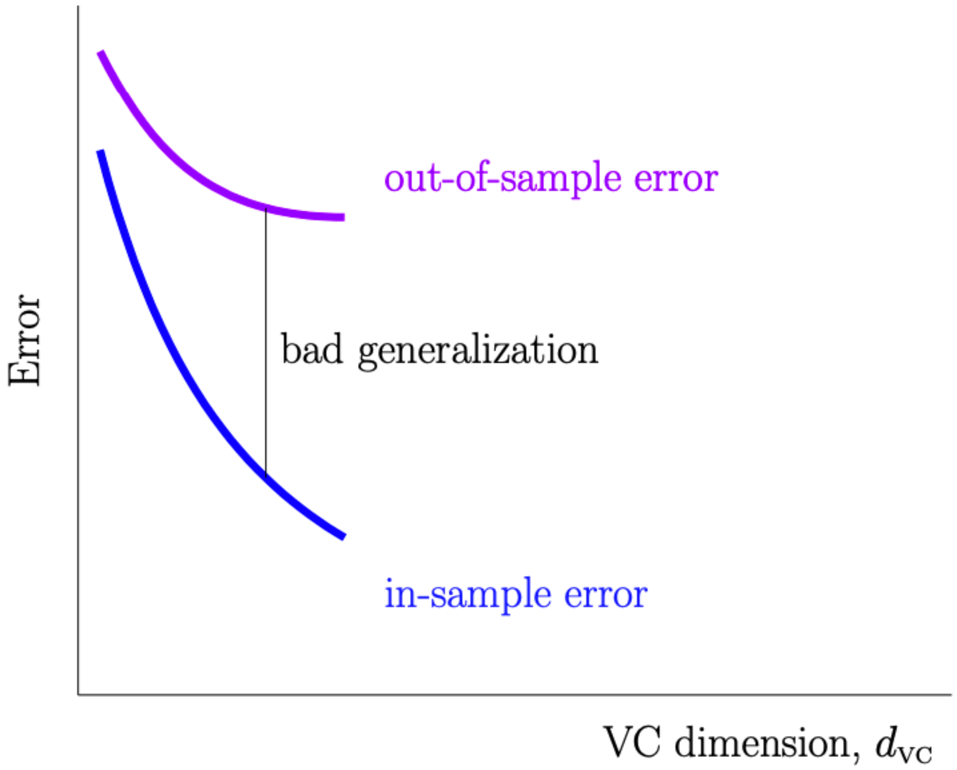
Classical overfitting: $E_{in} = 0$, but lead to a large E_{out}

Fitting the **noise** instead of the target

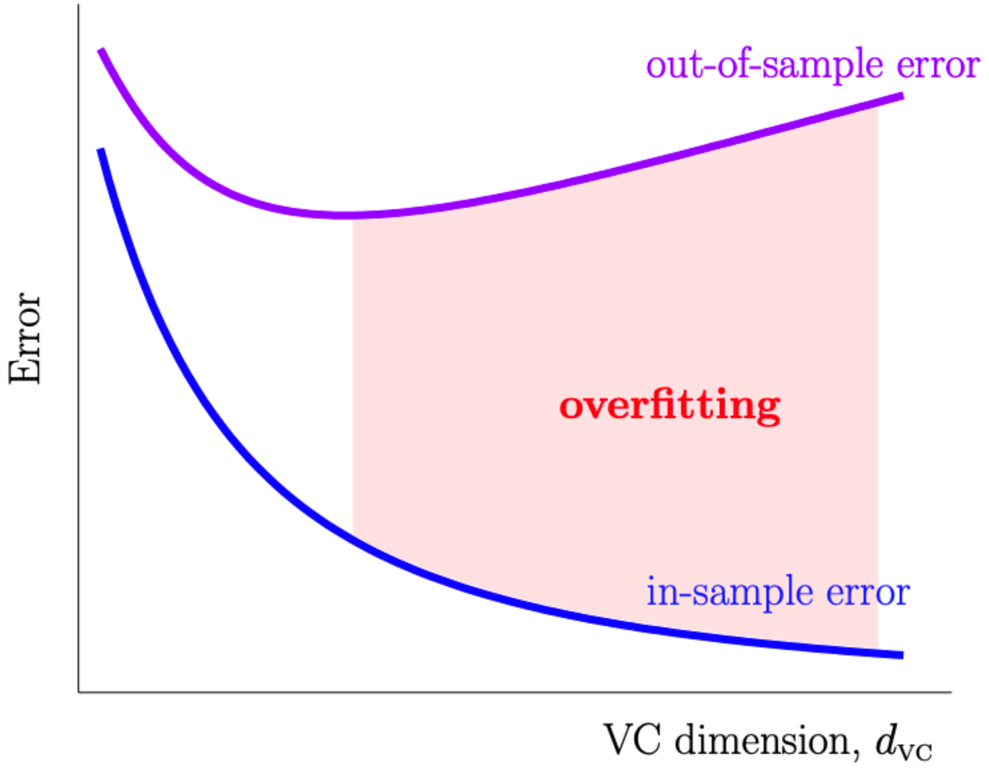
What is Overfitting?

Fitting the data more than is warranted

Overfitting is Not Just Bad Generalization



Overfitting is Not Just Bad Generalization

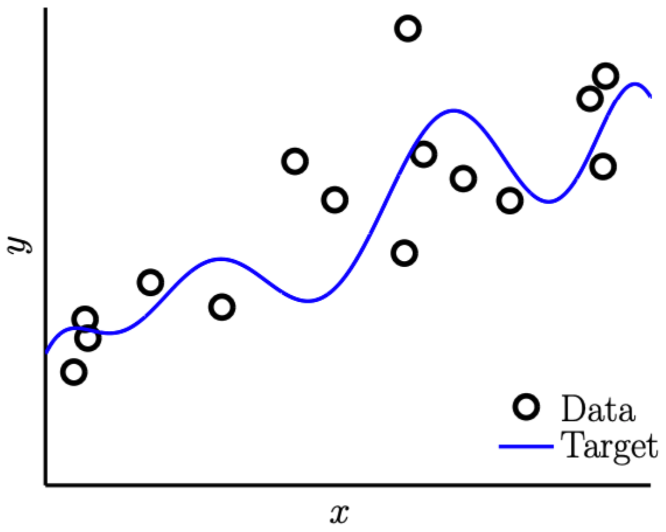


Overfitting

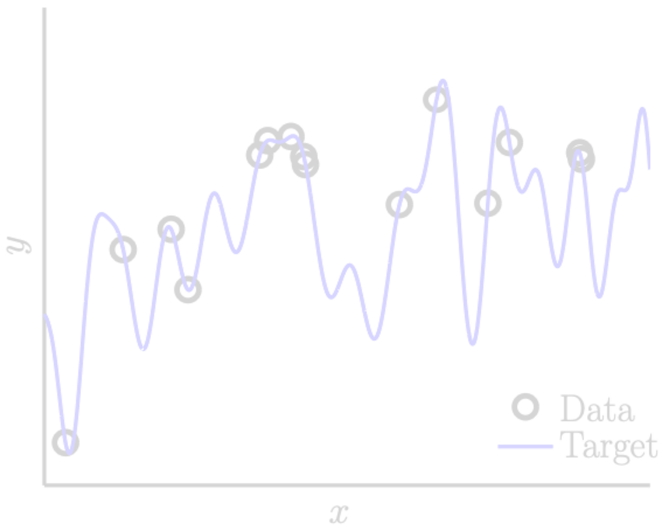
Going for lower and lower E_{in} results in higher and higher E_{out}

Case Study:
2nd vs 10th Order Polynomial Fit

N=15



10th order f with noise.



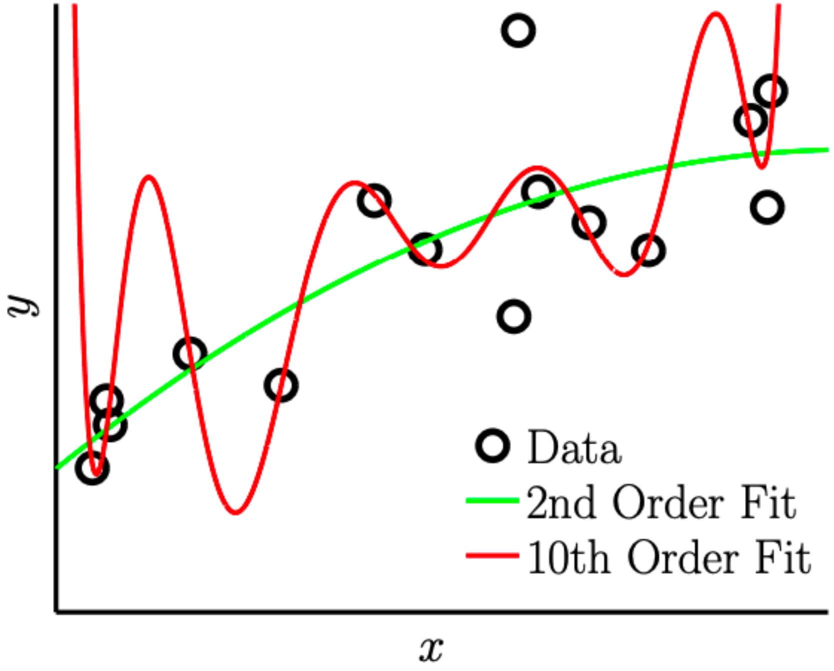
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

Which model would 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

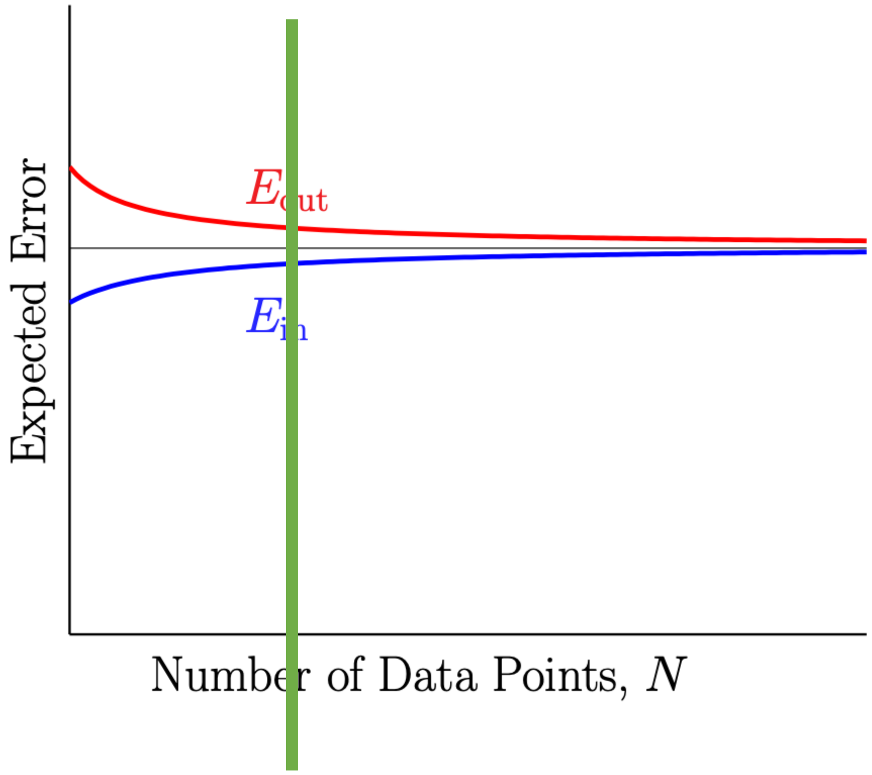
- Both **know** the target is 10^{th} order

- Red chooses H_{10}
- Green chooses H_2

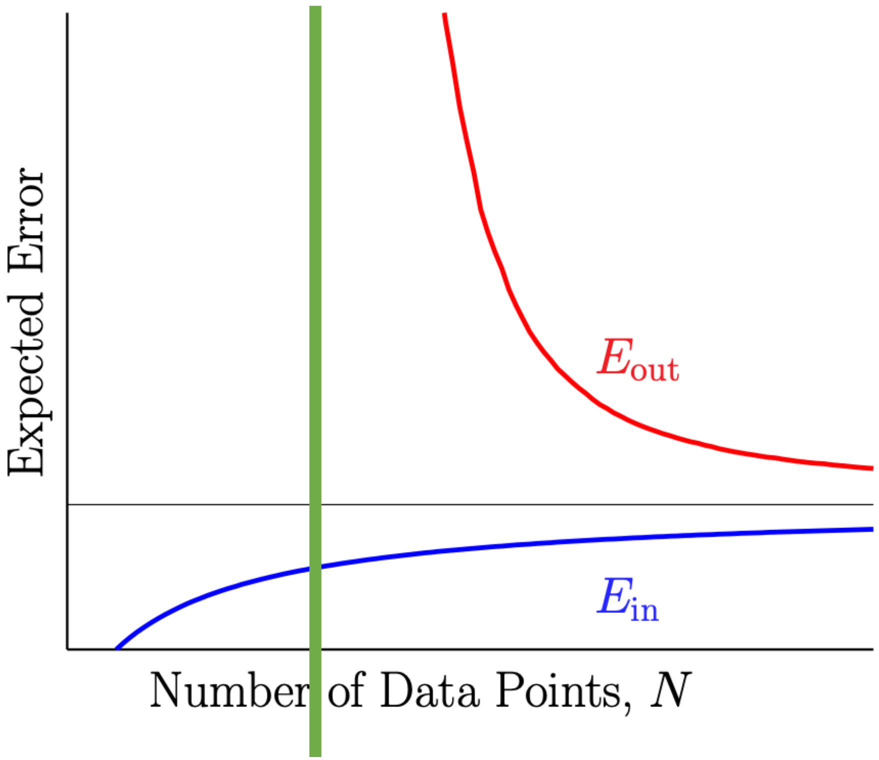
- Green outperforms Red

Why is H_2 Better than H_{10}?

Learning curve for H_2

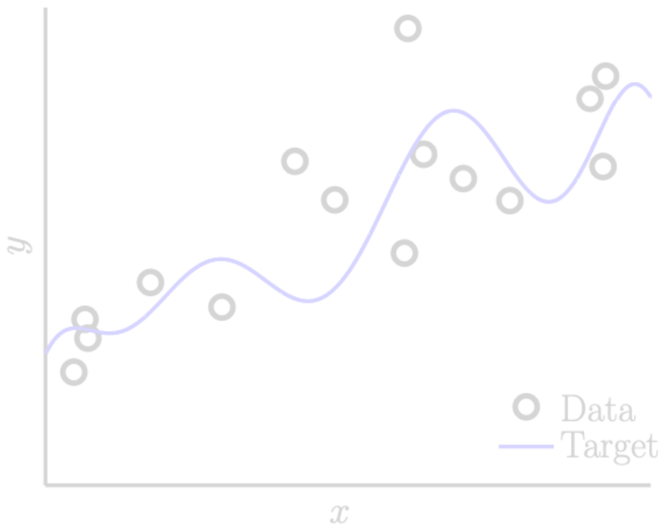


Learning curve for H_{10}

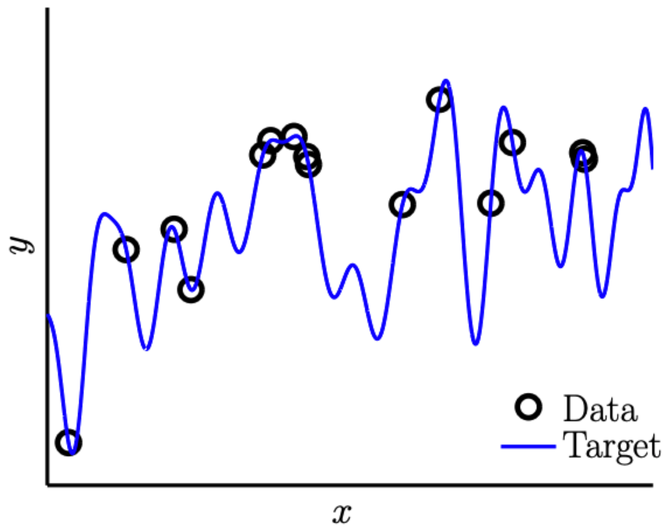


When *N* is small, $E_{out}(g_{10}) \geq E_{out}(g_2)$

N=15



10th order f with noise.



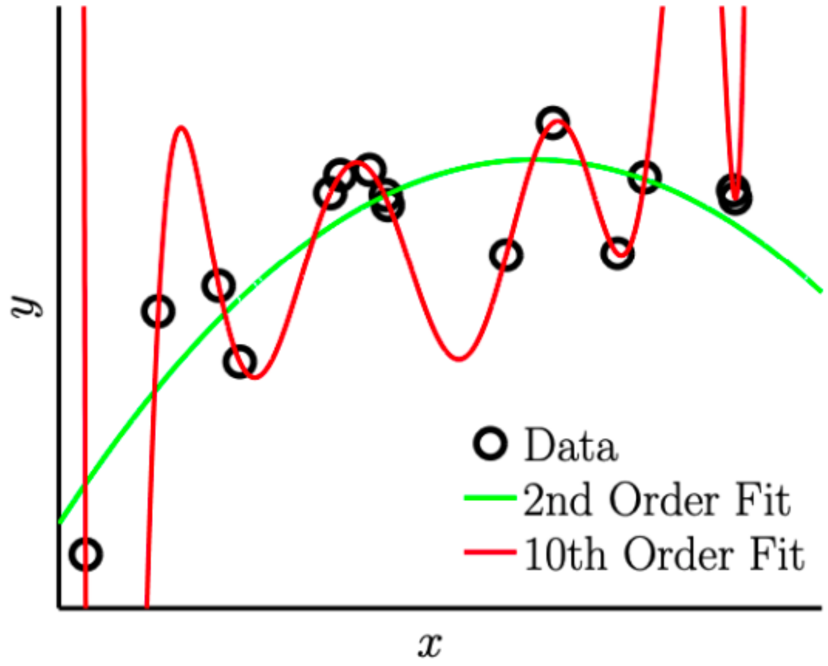
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

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

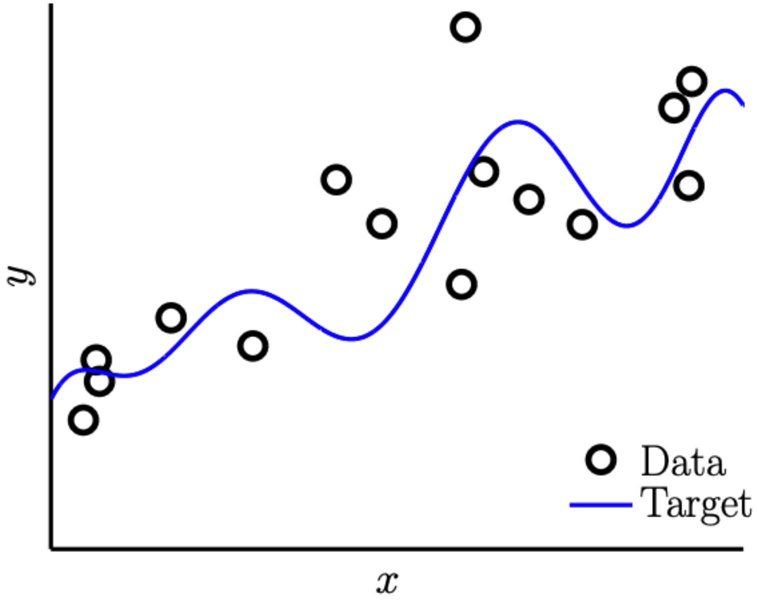
Simpler H is better even for complex target with no noise



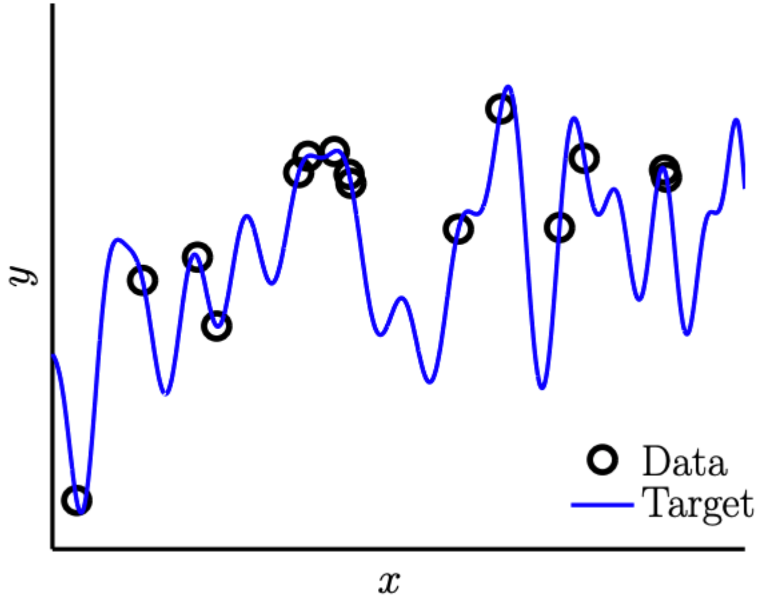
complex noiseless target

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

Is There Really "No Noise"?

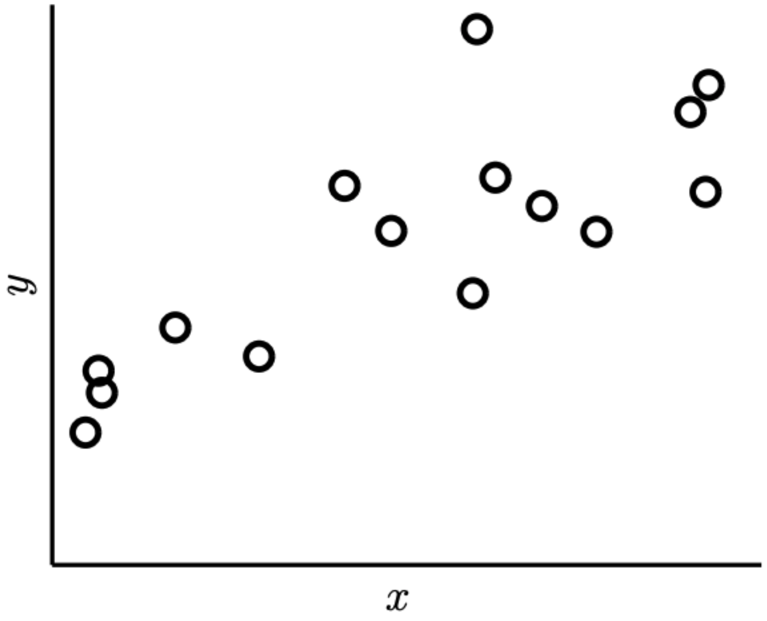


Simple f with noise.

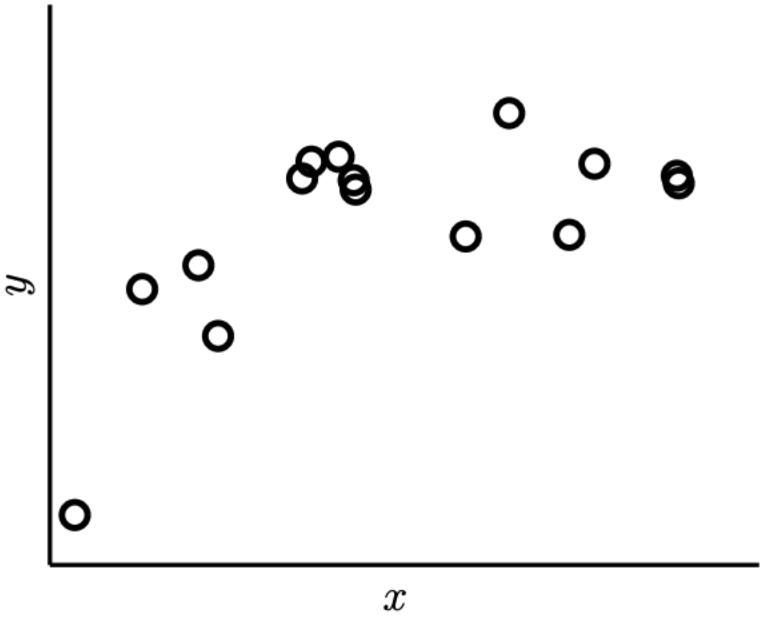


Complex f with no noise.

Is There Really “No Noise”?



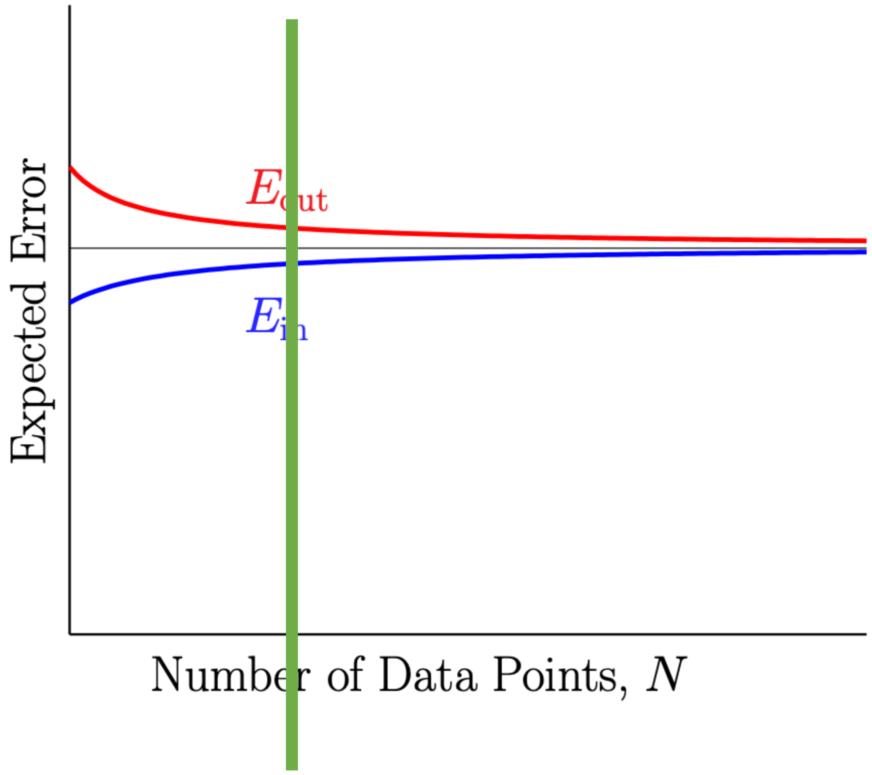
Simple f with noise.



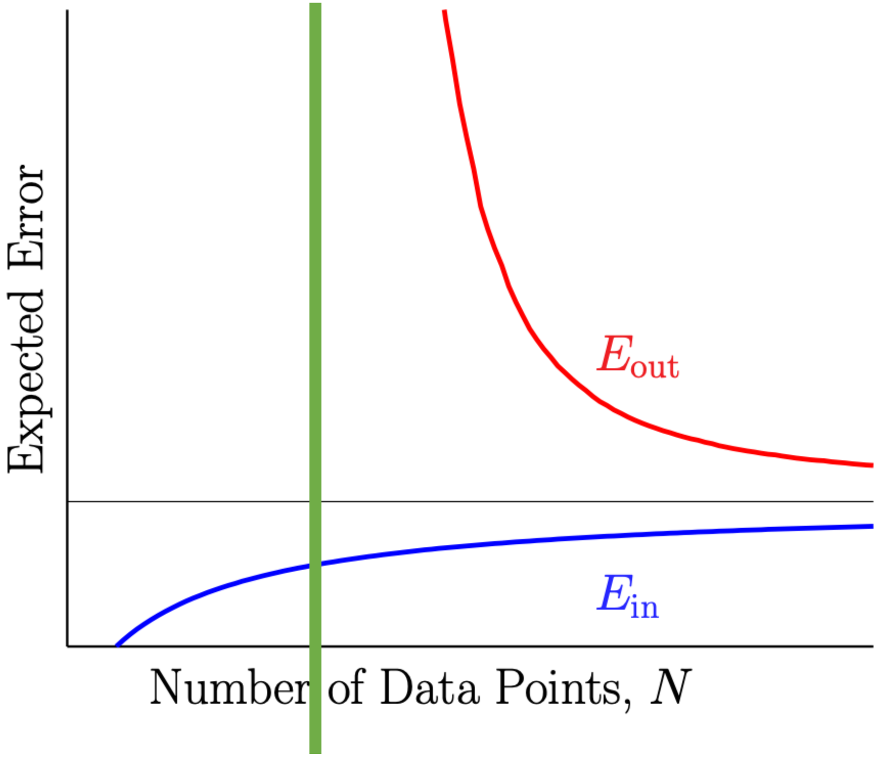
Complex f with no noise.

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

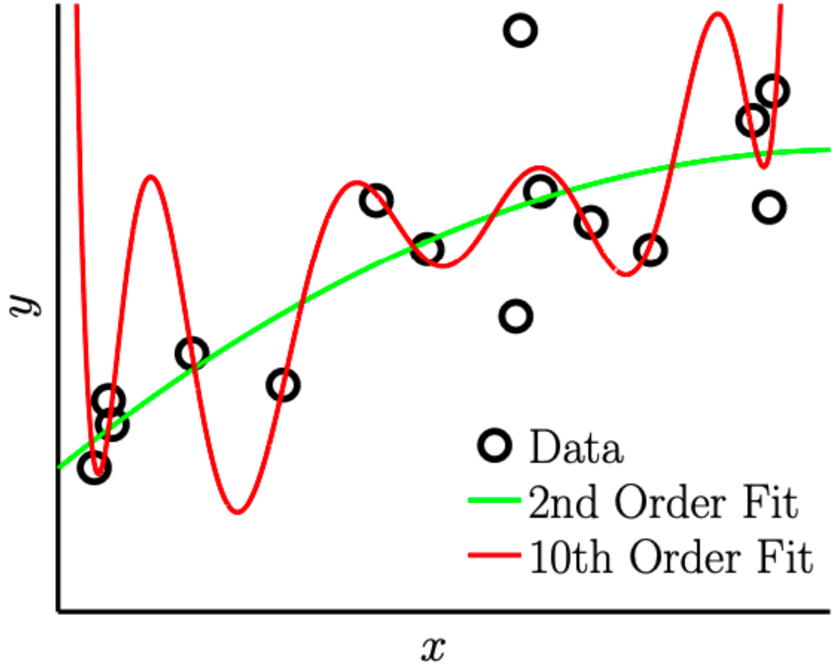
Data set size: N

The Overfit Measure

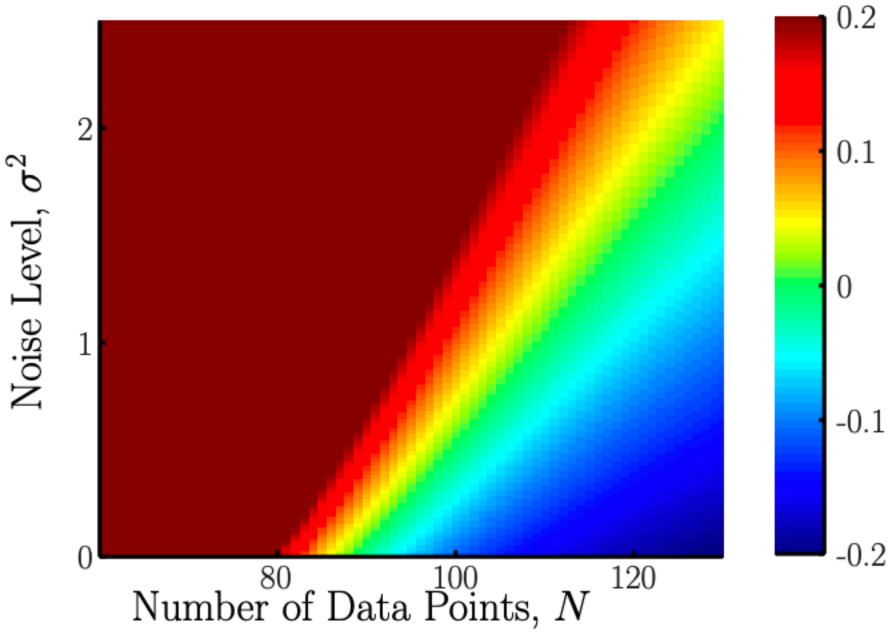
- Fit the data set using H_2 and H_{10}
  - Let g_2 and g_{10} be the learned hypothesis

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

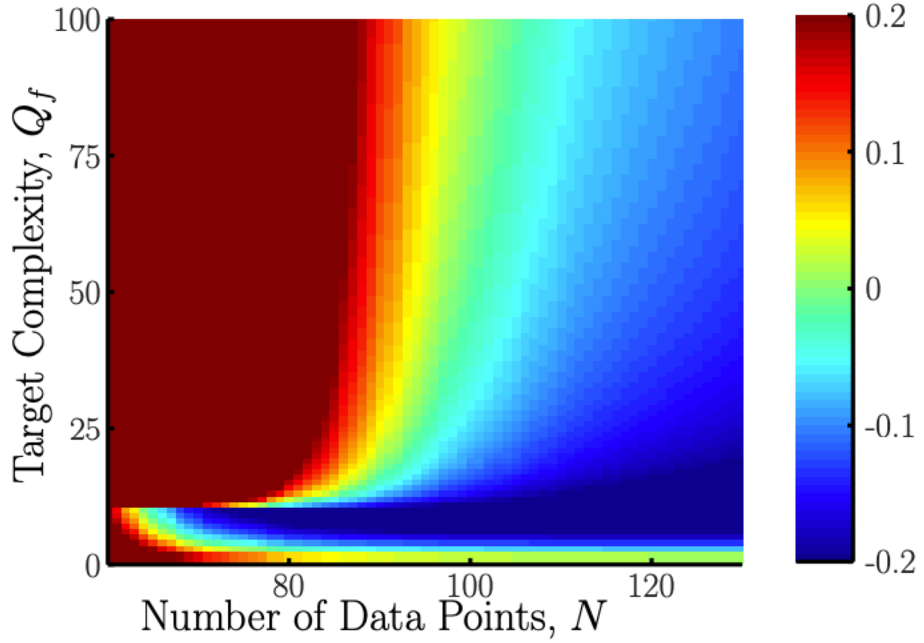
  - This value is large is overfitting happens



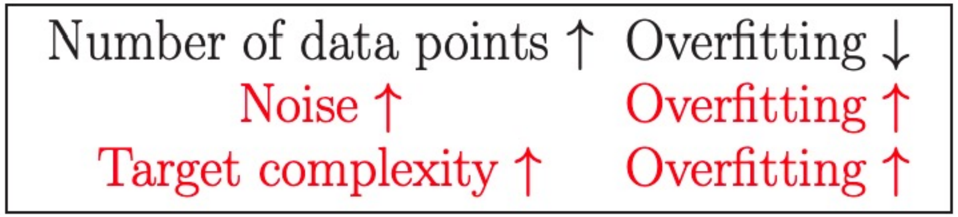
Overfit Measure: $E_{out}(g_{10}) - E_{out}(g_2)$



Stochastic noise



deterministic noise



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

Noise:
The part of y we cannot model

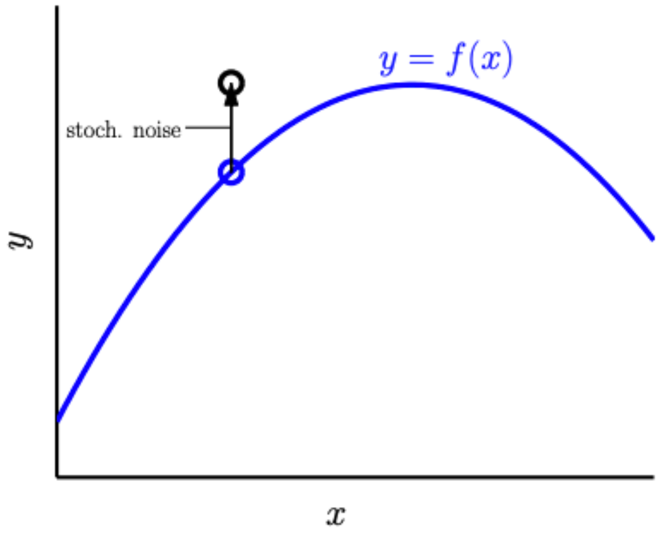
Stochastic Noise

We would like to learn from ○:

$$y_n = f(x_n)$$

Unfortunately, we only observe ○:

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



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

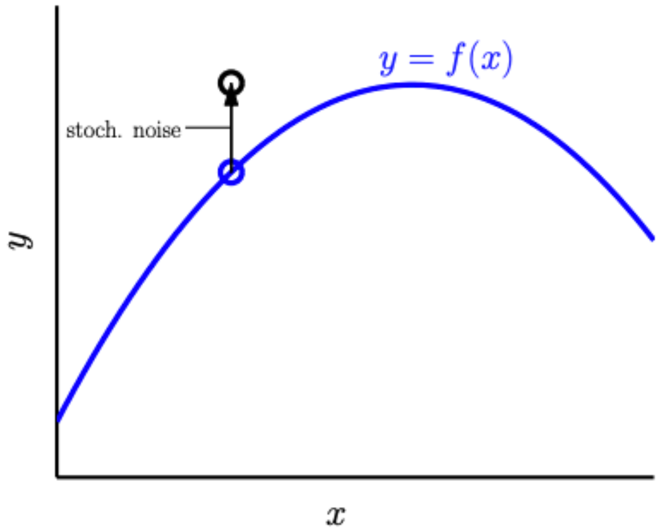
Stochastic Noise

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.**

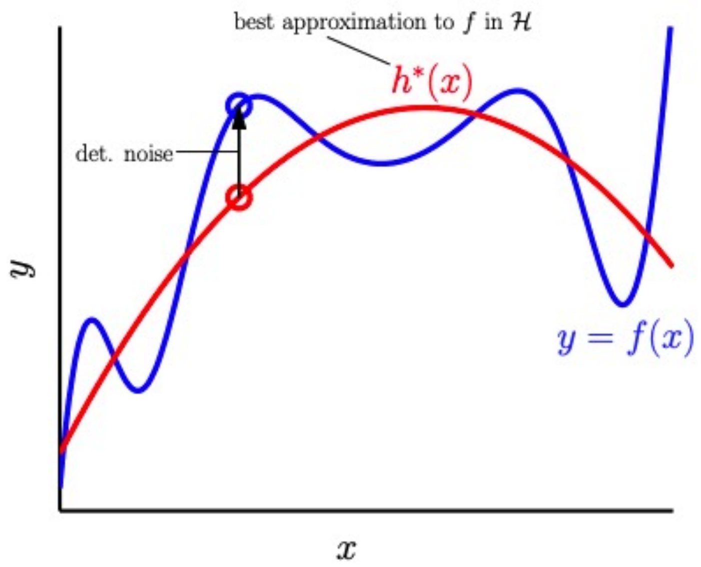
Deterministic Noise

We would like to learn from ○:

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

Unfortunately, we only observe ○:

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



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

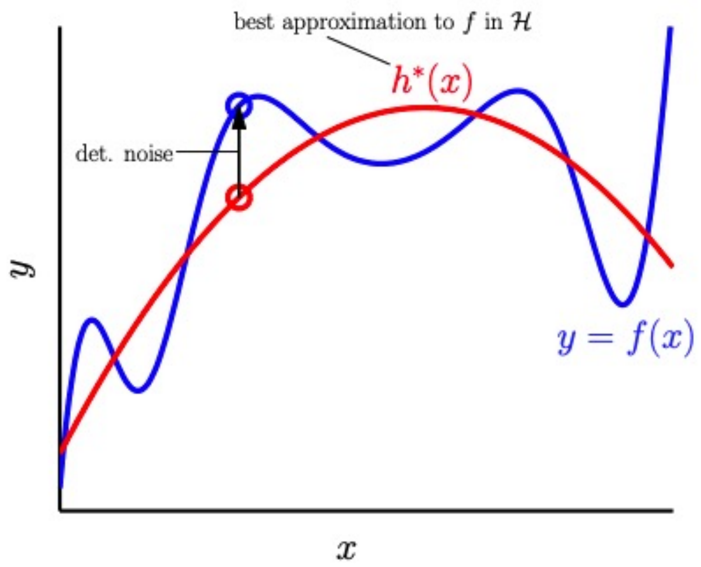
Deterministic Noise

We would like to learn from ○:

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

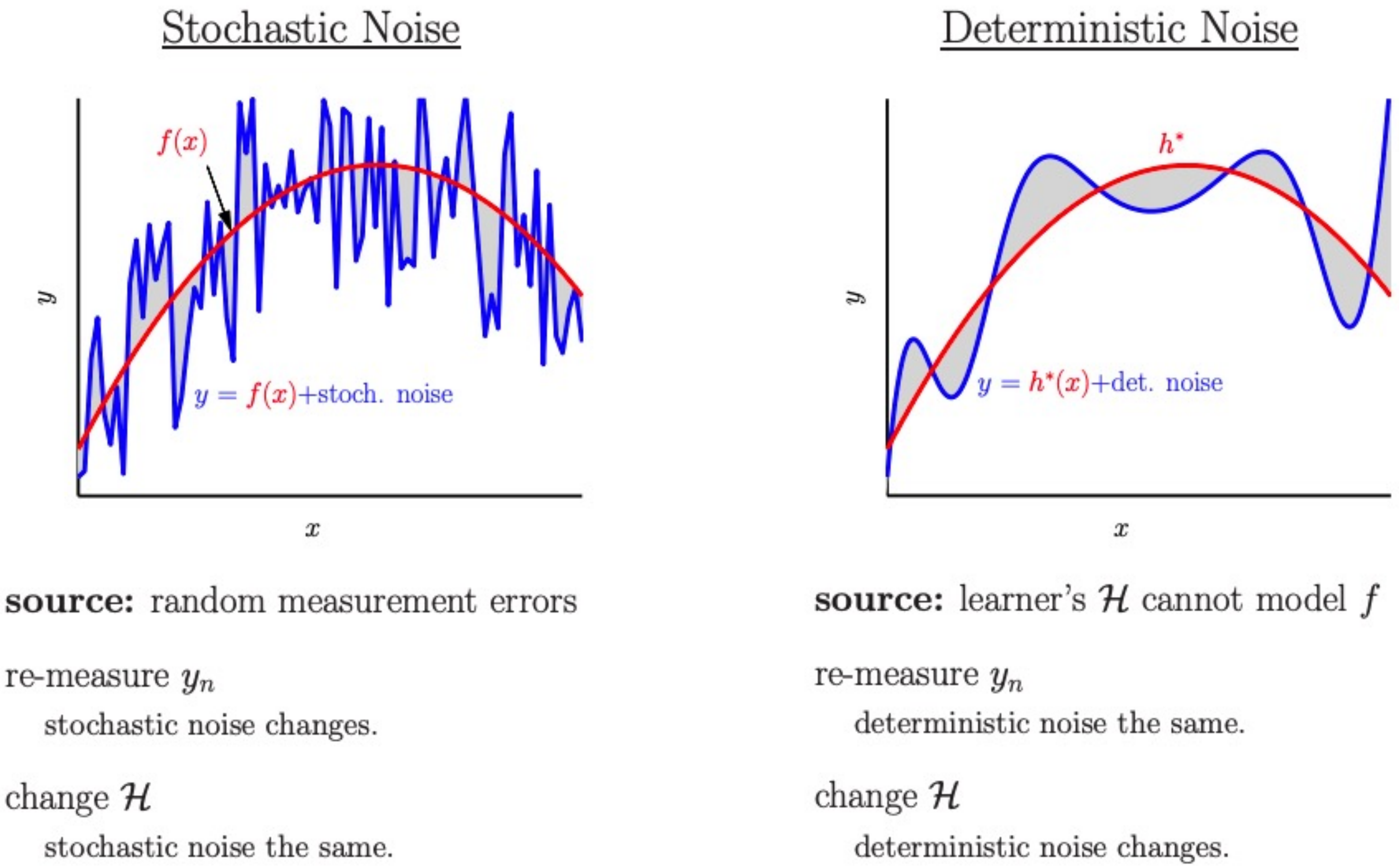
Unfortunately, we only observe ○:

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



Deterministic Noise: the part of f we cannot model.

Both sources of noises hurt learning



Stochastic Noise	Deterministic Noise
source: random measurement errors	**source:** learner's $\mathcal{H}$ cannot model f
re-measure y_n stochastic noise changes.	re-measure y_n deterministic noise the same.
change $\mathcal{H}$ stochastic 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

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

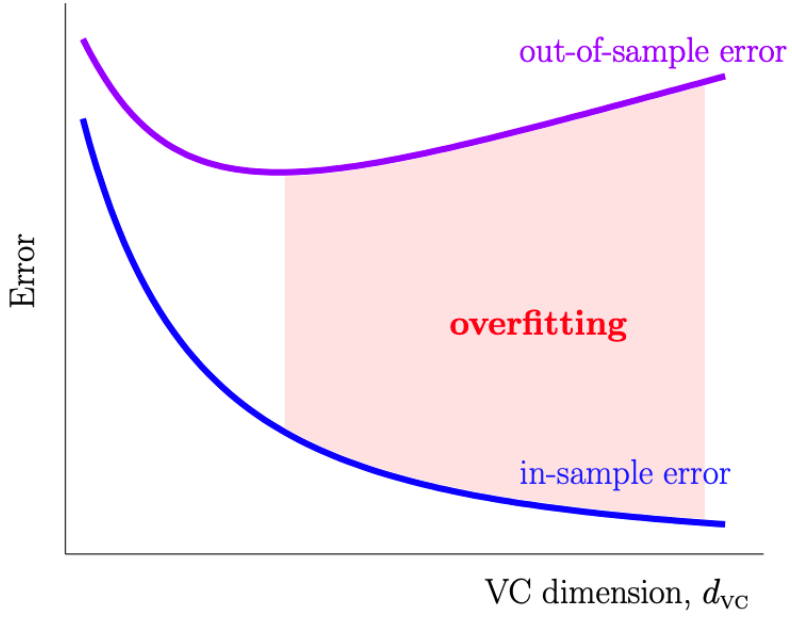
$$\mathbb{E}[E_{out}(\vec{x})] = \underset{\substack{\downarrow \\ \text{Stochastic Noise}}}{\sigma^2} + \underset{\substack{\downarrow \\ \text{Deterministic noise}}}{\text{bias}} + \text{variance}$$

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?

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  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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  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

<u>Proof Sketch:</u>

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

<u>Proof Sketch:</u>

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 $(y_1, \dots, y_{d+2}) = (\mathrm{sign}(\mathrm{a}_1), \dots, \mathrm{sign}(\mathrm{a}_{d+1}), -1)$, 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.