CSE 417T
Introduction to Machine Learning

Lecture 10

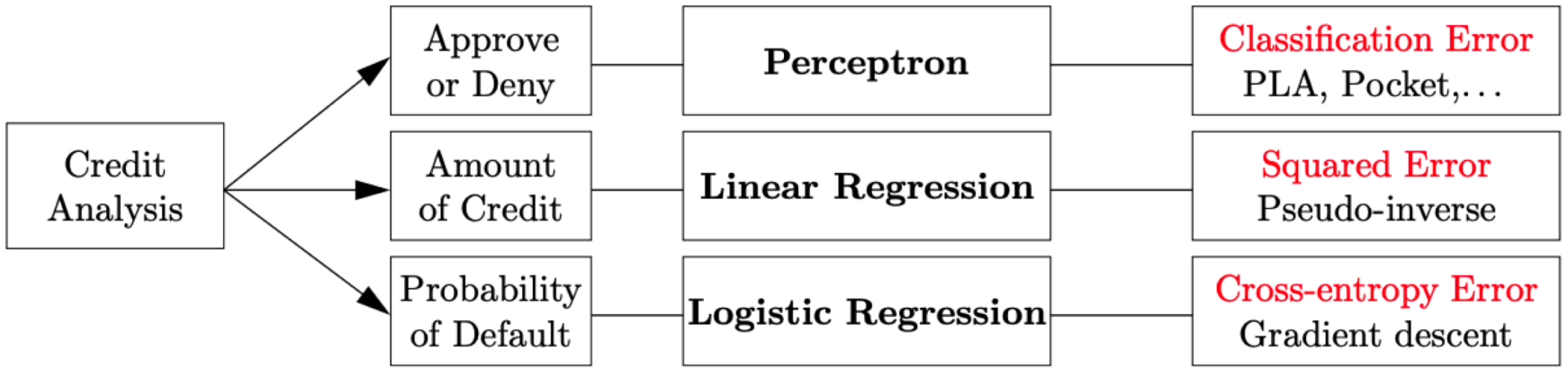
Instructor: Chien-Ju (CJ) Ho

Recap

Linear Models

This is why it's called linear models

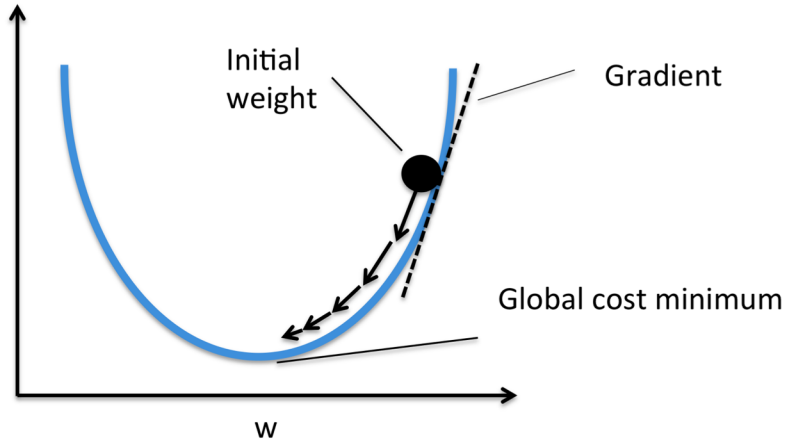
- H contains hypothesis $h(\vec{x})$ as **some function of $\vec{w}^T\vec{x}$**



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

Gradient Descent

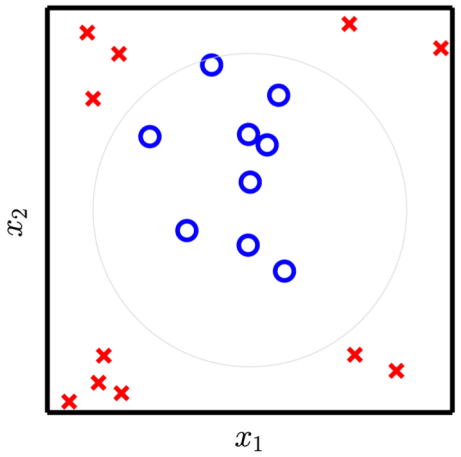
- Gradient descent algorithm
  - Initialize $\vec{w}(0)$
  - For $t = 0, \dots$
    - $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}(\vec{w}(t))$
    - Terminate if the stop conditions are met
  - Return the final weights



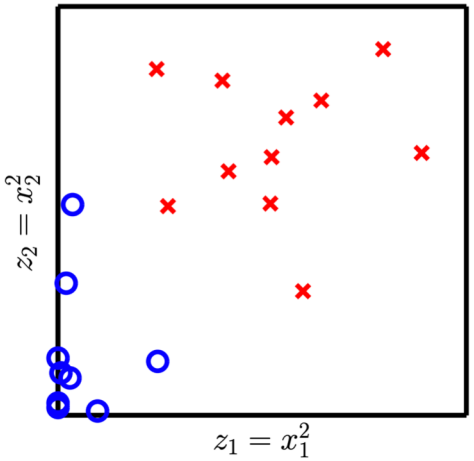
Works for functions where gradient exists everywhere

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

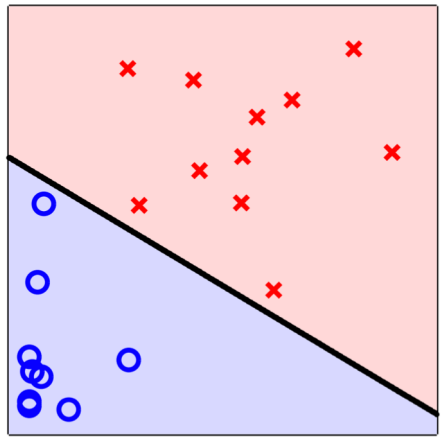
Nonlinear Transformation



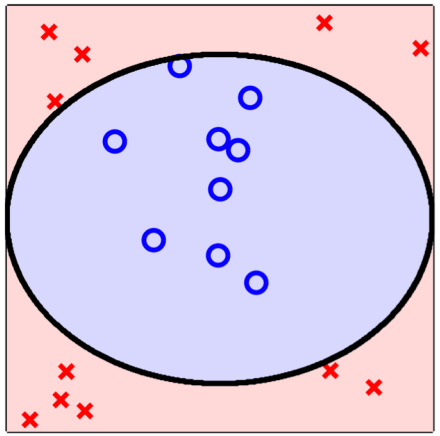
$$\vec{z} = \Phi(\vec{x})$$



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



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



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
    - $\vec{x} = (1, x_1, x_2),\ \Phi_2(\vec{x}) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$
    - 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

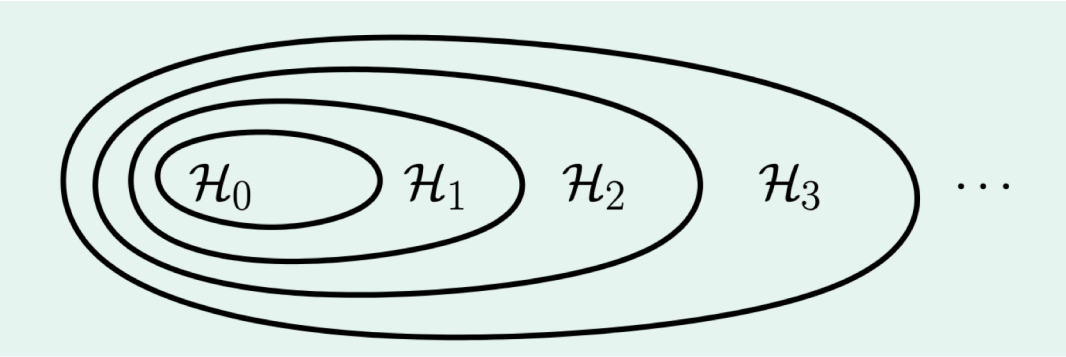
- $\vec{x} = (1, x_1, \ldots, x_d)$
- $\Phi_1(\vec{x}) = \vec{x}$
- $\Phi_Q(\vec{x}) = (\Phi_{Q-1}(\vec{x}), x_1^Q, x_1^{Q-1}x_2, \ldots, x_d^Q)$

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

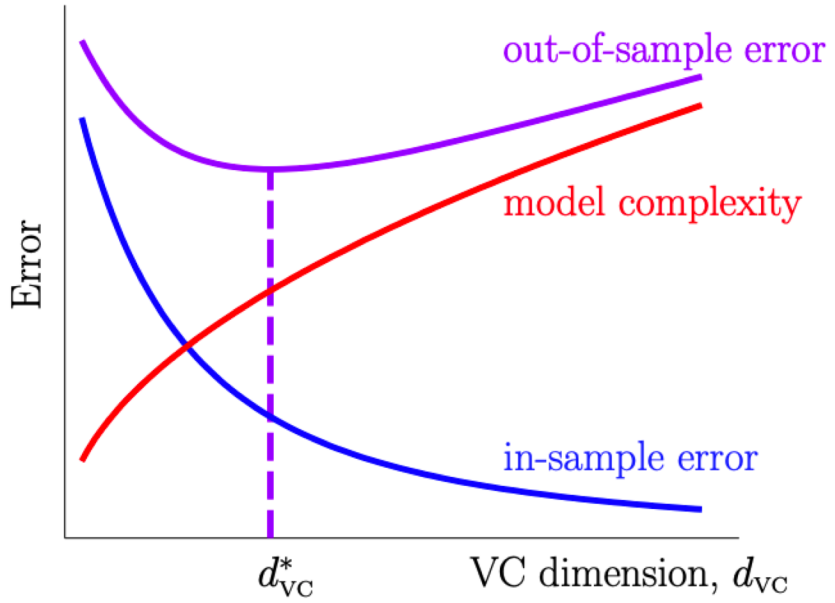
- Number of elements in $\Phi_Q(\vec{x})$: $\binom{Q+d}{Q}$ (including the initial 1)

Structural Hypothesis Sets

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



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



Brief Lecture Notes Today

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

Let me know if you spot errors.

Overfitting

[Adapted from the slides by Malik Magdon-Ismail]

Setup of the Discussion

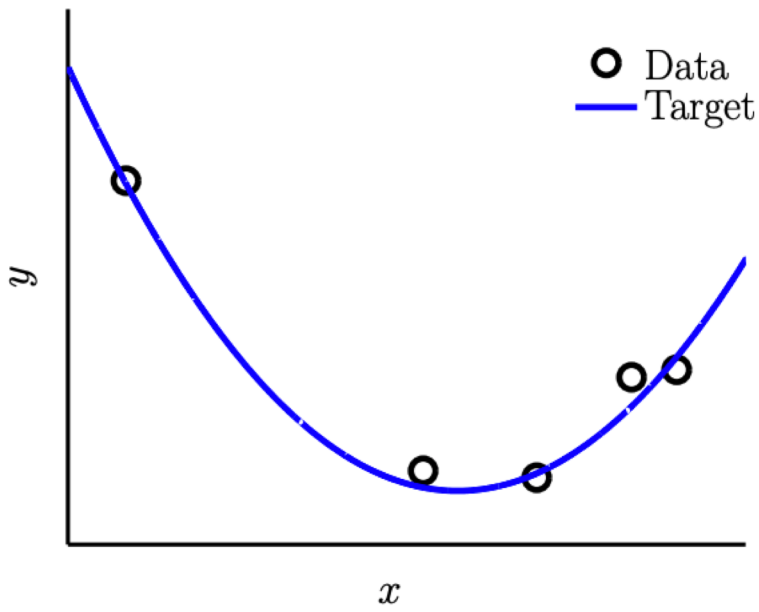
- Regression with polynomial transform
  - Input: 1-dimensional x
  - $\Phi_Q(x) = (1, x, x^2, x^3, \dots, x^Q)$
  - $H_Q = \{h(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_Q x^Q\}$

- 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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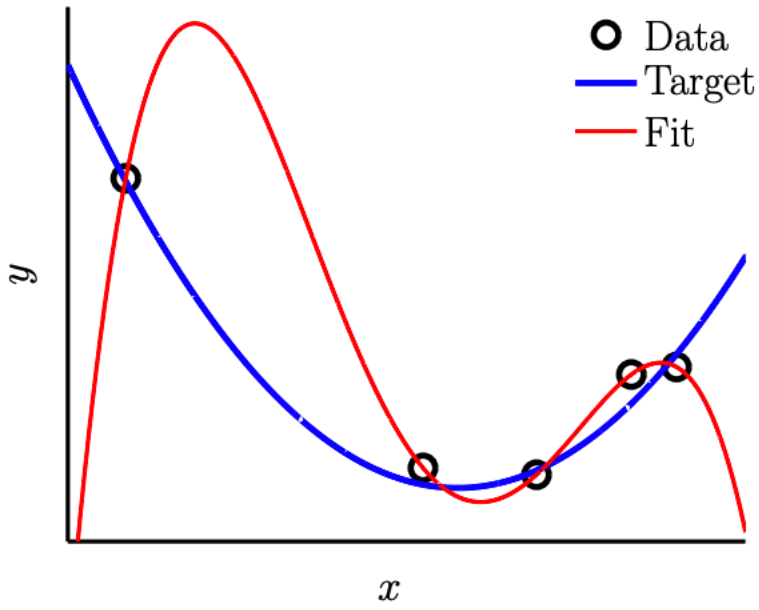


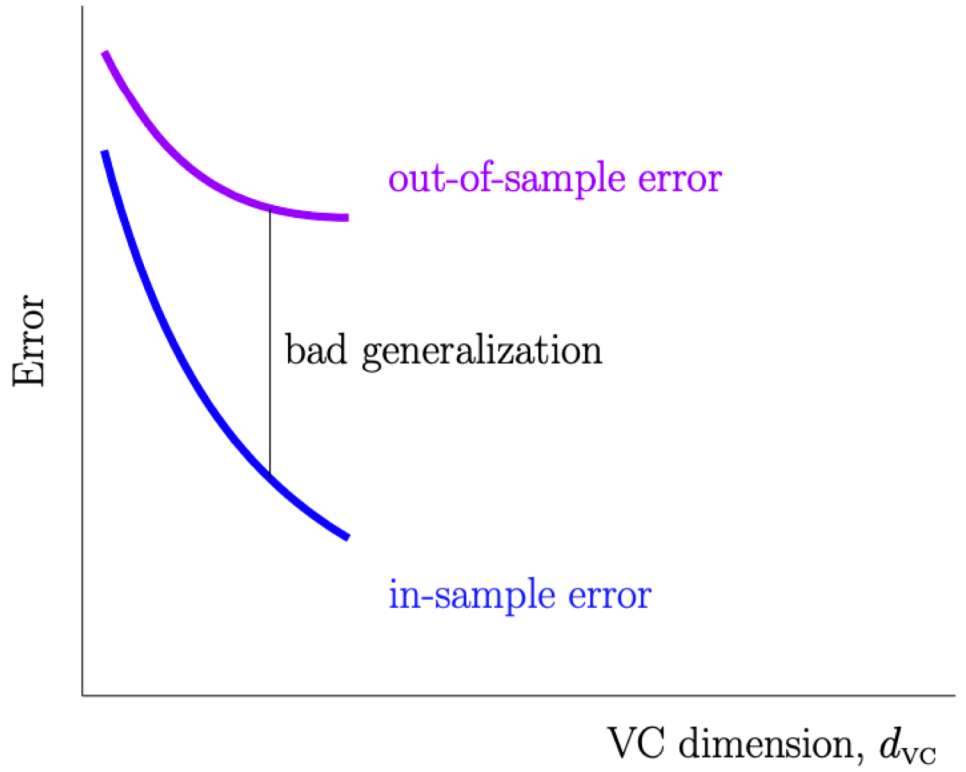
Classical overfitting: $E_{in} = 0$, but lead to a large E_{out}

Fitting the **noise** instead of the data

What is Overfitting?

Fitting the data more than is warranted

Overfitting is Not Just Bad Generalization



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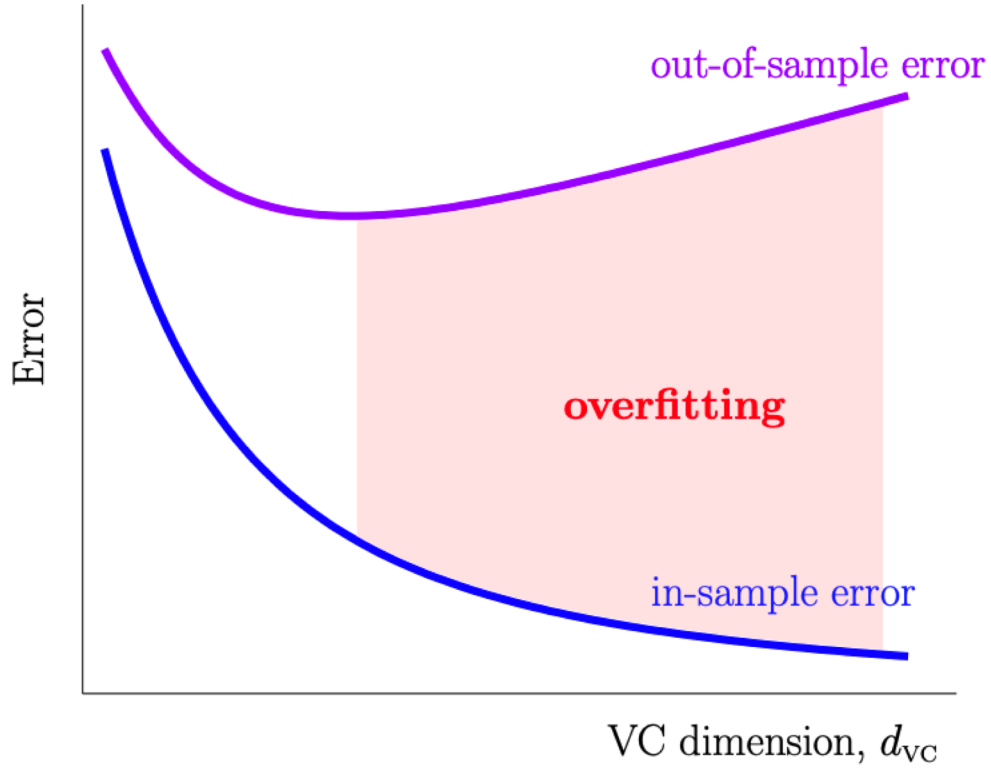
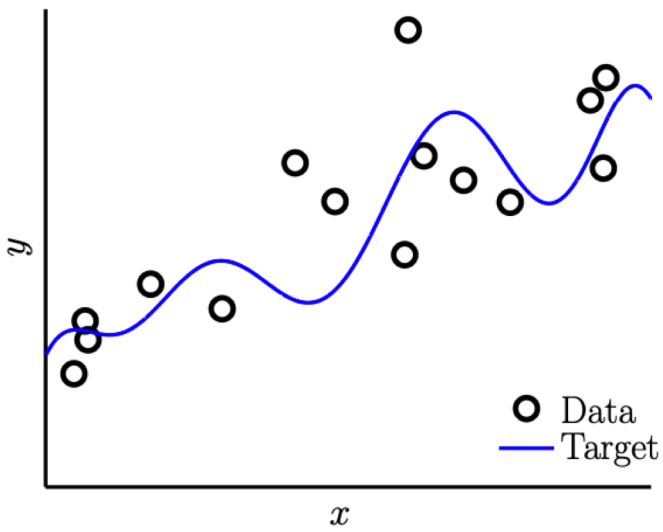


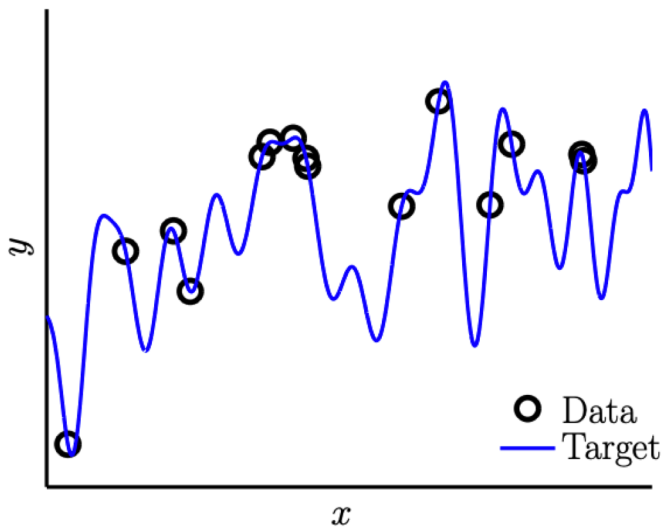
Overfitting

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

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



10th order f with noise.



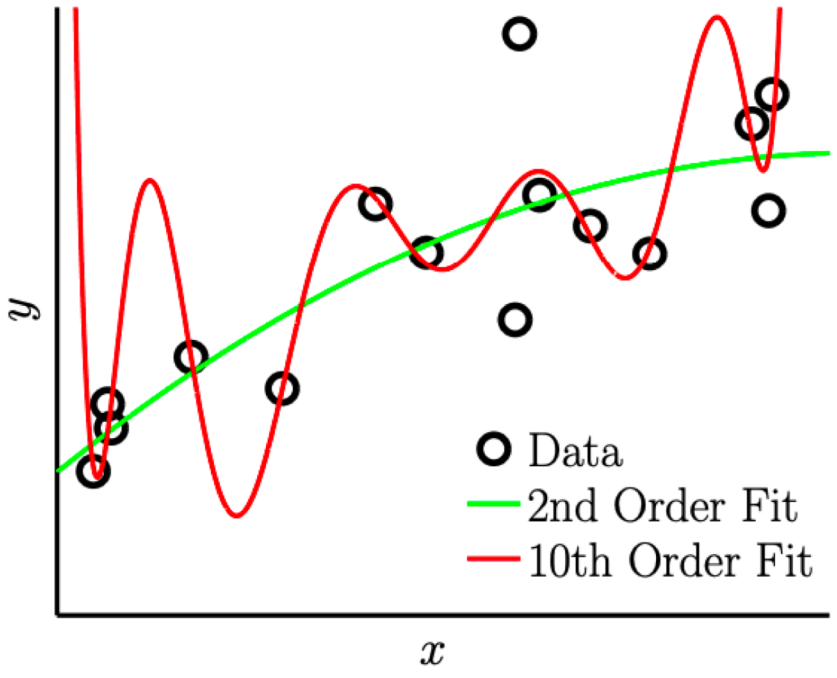
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

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

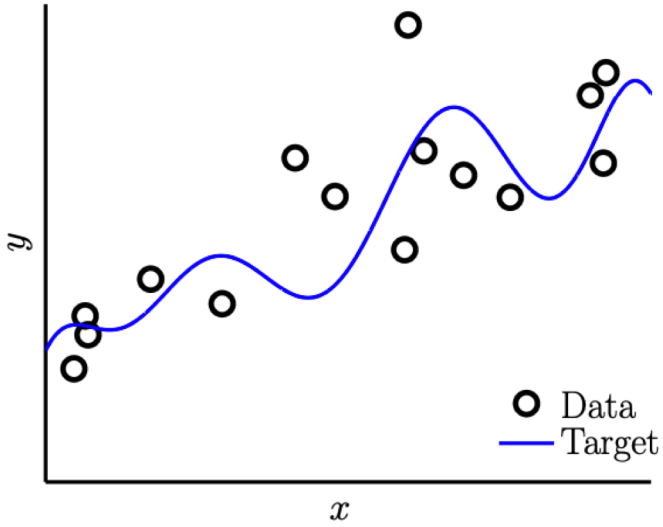
Target Function: 10^{th} Order f with Noise



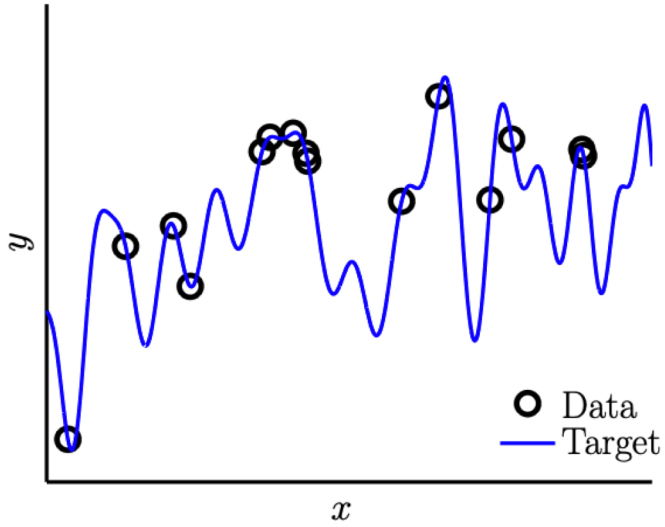
simple noisy target

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

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



10th order f with noise.



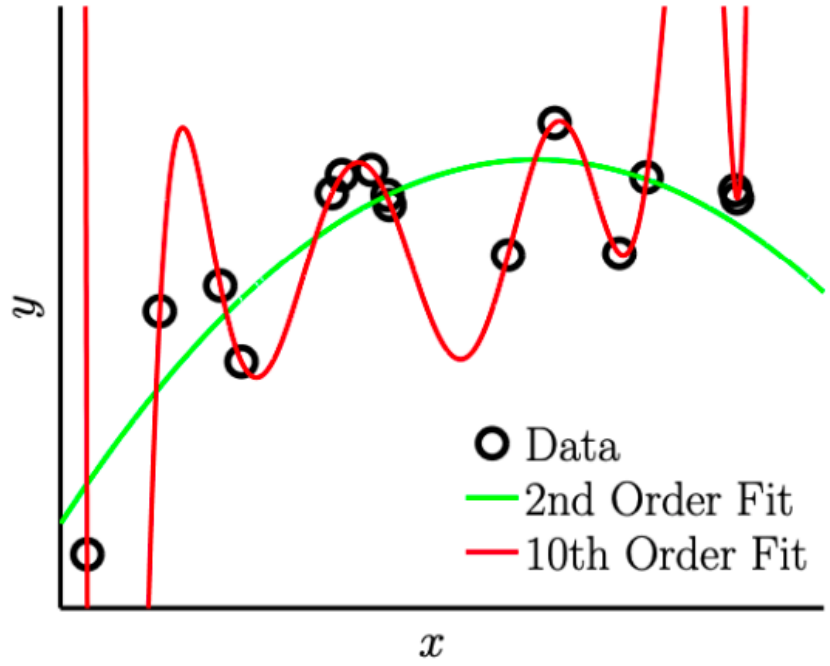
50th order f with no noise.

H_2: 2nd order polynomial fit

H_{10}: 10th order polynomial fit

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

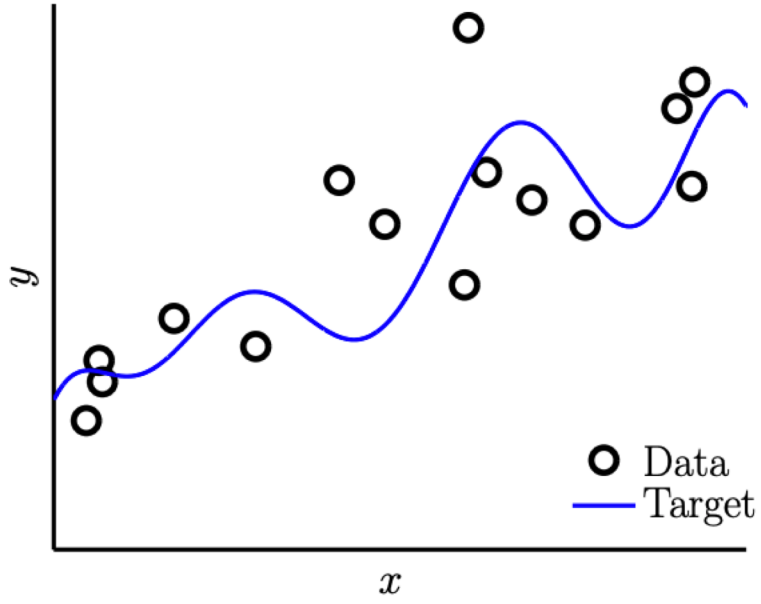
Simpler H is better even for complex target with no noise



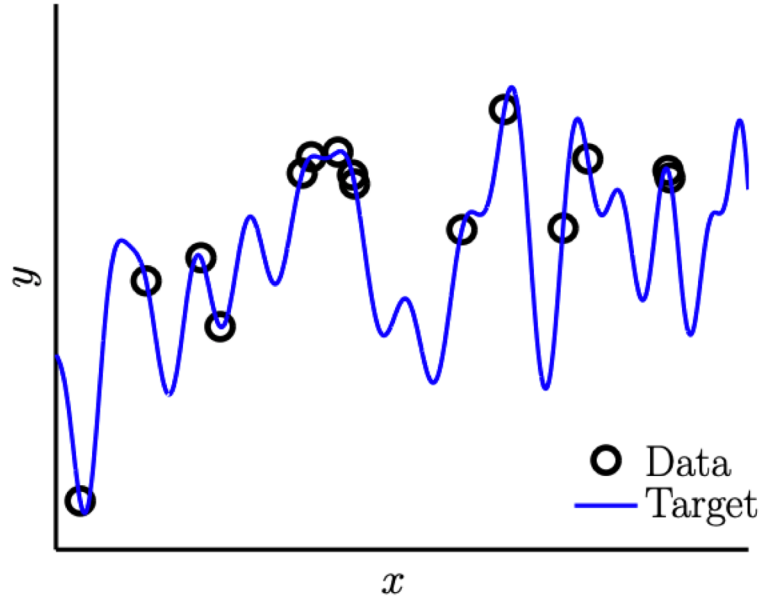
complex noiseless target

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

Is There Really “No Noise”?

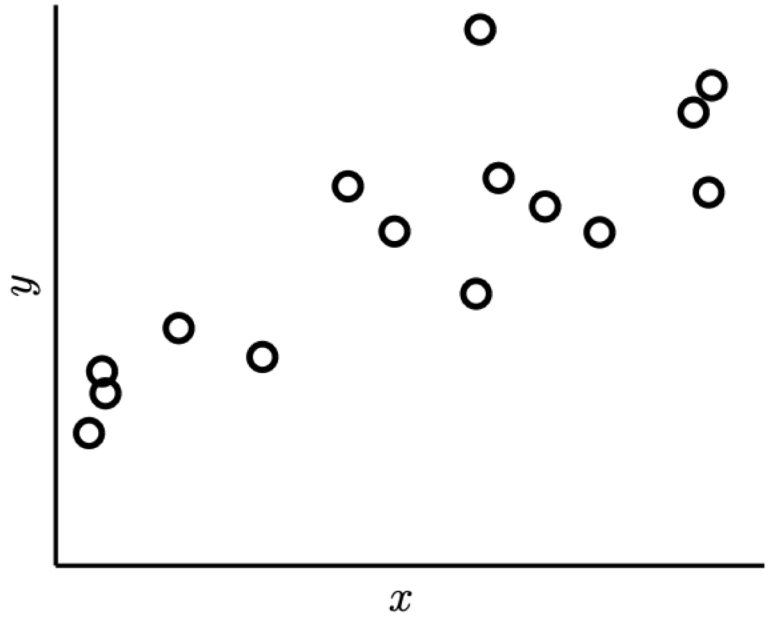


Simple f with noise.

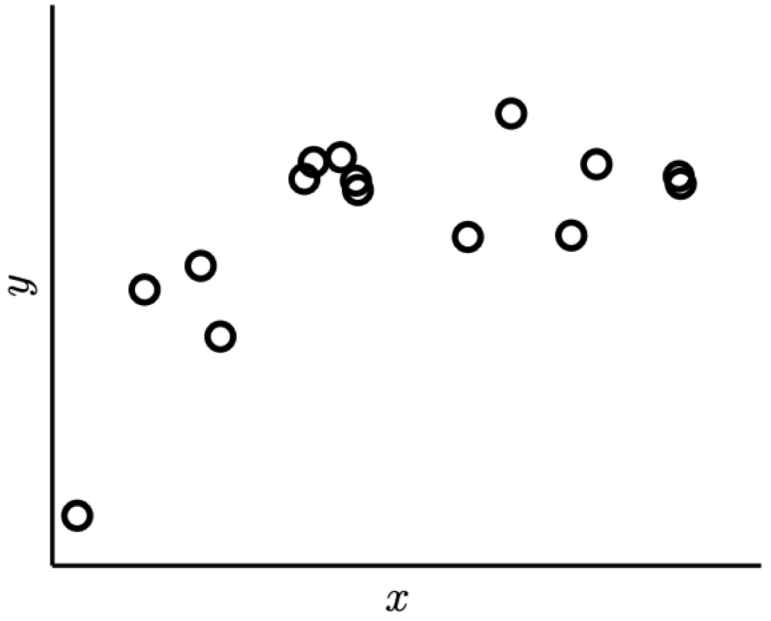


Complex f with no noise.

Is There Really "No Noise"?



Simple f with noise.

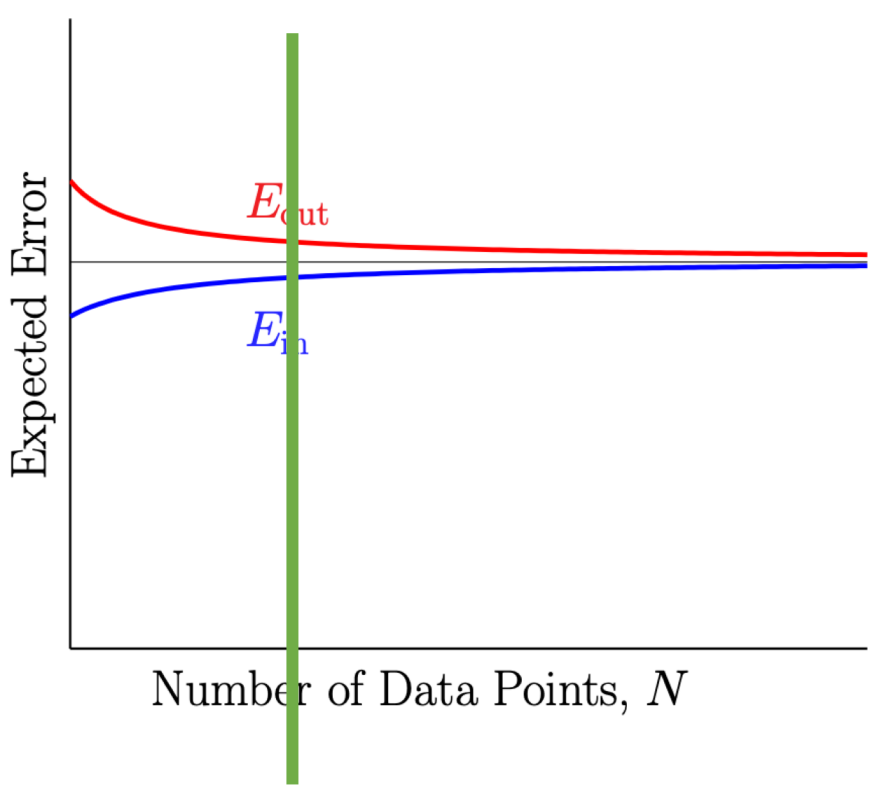


Complex f with no noise.

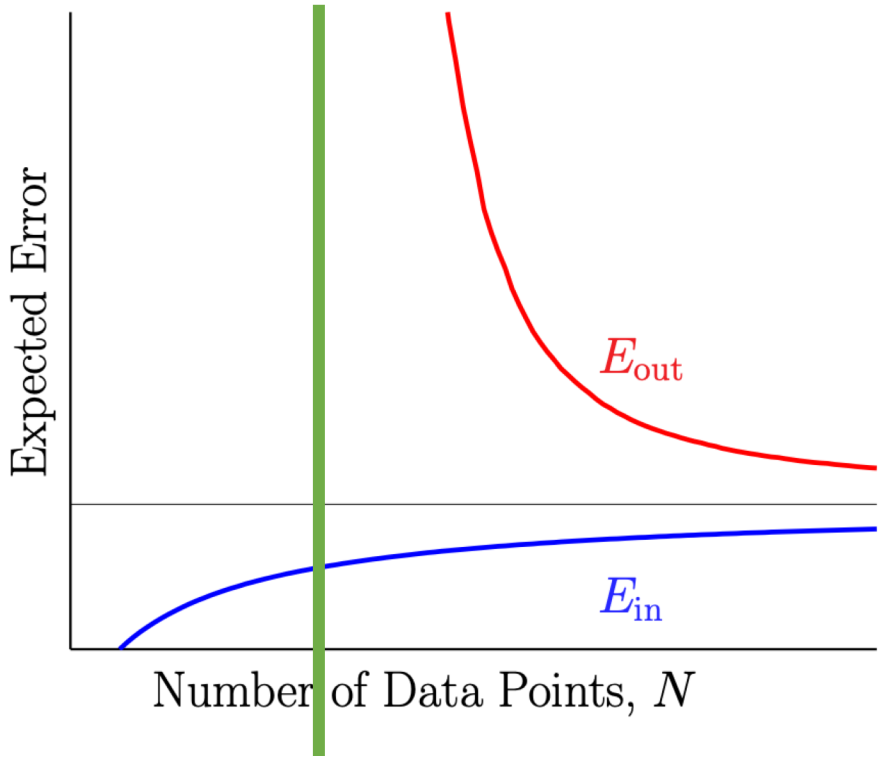
H should match **quantity and quality of data**, not (unknown)f

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

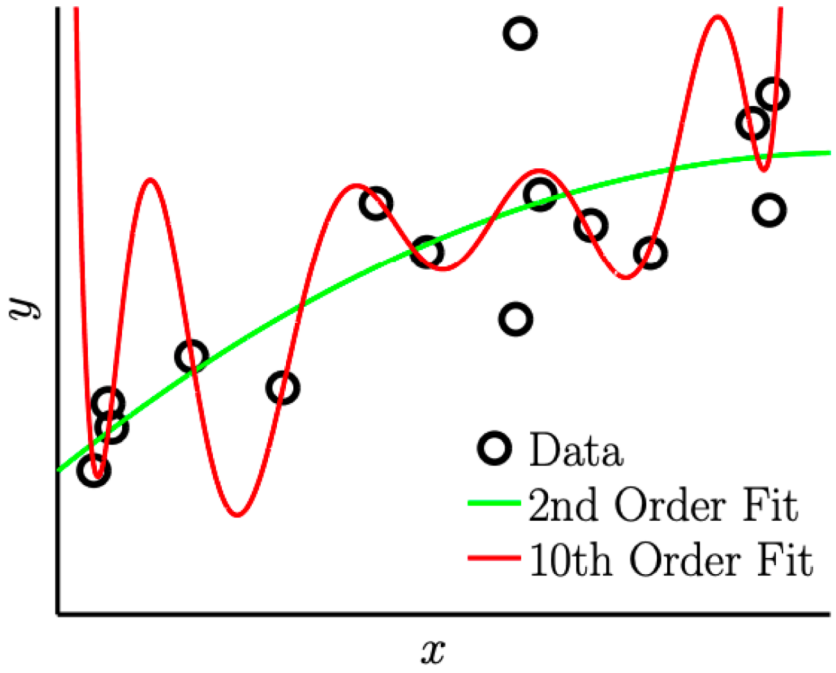
Data set size: N

The Overfit Measure

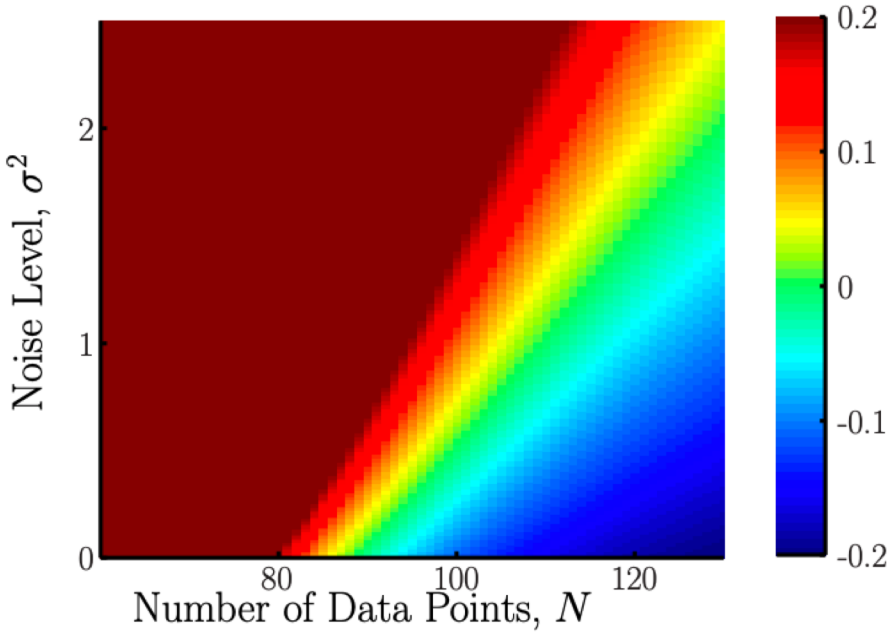
- Fit the data set using H_2 and H_{10}
  - Let g_2 and g_{10} be the learned hypothesis

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

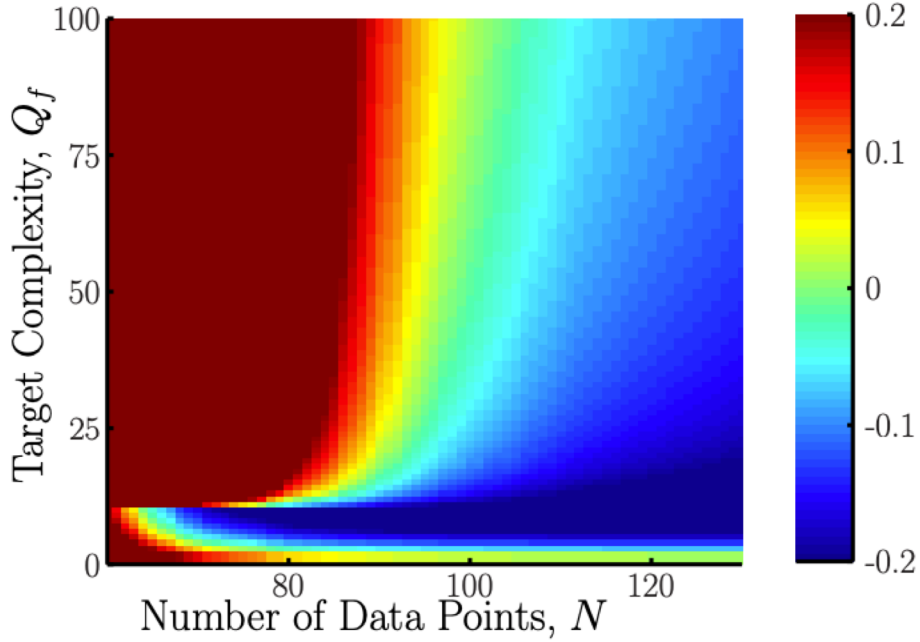
  - This value is large is overfit happens



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

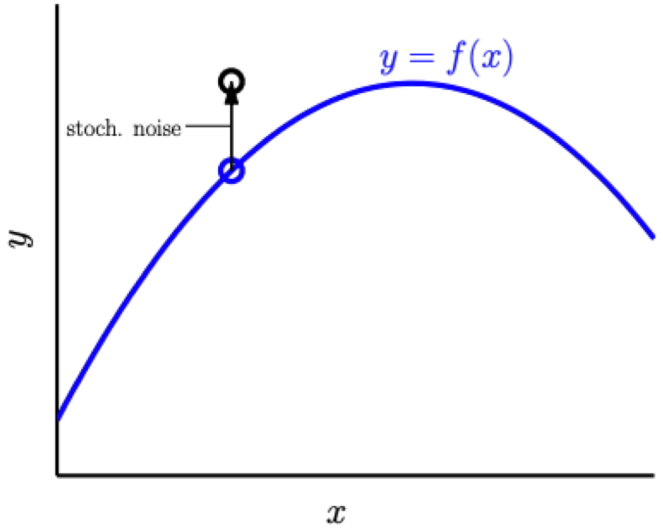
We would like to learn from ○:

$$y_n = f(x_n)$$

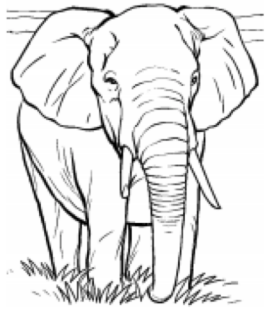
Unfortunately, we only observe ○:

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

↑ no one can model this



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



Deterministic Noise

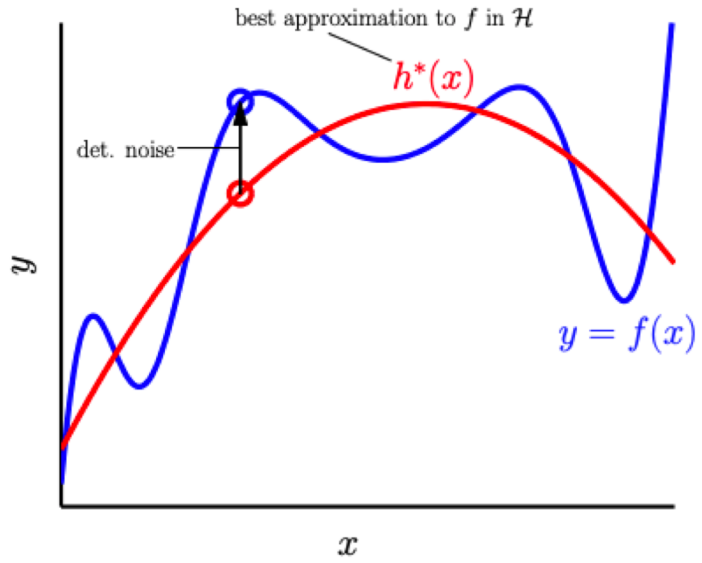
We would like to learn from ○:

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

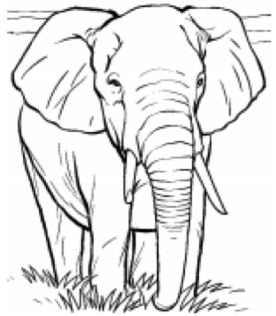
Unfortunately, we only observe ○:

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

↑ $\mathcal{H}$ cannot model this



Deterministic Noise: the part of f we cannot model.



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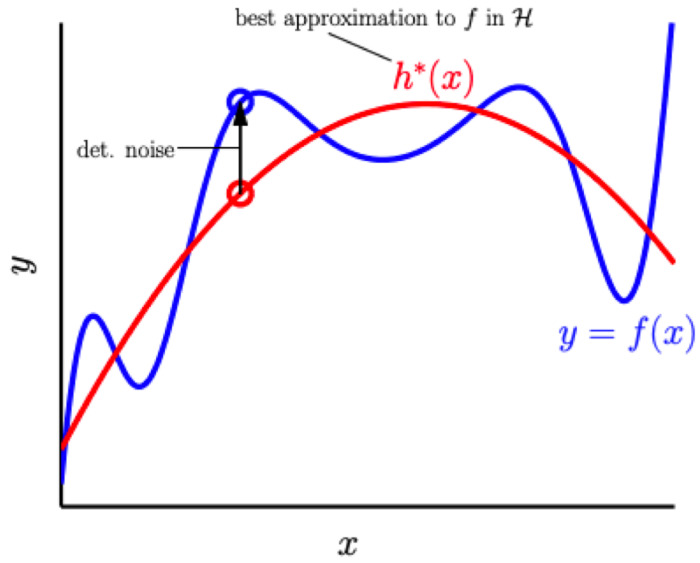

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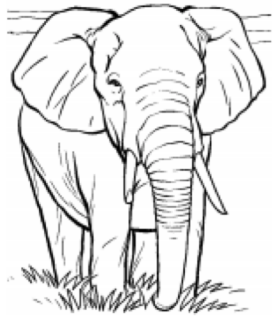
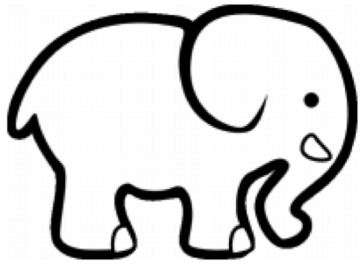
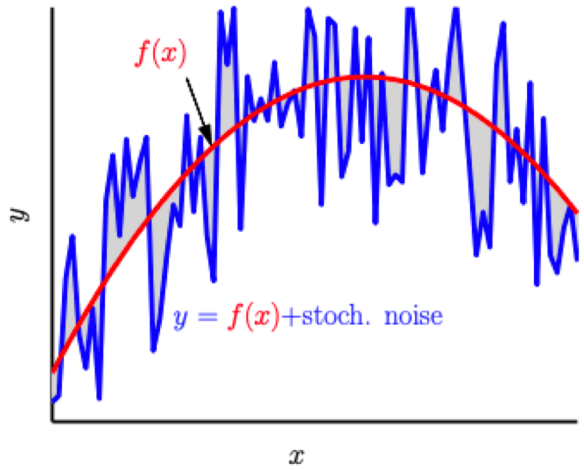




Both sources of noises hurt learning

Stochastic Noise



source: random measurement errors

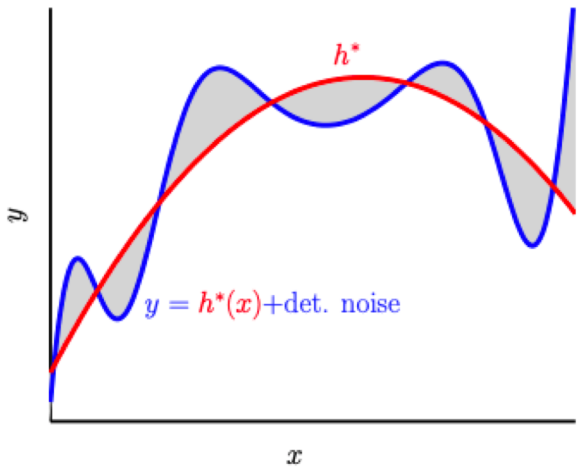
re-measure y_n

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

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