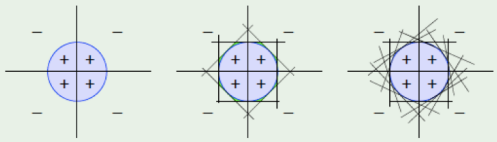
CSE4088 Introduction to Machine Learning

Overfitting

Slides are adopted from lecture notes of Yaser Abu-Mostafa

Review of last lecture

- Multilayer perceptrons

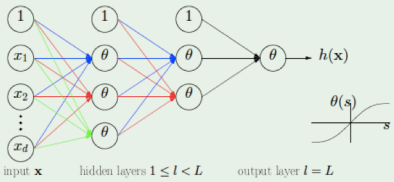


Logical combinations of perceptrons

- Neural networks

$$x_j^{(l)} = \theta\left(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)}\, x_i^{(l-1)}\right)$$

where $\theta(s) = \tanh(s)$



- Backpropagation

$$\Delta w_{ij}^{(l)} = -\eta\, x_i^{(l-1)} \delta_j^{(l)}$$

where

$$\delta_i^{(l-1)} = (1 - (x_i^{(l-1)})^2) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)}\, \delta_j^{(l)}$$

Outline

- What is overfitting?
- The role of noise
- Deterministic noise
- Dealing with overfitting

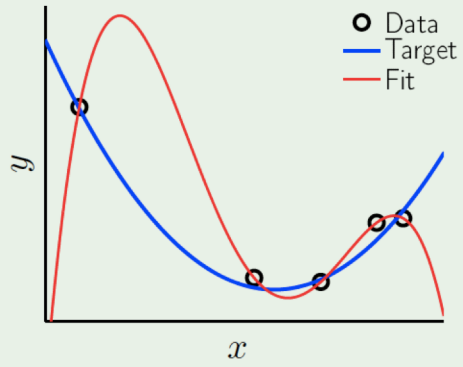
Illustration of overfitting

Simple target function

5 data points- **noisy**

4th-order polynomial fit

$E_{\text{in}} = 0, \;\; E_{\text{out}}$ is huge

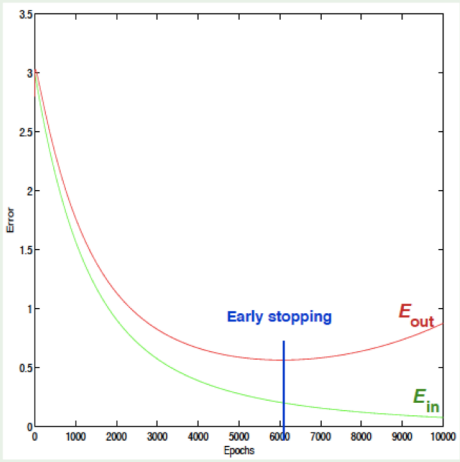


Overfitting can occur if you increase the model order.

Overfitting versus bad generalization

Neural network fitting noisy data

Overfitting: $E_{\text{in}} \downarrow$ $E_{\text{out}} \uparrow$



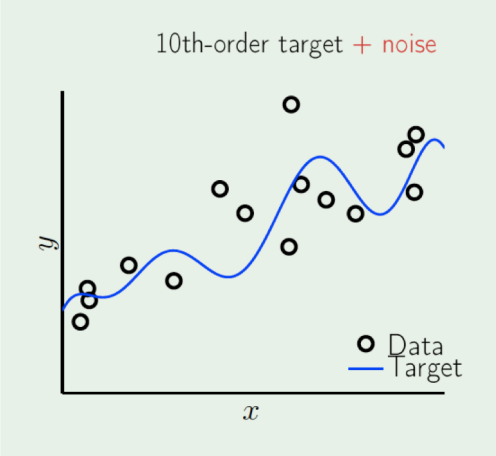
Overfitting can occur within the same model (e.g. neural network).

The culprit (source of the problem)

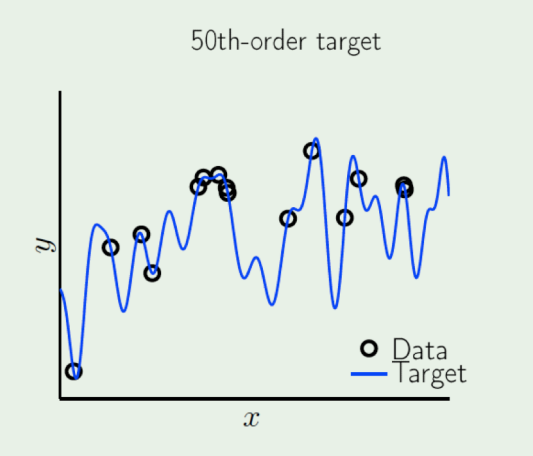
Overfitting: "fitting the data more than is warranted"

Culprit: fitting the noise - harmful

Case study

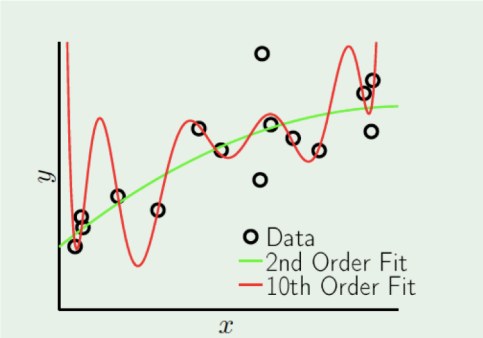


Generated 15 points **with noise**



Generated 15 points with **without noise** from the complex target

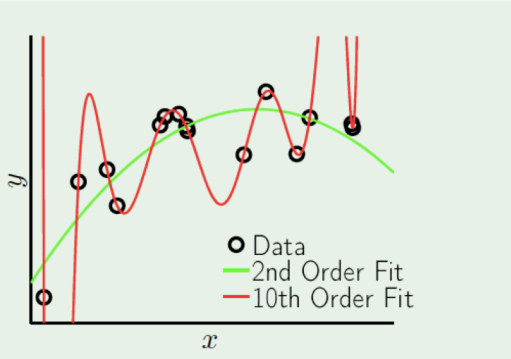
Two fits for each target



Noisy low-order target (10th order)

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

We are overfitting with the 10th order polynomial.
E_{in} decreased by E_{out} increased.



Noiseless high-order target (50th order)

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

We are overfitting with the 10th order polynomial.
E_{in} decreased by E_{out} increased !! But there is no noise here?

An irony of two learners

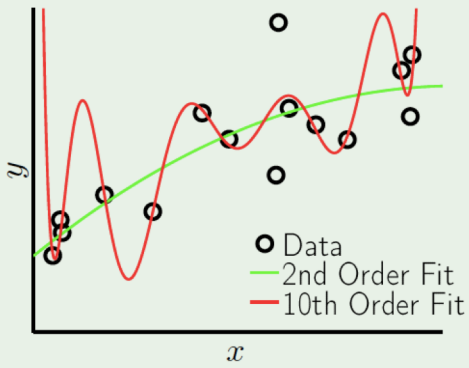
Two learners O and R

They know the target is 10th order

They have 15 **noisy samples**. They will choose a model.

O chooses $\mathcal{H}_{10}$ R chooses $\mathcal{H}_2$

There are 15 points (N), H_2 has 3 parameters, ratio = 15/3 = 5. Rule of thumb says ratio should be at least 10.
H_2 is more reasonable to learn as compared to H_{10}

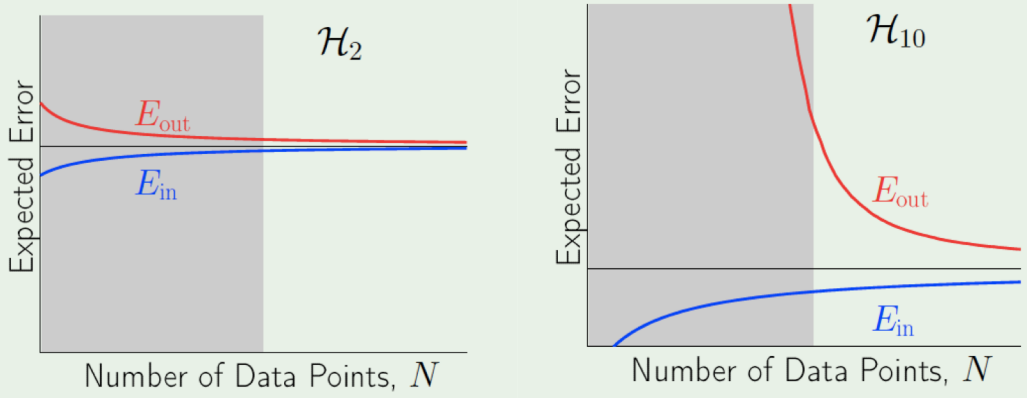


Learning a 10th-order target

Remember: You must match the complexity of your hypothesis to the data resources, not the complexity of the target function.

We have seen this case

Remember learning curves?



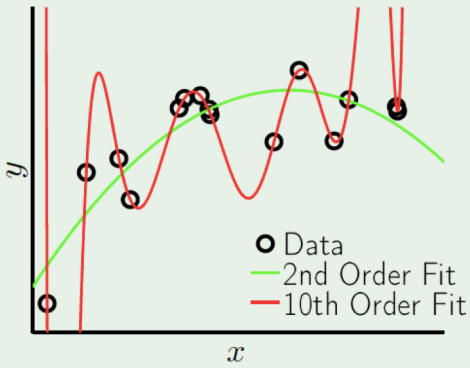
Even without noise

The two learners $\mathcal{H}_{10}$ and $\mathcal{H}_2$

They know there is no noise

Is there really no noise?

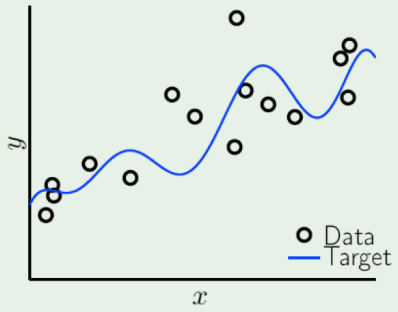
H_{10} has a better chance of getting closer to the target of 50th order polynomial. But it has larger E_{out}..



Learning a 50th-order target

A detailed experiment

Impact of **noise level** and **target complexity**



$$y = f(x) + \underbrace{\epsilon(x)}_{\sigma^2} = \underbrace{\sum_{q=0}^{Q_f} \alpha_q x^q}_{\text{normalized}} + \epsilon(x)$$

noise level: σ^2

target complexity: Q_f

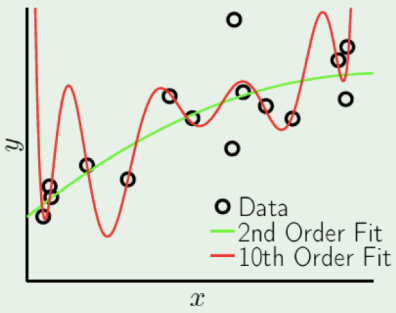
data set size: N

One instance: $Q_f = 10$, $N = 15$

The overfit measure

We fit the data set $(x_1, y_1), \cdots, (x_N, y_N)$ using our two models:

$\mathcal{H}_2$: 2nd-order polynomials $\mathcal{H}_{10}$: 10th-order polynomials

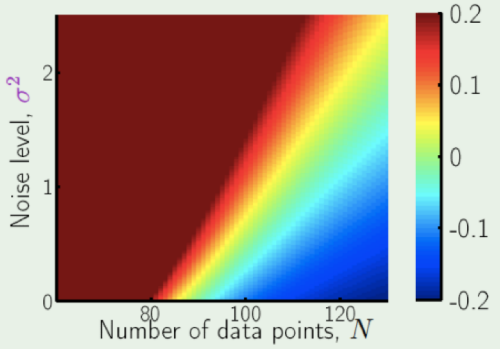


Compare out-of-sample errors of

$g_2 \in \mathcal{H}_2$ and $g_{10} \in \mathcal{H}_{10}$

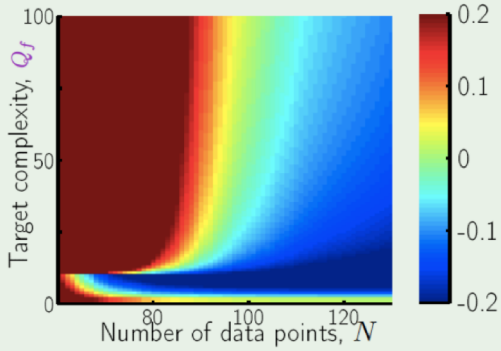
overfit measure: $E_{\text{out}}(g_{10}) - E_{\text{out}}(g_2)$

The results



Impact of σ^2

Q^f = 20 (order of target polynomial is fixed)



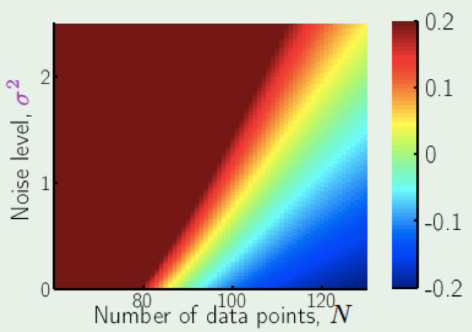
Impact of Q_f

Noise level $\sigma^2 = 1$ (fixed)

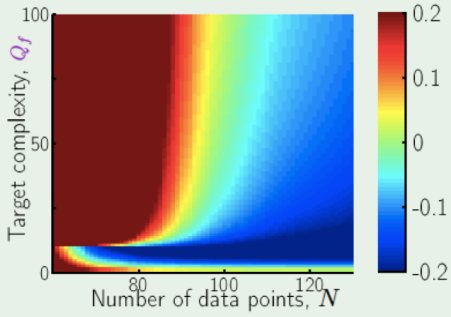
overfit measure: $E_{\text{out}}(g_{10}) - E_{\text{out}}(g_2)$

Red: more overfitting **Blue**: less overfitting

Impact of "noise"



Stochastic noise



Deterministic noise

number of data points	↑	Overfitting ↓
stochastic noise	↑	Overfitting ↑
deterministic noise	↑	Overfitting ↑

Outline

- What is overfitting?
- The role of noise
- **Deterministic noise**
- Dealing with overfitting

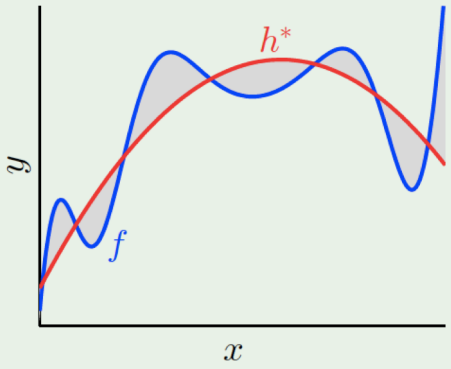
Definition of deterministic noise

The part of f that $\mathcal{H}$ cannot capture: $f(\mathbf{x}) - h^*(\mathbf{x})$

Why "noise"?

Main differences with stochastic noise:

1. depends on $\mathcal{H}$
2. fixed for a given $\mathbf{x}$

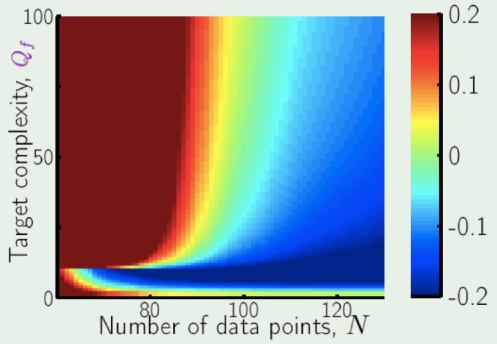


h* is the best possible approximation of *f* (target)

Impact on overfitting

Deterministic noise and Q_f

Finite N: $\mathcal{H}$ tries to fit the noise



how much overfit

overfit measure: $E_{\text{out}}(g_{10}) - E_{\text{out}}(g_2)$

Noise and bias-variance

Recall the decomposition:

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\text{var}(\mathbf{x})} + \underbrace{\left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]}_{\text{bias}(\mathbf{x})}$$

What if f is a noisy target?

$$y = f(\mathbf{x}) + \epsilon(\mathbf{x}) \qquad \mathbb{E}\left[\epsilon(\mathbf{x})\right] = 0$$

A noise term

$$\mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \quad y \quad\right)^2\right] = \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}) - \epsilon(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) + \bar{g}(\mathbf{x}) - f(\mathbf{x}) - \epsilon(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2 + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2 + \left(\epsilon(\mathbf{x})\right)^2\right.$$

$$\left. + \text{ cross terms }\right]$$

Actually, two noise terms

$$\underbrace{\mathbb{E}_{\mathcal{D},\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x})-\bar{g}(\mathbf{x})\right)^2\right]}_{\text{var}}+\underbrace{\mathbb{E}_{\mathbf{x}}\left[\left(\bar{g}(\mathbf{x})-f(\mathbf{x})\right)^2\right]}_{\text{bias}}+\underbrace{\mathbb{E}_{\epsilon,\mathbf{x}}\left[\left(\epsilon(\mathbf{x})\right)^2\right]}_{\sigma^2}$$

↑ deterministic noise

↑ stochastic noise

Outline

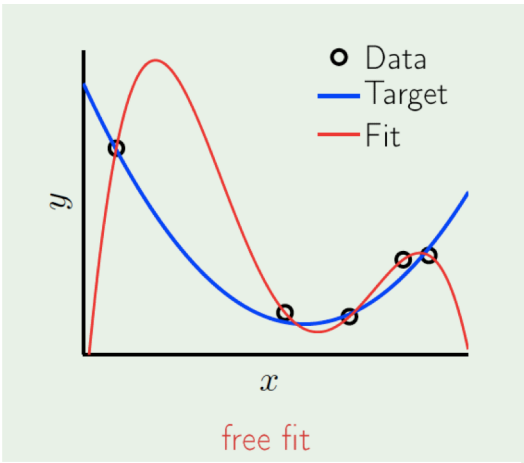
- What is overfitting?
- The role of noise
- Deterministic noise
- Dealing with overfitting

Two cures

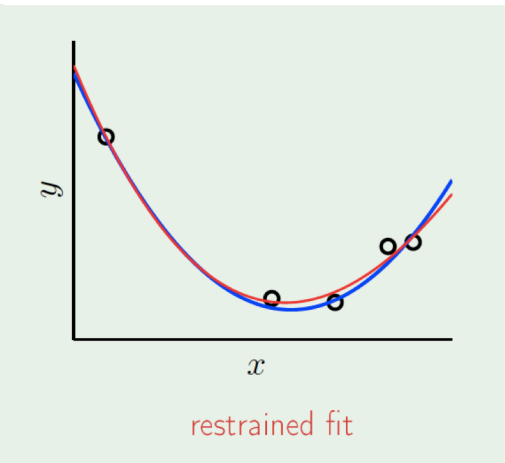
Regularization: Putting the brakes

Validation: Checking the bottom line

Putting the brakes



The fit is 4th order polynomial.



A 4th order polynomial is fit by restiring the curve not to pass through the points.