CSE4088 Introduction to Machine Learning

Bias-variance Tradeoff

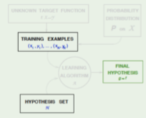
Slides are adopted from lecture notes of Yaser Abu-Mostafa

Review of last lecture

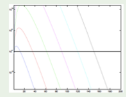
- VC dimension $d_{VC}(\mathcal{H})$

  most points $\mathcal{H}$ can shatter

- Scope of VC analysis



- Utility of VC dimension



$N \propto d_{VC}$

Rule of thumb: $N \geq 10\, d_{VC}$

- Generalization bound

  $E_{out} \leq E_{in} + \Omega$

Ω is a function of N (number of samples), VC dimension and δ (prob. of error)

Outline

- Bias and variance
- Learning curves

Approximation-generalization tradeoff

Small E_{out}: good approximation of f out of sample.

More complex $\mathcal{H} \Longrightarrow$ better chance of **approximating** f

Less complex $\mathcal{H} \Longrightarrow$ better chance of **generalizing** out of sample

Ideal $\mathcal{H} = \{f\}$ winning lottery ticket ☺

Quantifying the tradeoff

VC analysis was one approach: $E_{out} \leq E_{in} + \Omega$

Bias-variance analysis is another: decomposing E_{out} into

1. How well $\mathcal{H}$ can approximate f
2. How well we can zoom in on a good $h \in \mathcal{H}$

Applies to **real-valued targets** and uses **squared error**

Start with E_{out}

$$E_{out}(g^{(\mathcal{D})}) = \mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

E_{out} depends on the final hypothesis *g* and The dataset *D*

We want to release the dependency on the dataset by averaging out on D

$$\mathbb{E}_{\mathcal{D}}\left[E_{out}(g^{(\mathcal{D})})\right] = \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]$$

(We can change the order of the expectations since the integrand is non-negative)

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

Now, let us focus on:

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

The average hypothesis

To evaluate $\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$

we define the 'average' hypothesis $\bar{g}(\mathbf{x})$:

This will give us the correct value, in theory, if the noise is zero-mean.

$$\bar{g}(\mathbf{x}) = \mathbb{E}_{\mathcal{D}}\left[g^{(\mathcal{D})}(\mathbf{x})\right]$$

Imagine **many** data sets $\mathcal{D}_1, \mathcal{D}_2, \cdots, \mathcal{D}_K$

$$\bar{g}(\mathbf{x}) \approx \frac{1}{K}\sum_{k=1}^{K} g^{(\mathcal{D}_k)}(\mathbf{x})$$

Using $\bar{g}(\mathbf{x})$

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

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

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

Bias and variance

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

Therefore, $\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]$

$$= \mathbb{E}_{\mathbf{x}}[\text{bias}(\mathbf{x}) + \text{var}(\mathbf{x})]$$

$$= \text{bias} + \text{var}$$

Var: How far is your hypothesis *g* from the average hypothesis (the best possible one)? It is the variance of the model due to the finite dataset.

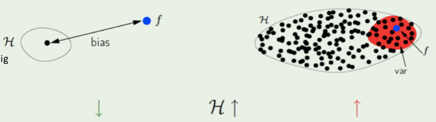
Bias: How far is your best hypothesis from the target function? (You did your best by averaging out but it is still far from the target function)

Interpretation: You learn from one dataset and calculate your error E_{out}. You do this for other possible datasets and take the average. Lets say your error is 0.3. Then, 0.05 of it might come from bias and 0.25 of it might come from variance.

The tradeoff

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

Small hypothesis set, bias is big



Huge hypothesis set includes *f* .

Bias diminishes, variance gets larger as the hypothesis set gets bigger since the red area gets bigger.

Example: sine target

$f : [-1, 1] \to \mathbb{R} \qquad f(x) = \sin(\pi x)$

Only two training examples! $N = 2$

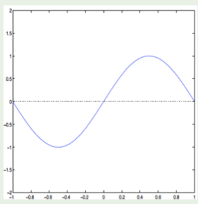
Two models used for learning:

$\mathcal{H}_0$: $h(x) = b$

$\mathcal{H}_1$: $h(x) = ax + b$

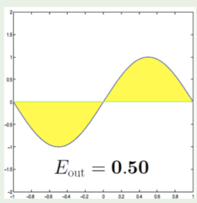
Which is better, $\mathcal{H}_0$ or $\mathcal{H}_1$?

f

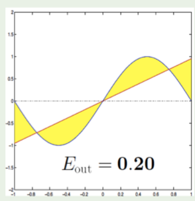


Approximation - $\mathcal{H}_0$ versus $\mathcal{H}_1$

$\mathcal{H}_0$

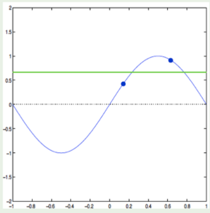


$\mathcal{H}_1$

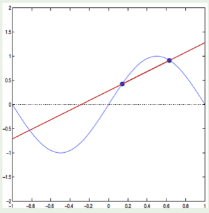


Learning - $\mathcal{H}_0$ versus $\mathcal{H}_1$

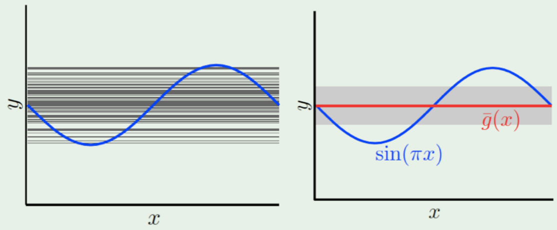
$\mathcal{H}_0$



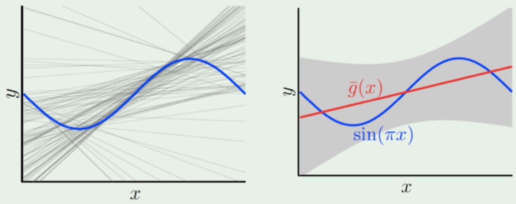
$\mathcal{H}_1$



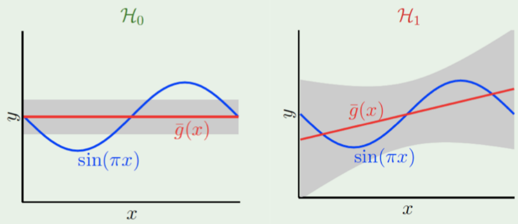
Bias and variance - $\mathcal{H}_0$



Bias and variance - $\mathcal{H}_1$



and the winner is ...



bias $= \mathbf{0.50}$ var $= \mathbf{0.25}$

bias $= \mathbf{0.21}$ var $= \mathbf{1.69}$

Lesson learned

Match the '**model complexity**'

to the **data resources**, not to the **target complexity**

Expected E_{out} and E_{in}

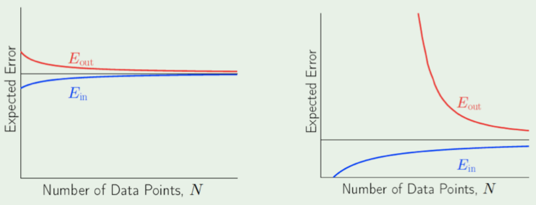
Data set $\mathcal{D}$ of size N

Expected out-of-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{out}}(g^{(\mathcal{D})})]$

Expected in-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{in}}(g^{(\mathcal{D})})]$

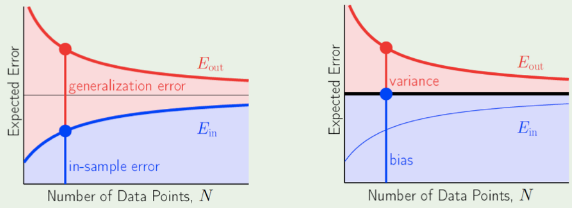
How do they vary with N?

The curves



Simple Model   Complex Model

VC versus bias-variance



VC analysis   bias-variance

Linear regression case

Data set $\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$

Linear regression solution: $\mathbf{w} = (\mathrm{X}^{\mathsf{T}}\mathrm{X})^{-1}\mathrm{X}^{\mathsf{T}}\mathbf{y}$

In-sample error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}$

'Out-of-sample' error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}'$

Learning curves for linear regression

Best approximation error $= \sigma^2$

Expected in-sample error $= \sigma^2 \left(1 - \frac{d+1}{N}\right)$

Expected out-of-sample error $= \sigma^2 \left(1 + \frac{d+1}{N}\right)$

Expected generalization error $= 2\sigma^2 \left(\frac{d+1}{N}\right)$