ECE595 / STAT598: Machine Learning I

Lecture 28.2: Sample and Model Complexity

Spring 2020

Stanley Chan

School of Electrical and Computer Engineering
Purdue University

PURDUE
UNIVERSITY

Outline

- Lecture 28 Sample and Model Complexity
- Lecture 29 Bias and Variance
- Lecture 30 Overfit

Today's Lecture:

- Generalization Bound using VC Dimension
  - Review of growth function and VC dimension
  - Generalization bound
- Sample and Model Complexity
  - Sample complexity
  - Model complexity
  - Trade off

Sample and Model Complexity

Sample Complexity

- What is the smallest number of samples required?
- Required to ensure training and testing error are close
- Close = within certain ϵ, with confidence $1 - \delta$
- Regardless of what learning algorithm you use

Model Complexity

- What is the largest model you can use?
- Refers to the hypothesis set
- With respect to the number of training samples
- Largest = measured in terms of VC dimension
- Can use = within certain ϵ, with confidence $1 - \delta$
- Regardless of what learning algorithm you use

Sample Complexity

- The generalization bound is

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{8}{N} \log \frac{4m_{\mathcal{H}}(2N)}{\delta}}.$$

- If you want the generalization error to be at most ϵ, then

$$\sqrt{\frac{8}{N} \log \frac{4m_{\mathcal{H}}(2N)}{\delta}} \leq \epsilon.$$

- Rearrange terms and use VC dimension,

$$N \geq \frac{8}{\epsilon^2} \log \left(\frac{4(2N)^{d_{\text{VC}}} + 1}{\delta} \right).$$

- Example. $d_{\text{VC}} = 3$. $\epsilon = 0.1$. $\delta = 0.1$ (90% confidence). Then the number of samples we need is

$$N \geq \frac{8}{0.1^2} \log \left(\frac{4(2N)^3 + 4}{0.1} \right).$$

Sample Complexity

- How to solve for N in this equation?

$$N \geq \frac{8}{0.1^2} \log \left(\frac{4(2N)^3 + 4}{0.1} \right).$$

- Put $N = 1000$ to the right hand side

$$N \geq \frac{8}{0.1^2} \log \left(\frac{4(2 \times 1000)^3 + 4}{0.1} \right) \approx 21,193.$$

- Not enough. So put $N = 21,193$ to the right hand side. Iterate.
- Then we get $N \approx 30,000$.
- So we need at least 30,000 samples.
- However, generalization bound is not tight. So our estimate is over-estimate.
- Rule of thumb, $10 \times d_{\text{VC}}$.

Error Bar

- The generalization bound is

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{8}{N} \log \left(\frac{4\left((2N)^{d_{\text{VC}}} + 1\right)}{\delta} \right)}.$$

- What error bar can we offer?
- Example. $N = 100$. $\delta = 0.1$ (90% confidence). $d_{\text{VC}} = 1$.
-

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{8}{100} \log \left(\frac{4\left((2 \times 100) + 1\right)}{0.1} \right)} \approx E_{\text{in}}(g) + 0.848.$$

- Close to useless.
- If we use $N = 1000$, then

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + 0.301.$$

- Somewhat more respectable estimate.

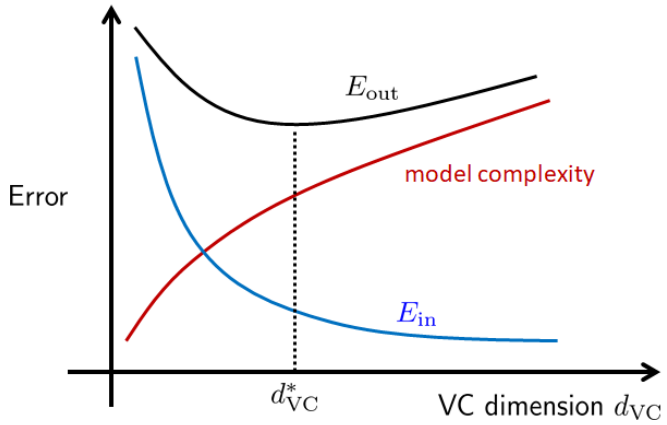
Model Complexity

- The generalization bound is

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \underbrace{\sqrt{\frac{8}{N}\log\frac{4\left((2N)^{d_{\text{VC}}}+1\right)}{\delta}}}_{=\epsilon(N,\mathcal{H},\delta)}$$

- $\epsilon(N,\mathcal{H},\delta)$ = penalty of the model complexity
- If d_{VC} is large, then $\epsilon(N,\mathcal{H},\delta)$ is big
- So the generalization error is large
- There is a trade-off curve

Trade-off Curve



Generalization Bound for Testing

- Testing Set: $\mathcal{D}_{\text{test}} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_L\}$.
- The final hypothesis g is already determined. So no need to use Union bound.
- The Hoeffding is as simple as

$$\mathbb{P}\Big\{ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon \Big\} \leq 2e^{-2\epsilon^2 L},$$

- The generalization bound is

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{1}{2L} \log \frac{2}{\delta}}.$$

- If you have a lot of testing samples, then $E_{\text{in}}(g)$ will be good estimate of $E_{\text{out}}(g)$
- Independent of model complexity
- Only δ and L

Reading List

- Yasar Abu-Mostafa, Learning from Data, chapter 2.1
- Mehrya Mohri, Foundations of Machine Learning, Chapter 3.2
- Stanford Note http://cs229.stanford.edu/notes/cs229-notes4.pdf