Machine Learning: Generalization 2

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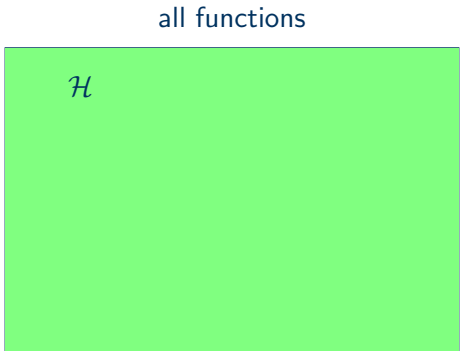
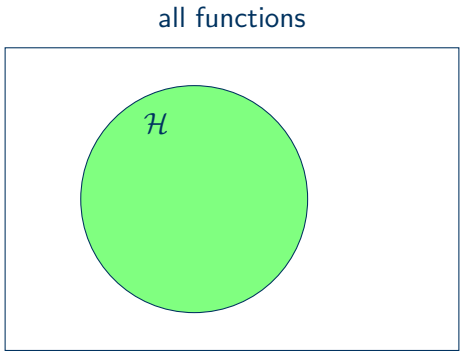
No free lunch theorem

all functions

No free lunch theorem



No free lunch theorem



No free lunch theorem

- If $\mathcal{H}$ is the set of all functions, $\mathcal{H}$ is not PAC learnable.
- If $\mathcal{H} = \{f\}$ where $L_{\mathcal{D}}(f) = 0$, then $\mathcal{H}$ is PAC learnable with ERM.

Error decomposition

$$L_{\mathcal{D}}(h) = \underbrace{L_{\mathcal{D}}(h) - \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h')}_{\text{estimation error}} + \underbrace{\min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h')}_{\text{approximation error}} \tag{1}$$

- Approximation error is due to the choice of $\mathcal{H}$.
- Estimation error is due to not finding the best program in $\mathcal{H}$.

Tradeoff between model complexity and generalization

- When we say we only compare to the best in $\mathcal{H}$, we are comparing against $\min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$.
- When $\mathcal{H}$ is large, $\min_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$ becomes lower.
- When $\mathcal{H}$ is the universe of all functions, we cannot learn.
- $\mathcal{H}$ needs to be about the right size.
- $\mathcal{H}$ can actually be a large, but the range of A needs to be about the right size.
- For example, we can only run a finite number of steps with stochastic gradient descent, so the range we can explore is limited by the algorithm.

Uniform convergence

A hypothesis class $\mathcal{H}$ has uniform convergence property if for any distribution $\mathcal{D}$, and any $\epsilon > 0$ and $0 \leq \delta \leq 1$, there exists $N > 0$ such that for every $h \in \mathcal{H}$,

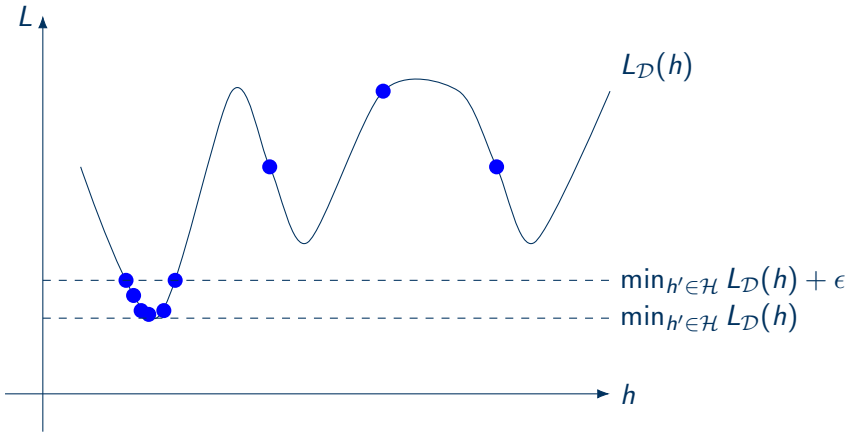
$$\mathbb{P}_{S \sim \mathcal{D}^n} \left[|L_S(h) - L_{\mathcal{D}}(h)| > \epsilon \right] < \delta \tag{2}$$

for all $n \geq N$.

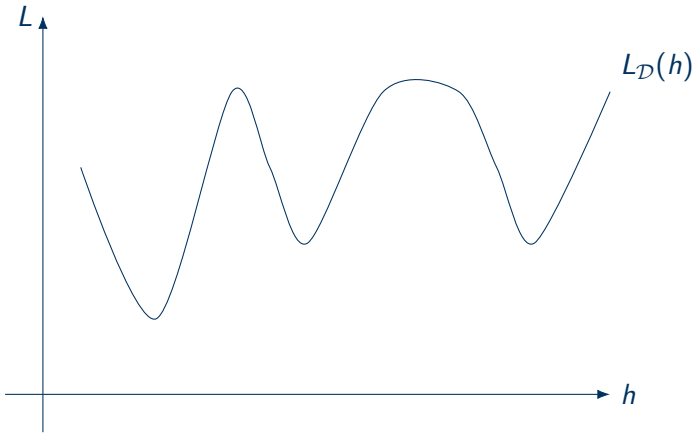
Uniform convergence

- Uniform convergence assures that the training error and generalization error are not far from each other.
- This has to happen for all $h \in \mathcal{H}$, the uniform part (and a strong requirement).

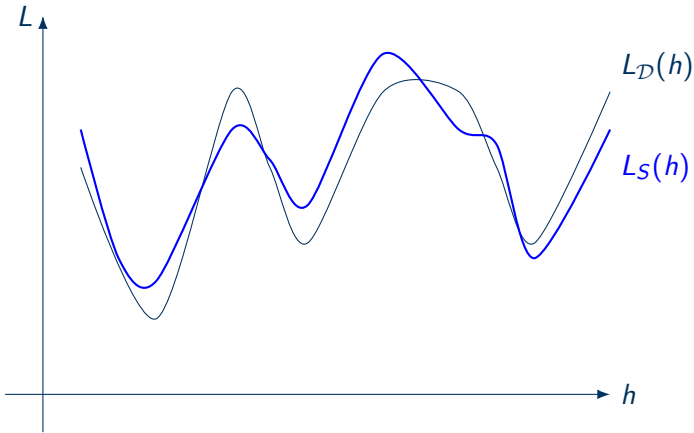
Comparing PAC learning and uniform convergence



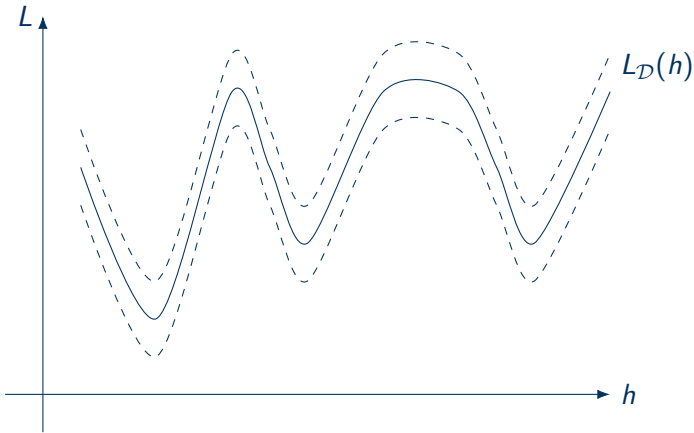
Comparing PAC learning and uniform convergence



Comparing PAC learning and uniform convergence



Comparing PAC learning and uniform convergence



Uniform convergence

- If we have uniform convergence,

$$L_{\mathcal{D}}(h_{\mathrm{ERM}}) \leq L_S(h_{\mathrm{ERM}}) + \epsilon \leq L_S(h) + \epsilon \leq L_{\mathcal{D}}(h) + \epsilon + \epsilon \tag{3}$$

  for any $h \in \mathcal{H}$.

- In particular,

$$L_{\mathcal{D}}(h_{\mathrm{ERM}}) \leq \min_{h' \in \mathcal{H}} L_{\mathcal{D}}(h') + 2\epsilon. \tag{4}$$

- If $\mathcal{H}$ has uniform convergence property, then $\mathcal{H}$ is PAC-learnable with ERM.

Fundamental theorem of statistical learning

Fundamental theorem of statistical learning

Vapnik–Chervonenkis dimension

- VC dimension is the largest number of points that $\mathcal{H}$ can shatter.
- Given n data points, there are 2^n ways of label them $\{+1, -1\}$.
- A set of n points is **shattered** by $\mathcal{H}$ if there is an arrangement of n points such that classifiers in $\mathcal{H}$ can produce all 2^n ways of labeling.

Shattering points in 2D

- We could shatter 3 points with a line in 2D.
- However, we cannot shatter 4 points with a line in 2D.
- The VC dimension of lines in 2D is 3.
- In general, linear classifiers with p parameters have VC dimension $p + 1$.
- We can again shatter 4 points with a 2-layer MLP in 2D.
- Neural networks have larger VC dimension than linear classifiers.
- The sine function has infinite VC dimension.

VC generalization bounds

- With probability $1 - \delta$, for all $h \in \mathcal{H}$

$$L_{\mathcal{D}}(h) \leq L_S(h) + 2\sqrt{\frac{8d \log(en/d) + 2\log(4/\delta)}{n}} \tag{5}$$

- d is called the VC dimension.
- For linear classifiers $\mathcal{H}_{\text{lin}} = \{x \mapsto w^\top x : w \in \mathbb{R}^p\}$, VC-dim$(\mathcal{H}_{\text{lin}}) = p + 1$.
- For multilayer perceptrons with p edges, VC-dim$(\mathcal{H}) = O(p \log p)$.
- These results are independent of learning algorithms.
- In particular, it is independent of how ERM is done.

Generalization bounds

- Many generalization bounds have the following form.
- With probability $1 - \delta$, for all $h \in \mathcal{H}$

$$L_{\mathcal{D}}(h) \leq L_S(h) + \sqrt{\frac{C(\mathcal{H})}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}. \tag{6}$$

- n is the number of samples.
- $C(\mathcal{H})$ is a capacity measure of $\mathcal{H}$.
- There is a family of uniform convergence results.

Sample complexity

- How many samples do we need to achieve a certain error?
- How large should n to get to ϵ?

$$\sqrt{\frac{C(\mathcal{H})}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}} \leq \epsilon \tag{7}$$

- In other words,

$$n = O\left(\frac{C(\mathcal{H}) + \log(1/\delta)}{\epsilon^2}\right) \tag{8}$$

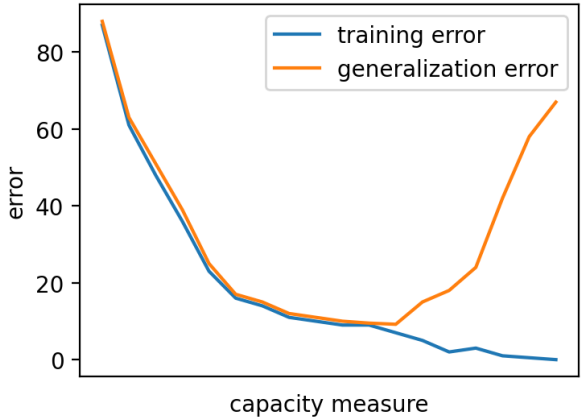
Interpreting generalization bounds

- VC generalization bounds

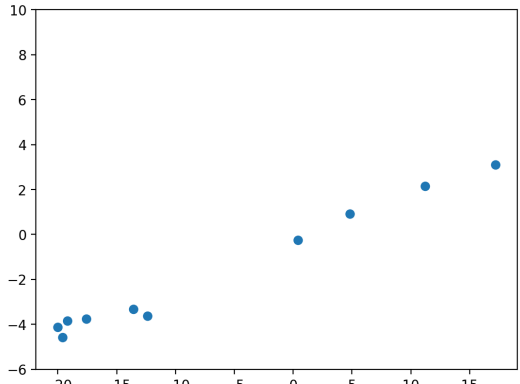
$$L_{\mathcal{D}}(h) \leq L_S(h) + 2\sqrt{\frac{8d\log(en/d) + 2\log(4/\delta)}{n}} \tag{9}$$

- When $\mathcal{H}$ is large, $\min_{h\in\mathcal{H}} L_S(h)$ can be low.
- When $\mathcal{H}$ is large, d becomes large.

Capacity-generalization tradeoff



Capacity-generalization tradeoff



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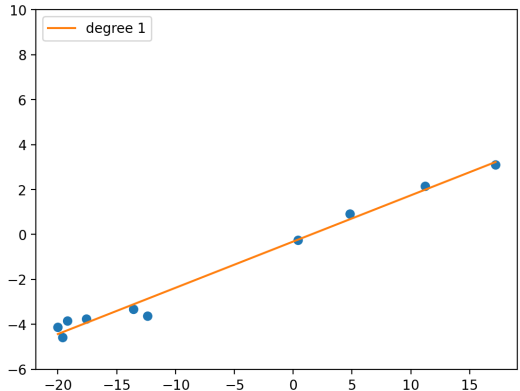

Capacity-generalization tradeoff