Recitation 7
Learning Theory and Generative Models

10-301/10-601: Introduction to Machine Learning

10/21/2021

1 Learning Theory

Some Important Definitions and Theorems

1. Basic notations:
   - **True function** (expert/oracle) $c^* : X \to Y$ (unknown)
   - **Hypothesis space** $\mathcal{H}$ and **hypothesis** $h \in \mathcal{H} : X \to Y$
   - Probability Distribution p^* (unknown)
   - Training Dataset $S = \{x^{(1)}, ...x^{(N)}\}$
2. **True Error (expected risk)**

$$R(h) = P_{x \sim p^*(x)}(c^*(x) \neq h(x))$$

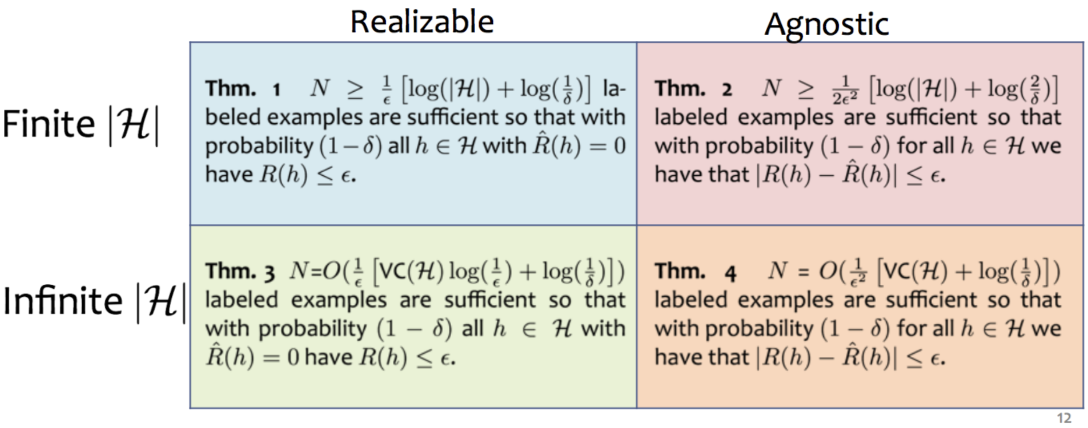
3. **Train Error (empirical risk)**

$$\begin{aligned}\hat{R}(h) &= P_{x \sim S}(c^*(x) \neq h(x)) \\ &= \frac{1}{N}\sum_{i=1}^{N} \mathbb{1}(c^*(x^{(i)}) \neq h(x^{(i)})) \\ &= \frac{1}{N}\sum_{i=1}^{N} \mathbb{1}(y^{(i)}) \neq h(x^{(i)}))\end{aligned}$$

4. **PAC criterion** is that we produce a high accuracy hypothesis with high probability. More formally,

$$P(\forall h \in \mathcal{H}, |R(h) - \hat{R}(h)| \leq \epsilon) \geq 1 - \delta$$

5. A hypothesis $h \in \mathcal{H}$ is **consistent** with training data S if $\hat{R}(h) = 0$ (zero training error/correctly classify)
6. **Sample Complexity** is the minimum number of training examples N such that PAC criterion is satisfied for a given ϵ (arbitrarily small error) and δ (with high probability)
7. Sample Complexity for 4 Cases: See Figure 1. Note that



	Realizable	Agnostic
Finite $\lvert\mathcal{H}\rvert$	**Thm. 1** $N \geq \frac{1}{\epsilon}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.	**Thm. 2** $N \geq \frac{1}{2\epsilon^2}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{2}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\lvert R(h) - \hat{R}(h)\rvert \leq \epsilon$.
Infinite $\lvert\mathcal{H}\rvert$	**Thm. 3** $N = O(\frac{1}{\epsilon}\left[\mathrm{VC}(\mathcal{H})\log(\frac{1}{\epsilon}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$.	**Thm. 4** $N = O(\frac{1}{\epsilon^2}\left[\mathrm{VC}(\mathcal{H}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\lvert R(h) - \hat{R}(h)\rvert \leq \epsilon$.

12

Figure 1

- **Realizable** means $c^* \in \mathcal{H}$
- **Agnostic** means c^* may or may not be in $\mathcal{H}$

8. **VC dimension** of a hypothesis space $\mathcal{H}$ is the maximum number of points such that there exists at least one arrangement of these points and a hypothesis $h \in \mathcal{H}$ that is consistent with any labelling of this arrangement of points.

9. If $\mathrm{VC}(\mathcal{H}) = n$, then for all placements of $n+1$ points, there exists no hypothesis $h \in \mathcal{H}$ that can shatter any of it.

Questions

1. For the following examples, write whether or not the data points can be shattered using a linear classifier

   - 2 points in 1D
   - 3 points in 1D
   - 3 points in 2D
   - 4 points in 2D

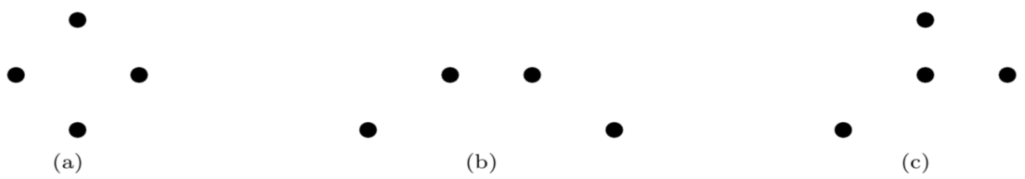
   How many points can a linear boundary (with bias) classify exactly for d-Dimensions?

   - Yes
   - No
   - Yes
   - No

   $$d + 1$$

2. Consider a semicircle classifier, where all points within the semicircle must equal 1 and all points outside must equal -1 (Rotated and scaled semi-circles are valid)

   (a) Which of the configurations of 4 points in figure 2 can a semicircle shatter?

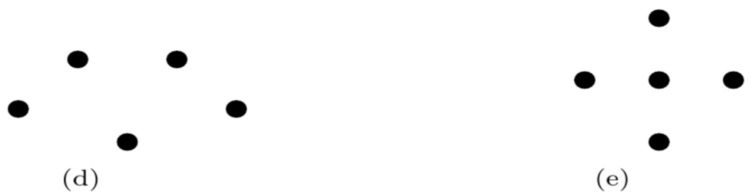


(a) (b) (c)

Figure 2

(a), (b), since the semi-circle can be scaled and rotated it can always perfectly classify the points. (c) is not perfectly classifiable in the case that all the exterior points are positive and the interior point is negative.

   (b) What about the configurations of 5 points in figure 3?



(d) (e)

Figure 3

None of the above. For (d), consider (from left to right) the labeling 1, 1 -1, -1, 1. For (e), same issue as (c).

3. Let $x_1, x_2, ..., x_n$ be n random variables that represent binary literals ($x \in \{0,1\}^n$). Let the hypothesis class H_d denote the class of depth $= d$ decision trees.

   Find the minimum number of examples required to learn $h \in H_3$ which guarantees at least 99% accuracy with at least 98% confidence.

   The number of depth d decision trees is actually quite tricky and is generally out of scope for this class.

   Let $|H_d|$ be the number of decision trees with depth d. We can see that $|H_0| = 2$, since for a depth 0 decision tree all we do is a majority vote classifier. We can then use a recursive definition for the number of trees at an arbitrary depth:

$$\begin{aligned}|H_d| &= (\text{\# choices of root attribute}) * (\text{\# possible left subtrees}) * (\text{\# possible right subtrees}) \\ &= n|H_{d-1}|^2\end{aligned}$$

It'll be easier to deal with this in log space, so let $L_d = \log_2 |H_d|$. $L_0 = 1$ trivially. For an arbitrary d:

$$\begin{aligned} L_d &= \log_2 n + 2L_{d-1} \\ &= \log_2 n + 2(\log_2 n + 2L_{d-2}) \\ &= \log_2 n + 2\log_2 n + 2^2\log_2 n + \cdots + 2^{d-1}(\log_2 n + 2L_0) \\ &= (2^d - 1)(1 + \log_2 n) + 1 \\ \implies |H_d| &= 2^{(2^d-1)(1+\log_2 n)+1} \end{aligned}$$

$|H_3| = 2^{8+7\log_2 n}, \epsilon = 0.01, \delta = 0.02$

$N(H_3, \epsilon, \delta) \geq \lceil \frac{1}{2\epsilon^2}[\ln(2^{8+7\log_2 n}) + \ln\frac{2}{\delta}]\rceil = \lceil \frac{1}{0.0002}\ln(25600n^7)\rceil$

Thus, in the case that $n = 10$, for instance, you would need: $\lceil \frac{1}{0.0002}\ln(25600(10)^7)\rceil = \lceil 131342.22 \rceil = 131343$ training examples.

2 MLE/MAP

As a reminder, in MLE, we have

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg\max_{\theta} p(\mathcal{D}|\theta) \\ &= \arg\min_{\theta} -\log\left(p(\mathcal{D}|\theta)\right)\end{aligned}$$

For MAP, we have

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg\max_{\theta} p(\theta|\mathcal{D}) \\ &= \arg\max_{\theta} \frac{p(\mathcal{D}|\theta)p(\theta)}{\text{Normalizing Constant}} \\ &= \arg\max_{\theta} p(\mathcal{D}|\theta)p(\theta) \\ &= \arg\min_{\theta} -\log\left(p(\mathcal{D}|\theta)p(\theta)\right)\end{aligned}$$

Imagine you are a data scientist working for an advertising company. The advertising company has recently run an ad and they want you to estimate it's performance. The ad was shown to N people. $Y^{(i)} = 1$ if person i clicked on the ad and 0 otherwise. Thus $\sum_i^N y^{(i)} = k$ people decided to click on the ad. Assume that the probability that the i-th person clicks on the ad is θ and the probability that the i-th person does not click on the ad is $1 - \theta$.

1. Note

$$p(\mathcal{D}|\theta) = p((Y^{(1)}, Y^{(2)}, ..., Y^{(k)}|\theta) = \theta^k(1-\theta)^{N-k}$$

Calculate $\hat{\theta}_{MLE}$.

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg\min_{\theta} -\log\left(p(\mathcal{D}|\theta)\right) \\ &= \arg\min_{\theta} -\log\left(\theta^k(1-\theta)^{N-k})\right) \\ &= \arg\min_{\theta} -k * \log(\theta) - (N-k)\log(1-\theta)\end{aligned}$$

Setting the derivative equal to zero yields

$$\begin{aligned}0 &= \frac{-k}{\theta} + \frac{(N-K)}{1-\theta} \\ \implies \theta_{MLE} &= \frac{k}{N}\end{aligned}$$

2. Suppose $N = 100$ and $k = 10$. Calculate $\hat{\theta}_{MLE}$.

$\hat{\theta}_{MLE} = \frac{k}{N} = 0.10$

3. Your coworker tells you that $\theta \sim \text{Beta}(\alpha, \beta)$. That is:

$$p(\theta) = \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{B(\alpha,\beta)}$$

Recall from lecture that $\hat{\theta}_{MAP}$ for a Bernoulli random variable with a Beta prior is given by:

$$\hat{\theta}_{MAP} = \frac{k+\alpha+1}{N+\alpha+\beta-2}$$

Suppose $N = 100$ and $k = 10$. Furthermore, you believe that in general people click on ads about 6 percent of the time, so you, somewhat naively, decide to set $\alpha = 6+1 = 7$, and $\beta = 100-6+1 = 95$. Calculate $\hat{\theta}_{MAP}$.

$\hat{\theta}_{MAP} = \frac{k+\alpha-1}{N+\alpha+\beta-2} = \frac{10+7-1}{100+102-2} = \frac{16}{200} = 0.08$

4. How do $\hat{\theta}_{MLE}$ and $\hat{\theta}_{MAP}$ differ? Argue which estimate you think is better.

Both estimates are reasonable given the available information. Note that $\hat{\theta}_{MAP}$ has lower variance than $\hat{\theta}_{MLE}$, but $\hat{\theta}_{MAP}$ is more biased. If you believe that this advertisement is similar to advertisements with a 6 percent click rate, then $\hat{\theta}_{MAP}$ may be a superior estimate, but if the circumstances under which the advertisement was shown were different from the usual, then $\hat{\theta}_{MLE}$ might be a better choice.

5. Suppose a rental car service operates in your city. Drivers can drop off and pick up cars anywhere inside the city limits. You can find and rent cars using an app. Suppose you wish to find the probability that you can find a rental car within a short distance of your home address at any time of day. Over three days you look at the app and find the following number of cars within a short distance of your home address:

$$x = [3, 4, 1].$$

Your coworker tells you that this comes from a Poisson distribution. That is:

$$p(x|\theta) = \frac{e^{-\theta}\theta^{x}}{x!}$$

Also, you are told that

$$\theta \sim \text{Gamma}(2, 2)$$

That is:

$$p(\theta) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}}\theta^{(\alpha-1)}e^{\frac{-\theta}{\beta}}, \quad \theta > 0$$

Calculate $\hat{\theta}_{MAP}$.

(Writeup from https://en.wikipedia.org/wiki/Conjugate_prior#Practical_example)

Note:

$$p(\mathcal{D}|\theta) = \frac{e^{-\theta}\theta^3}{3!}\frac{e^{-\theta}\theta^4}{4!}\frac{e^{-\theta}\theta^1}{1!}$$

$$\begin{aligned}
\hat{\theta}_{MAP} &= \arg\min_{\theta} -\log\left(p(\mathcal{D}|\theta)p(\theta)\right) \\
&= \arg\min_{\theta} -\log\left(\frac{e^{-\theta}\theta^3}{3!}\frac{e^{-\theta}\theta^4}{4!}\frac{e^{-\theta}\theta^1}{1!}\frac{1}{\Gamma(2)2^2}\theta^{(2-1)}e^{\frac{-\theta}{2}}\right) \\
&= \arg\min_{\theta} -\log e^{-3\theta}\theta^8\theta^{(2-1)}e^{\frac{-\theta}{2}} \\
&= \arg\min_{\theta} -\log e^{-3\theta-\frac{\theta}{\beta}}\theta^{8+\alpha-1} \\
&= \arg\min_{\theta} -((-3\theta - \frac{\theta}{2}) + (8+2-1)\log(\theta))
\end{aligned}$$

Setting the derivative equal to zero yields

$$\begin{aligned}
0 &= -3 - \frac{1}{2} + \frac{(7+2)}{\theta} \\
\implies \theta_{MAP} &= \frac{7+2}{3+\frac{1}{2}} = 2.57142857143
\end{aligned}$$

3 Convolutional Neural Network

3.1 Concepts

What are filters?

Filters (also called kernels) are feature extractors in the form of a small matrix used in convolutional neural layers. They usually have a width, height, depth, stride, padding, channels (output) associated with them.

What are convolutions?

We sweep the filter around the input tensor and take matrix dot products based on factors such as filter size, stride, padding. The matrix dot products form a new tensor, which is the output of a convolutional layer.

What are the shapes of the input and output tensors[1] of a CNN layer?

Two acceptable answers, with or without batches.

Input (no batches): (channels x height x width)

Output (no batches): (channels x height x width)

Input (with batches): (batch size x channels x height x width)

Output (with batches): (batch size x channels x height x width)

(Note that the channels, height, and width may change when going from input to output)

What are some benefits of CNNs over fully connected (also called dense) layers?

- Good for image-related machine learning (learns the kernels that do feature engineering)
- Pseudo translational invariance (local spatial coherence from convolutions and pooling)
- Parameter efficient

3.2 Parameters

Suppose that we want to classify images that belong to one of ten possible classes (i.e. `[cat, dog, bird, turtle, ..., horse]`). The images come in RGB format (one channel for each color), and are downsampled to dimension `128x128`.

Figure 4 illustrates one such image from the MS-COCO dataset[2].

[1] tensors are the generalization of matrices to multi-dimensions

[2] https://cocodataset.org/

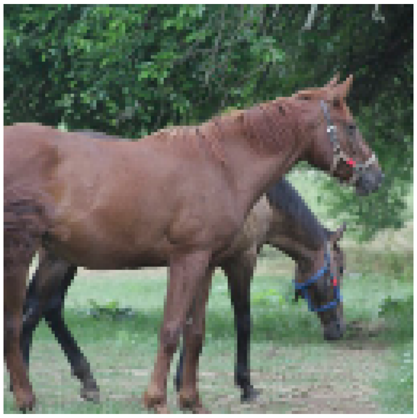


Figure 4: Image of a horse from the MS-COCO dataset, downsampled to 128x128

We construct a Convolutional Neural Network that has the following structure: the input is first max-pooled with a 2x2 filter with stride 2 and 3 output channels. The results are then sent to a convolutional layer that uses a 17x17 filter of stride 1 and 12 output channels. Those values are then passed through a max-pool with a 3x3 filter with stride 3 and also 12 output channels. The result is then flattened and passed through a fully connected layer (ReLU activation) with 128 hidden units followed by a fully connected layer (softmax activation) with 10 hidden units. We say that the final 10 hidden units thus represent the categorical probability for each of the ten classes. With enough labeled data, we can simply use some optimizer like SGD to train this model through backprogation.

Note: By default, please assume we have bias terms in all neural network layers unless explicitly stated otherwise.

1. **Draw a diagram that illustrates the channels and dimensions of the tensors before and after every neural net operation.**

   Step 1:

   ```
   [3@128x128](input) -> [3@?x?](maxpool) -> [12@?x?](conv)
   -> [12@?x?](maxpool) -> [?](flatten) -> [128](fc) -> [128](ReLU)
   -> [10](fc) -> [10](softmax)
   ```

   Step 2:

   ```
   [3@128x128](input) -> [3@64x64](maxpool) -> [12@48x48](conv)
   -> [12@16x16](maxpool) -> [3072](flatten) -> [128](fc) -> [128](ReLU)
   -> [10](fc) -> [10](softmax)
   ```

   Step 3:

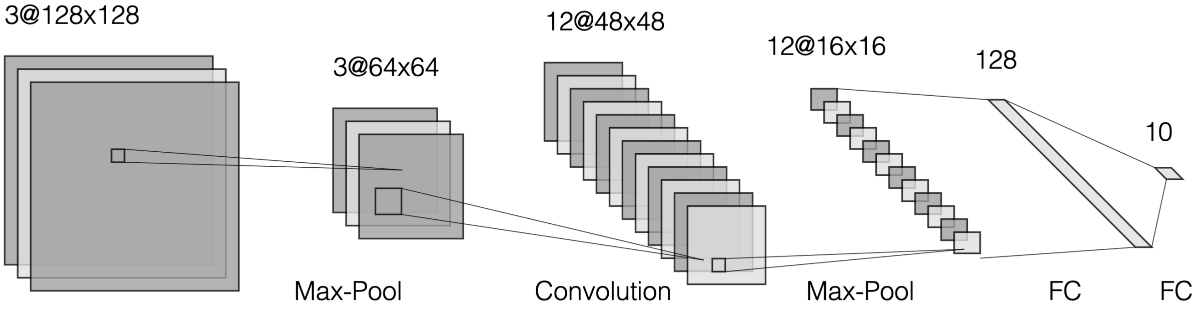


Figure 5: Full CNN structure, illustrated

2. **How many parameters are in this network for the convolutional components?**

$$\begin{aligned} N_{\text{conv}} &= (3 \times 12 \times 17 \times 17 + 12) \\ &= 10416 \end{aligned}$$

3. **How many parameters are in this network for the fully connected (also called dense) components?**

$$\begin{aligned} N_{\text{fc}} &= (3072 \times 128 + 128) + (128 * 10 + 10) \\ &= 393344 + 1290 \\ &= 394634 \end{aligned}$$

4. **From these parameter calculations, what can you say about convolutional layers and fully connected layers in terms of parameter efficiency[3]? Why do you think this is the case?**

$$\begin{aligned} N_{\text{total}} &= 10416 + 394634 \\ &= 405050 \end{aligned}$$

$$\begin{aligned} {}^{N_{\text{conv}}}/_{N_{\text{total}}} &= 2.57\% \\ {}^{N_{\text{fc}}}/_{N_{\text{total}}} &= 97.43\% \end{aligned}$$

Convolutional layers are much more parameter efficient, mainly because we are reusing the convolutional filter repeatedly for each convolutional layer (we only need to train one kernel per channel per layer). In comparison, the fully connected layer requires all nodes between two layers to be fully connected.

[3] the ratio between the number of parameters from some layer type and the total number of parameters.

3.3 Links

Visualization of convolutional filter sweep steps https://github.com/vdumoulin/conv_arithmetic

Visualization of convolutional filter smooth sweep with outputs https://www.youtube.com/watch?v=f0t-OCG79-U

Visualization of neural network layer outputs http://cs231n.stanford.edu/

The architecture used there is (conv→ relu → conv → relu → pool) x3 → fc → softmax