

# **Chapter 13**

## **Generalization performance of machine learning models**

4 This chapter gives a preview of generalization performance of deep networks.  
5 We will take a more abstract view of learning algorithms here and focus only on  
6 binary classification. We will first introduce a “learning model”, i.e., a formal  
7 description of what learning means. The topics we will discuss stem from the  
8 work of two people: **Leslie Valiant** who developed the most popular learning  
9 model called Probably Approximately Correct Learning (PAC-learning) and  
10 **Vladimir Vapnik** who is a Russian statistician who developed a theory (called  
11 the VC-theory) that provided a definitive answer on the class of hypotheses  
12 that were learnable under the PAC model.

### **13.1 The PAC-Learning model**

14 Our goal in machine learning is to use the training data in order to construct a  
15 model that generalizes well, i.e., has good performance outside of the training  
16 data. Formally, we search over a hypothesis space  $\mathcal{F}$ , e.g., a specific neural net  
17 architecture, using the available data to find a good hypothesis  $f \in \mathcal{F}$ . As we  
18 motivated in Chapter 2, without further assumptions, we cannot guarantee that  
19 this hypothesis works well on test data. We therefore assume two things in this  
20 chapter:

- 21 1. Nature provides independent and identically distributed samples  $x \in \mathcal{X}$   
22 from some (unknown to the learner) distribution  $P$ .
- 23 2. Nature labels these samples with  $c(x)$  which is again unknown to the  
24 learner.

25 Both training and test data are samples from Nature’s distribution  $P$ . We  
26 will also assume that even if the true labeler  $c(x)$  is unknown to us, we know  
27 that it belongs to a chosen hypothesis class  $c(x) \in \mathcal{C}$  and is deterministic, i.e.,  
28 Bayes error is zero. Changing this assumption does not change the crux of this  
29 theory.

30 Consider a learning algorithm, denoted by  $L$ . Given a dataset  $D = \{(x^i, c(x^i))\}_{i=1}^n$   
31 and a hypothesis class  $\mathcal{C}$ , the population risk (for classification) of the hypoth-

32   esis output by this learning algorithm is

$$R(h) = \mathbb{E}_{x \sim P} [\mathbf{1}_{\{f(x) \neq c(x)\}}]$$

33   Let us assume that the learning algorithm is deterministic for now, i.e., given  
 34   a training dataset  $D$  it returns a unique answer  $f$ . Let us assume that the  
 35   hypothesis class that the learner searches over, named  $\mathcal{F}$  is the same as the  
 36   hypothesis class  $\mathcal{C}$ . What do we want from this algorithm?

37   We expect that it works well for all hypotheses Nature could use to label  
 38   data  $c \in \mathcal{C}$  and all datasets  $D$  drawn from  $P$ . The PAC-Learning model  
 39   postulates the following desiderata upon the learning algorithm.

40   1. We are okay with an answer  $f$  with error

$$R(f) \in [0, 1/2)$$

41   because we only have access to finitely many training data. This is  
 42   the “approximate correct” part of the PAC-Learning. However the error  
 43   should decrease as  $n$  increases.

44   2. The dataset  $D$  is a random variable. This implies that the hypothesis  
 45   outputted by the learning algorithm  $f(D)$  is also a random variable. The  
 46   above statement therefore should hold with some large probability over  
 47   draws of the dataset  $D$ . In other words, there can be a small probability  
 48   that a non-representative dataset  $D$  is drawn and we do not expect  
 49   the learner to output a good hypothesis with  $R(f) < 1/2$ . However  
 50   the probability of such failure, let us call it  $\delta \in [0, 1/2)$ , should also  
 51   become smaller if more data is provided. This is the “probably” part of  
 52   PAC-Learning.

53   We now have a definition of what it means to be a good learning algorithm.

54   **Definition 13.1 (PAC-learnable hypothesis class).** A hypothesis class  $\mathcal{C}$  is  
 55   PAC-learnable if there exists an algorithm  $L$  such that for every  $c \in \mathcal{C}$ , for  
 56   every  $\epsilon, \delta \in [0, 1/2)$ , if  $L$  is given access to  $n(\epsilon, \delta)$  i.i.d. training data from  $P$   
 57   and their corresponding labels  $c$  then it outputs a hypothesis  $h_D \in \mathcal{C}$  such that

$$\mathbb{P}_D (R(f) < \epsilon) \geq 1 - \delta.$$

58   We want the learner to be statistically efficient, i.e., as our desiderata  $\epsilon, \delta$   
 59   get smaller, we should expect  $n(\epsilon, \delta)$  to not grow too quickly. For instance, we  
 60   would like  $n(\epsilon, \delta)$  to be a polynomial function of  $1/\epsilon$  and  $1/\delta$ . The minimum  
 61   number of samples  $n(\epsilon, \delta)$  required to learn a hypothesis class  $\mathcal{C}$  is called the  
 62   sample complexity of  $\mathcal{C}$ . One is also typically interested in the computational  
 63   complexity of finding  $f$ , e.g., to avoid a brute-force algorithm  $L$  that searches  
 64   over the entire hypothesis class  $\mathcal{F} = \mathcal{C}$ ; we will not worry about it here.

65   It is important to notice that PAC-learning assumes nothing about *how*  $L$  is  
 66   going to use the data, e.g., whether it runs SGD or what surrogate loss it uses,  
 67   or even whether it performs Empirical Risk Minimization. In this sense, the  
 68   above learning model is very abstract and we should expect only qualitative  
 69   answers from this theory.

70   **Example 13.2 (Learning Monotone Boolean Formulae).** Let  $x = [x_1, \dots, x_d]$   
 71   be the datum and  $c(x)$  be a conjunction, e.g.,

$$c(x) = x_1 \wedge x_3 \wedge x_4.$$

72 To take a few examples,  $c(10011) = 0$  and  $c(11110) = 1$ . Such formulae are  
 73 called monotone because no literals show up as negated in the formula.

74 We can have the hypothesis class  $\mathcal{F}$  to be the set of all possible conjunctions  
 75 of  $d$  variables  $x_1, \dots, x_d$ . Each literal  $x_i$  can be in the conjunction or not,  
 76 so the total number of hypotheses in  $\mathcal{F}$  is  $2^d$ .<sup>1</sup> Observe that since this is  
 77 exponential in  $d$ , an algorithm  $L$  that brute-force searches over  $\mathcal{F}$  will have a  
 78 large computational complexity. Also observe that since the true hypothesis  
 79  $c \in \mathcal{F}$ , there exists an answer  $f$  that the algorithm  $L$  can output that achieves  
 80 zero training error, i.e.,

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{\{f(x^i) \neq c(x^i)\}} = 0.$$

81 But for a fixed amount of data  $n$ , there is some probability that the minimizing  
 82 hypothesis  $f$  has zero training error but large population risk. As the number  
 83 of data  $n$  is large, we expect this event to be less and less probable.

84 Consider an algorithm  $L$  that does the following. It starts with the hypoth-  
 85 esis

$$f^0(x) = x_1 \wedge x_2 \wedge \dots \wedge x_d$$

86 with all literals and for every datum with a label 1, it deletes all literals  $x_i$  that  
 87 are not in this datum to update the hypothesis  $f$ ; this makes sense because if  
 88 the deleted literals were zero in some input,  $f$  and  $c$  would predict different  
 89 outputs. Remember that since  $c(x) \in \mathcal{F}$ , we cannot have a datum with input  
 90 1111...1 and output 0.

91 What kind of errors does this algorithm make? If some literal  $x_i$  was  
 92 deleted, it is because it had the value  $x_i = 0$  on a positively labeled sample.  
 93 So, it should be deleted, otherwise the hypothesis will output 0. So, we only  
 94 output a wrong hypothesis if more literals present than those in  $c(x)$ . So, the  
 95 output  $f(x)$  can only make an error on data labeled 1 by  $c(x)$ , never on the  
 96 ones labeled zero. Our algorithm therefore only has false negatives.

97 We now see why requesting more samples diminishes the probability of  
 98 this event happening. Let  $p_i = \mathbb{P}_{x \sim P} [c(x) = 1, x_i = 0]$ . Therefore

$$R(h) \leq \sum_{x_i \in f} p_i$$

99 If some  $p_i$  is small, then it does not contribute much to the error. If some  
 100  $p_i$  is large then we make sure to see enough samples so that we remove that  $x_i$   
 101 from  $f$ . After all, it only takes one appearance of this event to delete this  $x_i$ ,  
 102 and the event has probability  $p_i$  which is large. Rigorously, if all  $x_i$  in  $f$  have  
 103  $p_i < \epsilon/d$  then  $R(h) < \epsilon$ . On the other hand, if some  $x_i$  has  $p_i > \epsilon/d$  then the  
 104 probability of having this  $x_i$  in  $f$  is the probability that the event of  $p_i$  never  
 105 happens in the draw of  $n$  samples. But this new probability is smaller than  
 106  $1 - \epsilon/d$ . And the event will never happen in  $n$  i.i.d. draws with probability at  
 107 most  $(1 - \epsilon/d)^n \leq e^{-n\epsilon/d}$ . Using the union bound, since there are at most  
 108  $d$  literals in  $f$ , the probability that there is at least one such “bad event” is at  
 109 most  $de^{-n\epsilon/d}$ .

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<sup>1</sup>Actually the total number of conjunctions is  $2^d + 1$  because for the null-conjunction (without any literals) we can have the constant  $c(x) = 0$  or  $c(x) = 1$  for all  $x$ . We should therefore explicitly make sure  $c(111\dots11) = 0$  is not in the true labeling function. But we ignore this corner case, and silently assume that only the hypothesis  $c(x) = 1 \forall x$  is in our class  $\mathcal{C}$ .

110 If this bad event never happens the population risk is less than  $\epsilon$ . Of course,  
 111 such a bad event happening would be devastating. For some distributions it  
 112 could lead the error up to 1. However, in our PAC-learning setting we can  
 113 accept this as long as it happens rarely with probability at most  $\delta$ . Since

$$de^{-n\epsilon/d} < \delta \iff n \geq \frac{d}{\epsilon} \log \frac{d}{\delta}$$

114 we are guaranteed to meet the PAC criteria: of error less than  $\epsilon$  with probability  
 115 at least  $1 - \delta$ .

116 Note that both the sample complexity and computational complexity are  
 117 polynomial. We have thus shown that the class of Monotone Boolean Formulae  
 118 is  $(\epsilon, \delta)$ -PAC learnable.

## 119 13.2 Concentration of Measure

120 Two very important results from probability theory that we will use are the  
 121 Union Bound and the Chernoff Bound.

### 122 13.2.1 Union Bound (or Boole's Inequality)

123 For any countable set of events,  $\{A_1, \dots, A_n, \dots\}$ ,

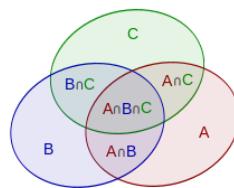
$$\mathbb{P}\left(\bigcup_i A_i\right) \leq \sum_i \mathbb{P}[A_i].$$

124 This is a rather loose, but useful, upper bound and is (mostly) embedded in  
 125 the assumptions of what we call a “probability measure” in probability theory  
 126 ( $\sigma$ -subadditivity). This essentially means that it can be used without any extra  
 127 assumptions in practice.

128 By the inclusion-exclusion principle for finite set of events  $\{A_1, \dots, A_n\}$ ,

$$\mathbb{P}\left(\bigcup_{i=1}^n A_i\right) = \sum_{i=1}^n \mathbb{P}(A_i) - \sum_{1 \leq i < j \leq n} \mathbb{P}(A_i, A_j) + \dots + (-1)^{n-1} \mathbb{P}(A_1, A_2, \dots, A_n)$$

129 We can get better approximations of the union, if we use the first  $k \leq n$  terms  
 130 above. If we stop at odd  $k$ , we get an upper bound. If we stop at even  $k$  we get  
 131 a lower bound. The error of the approximation is decreasing with  $k$ .



132

**▲** If we want a better approximation of the probability of the union of multiple events and we know more about the problem at hand we can use what are called Bonferroni inequalities.

**?** Where did we use the union bound in the proof for the PAC-learnability of the class of monotone Boolean functions?

### 133 13.2.2 Chernoff Bound

134 Let  $A_1, \dots, A_n$  be a sequence of i.i.d. random variables. We focus on the  
 135 case of Bernoulli random variables where  $\mathbb{P}(A_i = 1) = p$ . We would like

**?** Try to prove that  

$$\mathbb{P}\left(\bigcap_{i=1}^n A_i\right) \geq 1 - \sum_{i=1}^n \mathbb{P}(A_i^c)$$

136 to estimate  $p$  from samples. One way to do this is to compute the empirical  
 137 average

$$\hat{p} = \frac{1}{n} \sum_{i=1}^n A_i$$

138 and estimate how close it is to the true  $p$ . We know that as  $n \rightarrow \infty$

139 **Weak Law** For all  $\epsilon > 0$  we have

$$\mathbb{P}(|\hat{p} - p| > \epsilon) \rightarrow 0.$$

140 This is also known as convergence in probability.

141 **Strong Law** We have almost sure convergence, i.e.,

$$\mathbb{P}\left(\lim_{n \rightarrow \infty} \hat{p} = p\right) = 1.$$

142 **Central Limit Theorem** As  $n \rightarrow \infty$ , the quantity  $\sqrt{n}(\hat{p} - p)$  is distributed  
 143 as a Normal distribution with mean zero and variance  $p(1 - p)$ . Notice that  
 144 as opposed to the law of large numbers, the central limit theorem also gives  
 145 us a rate of convergence, i.e., how many samples  $n$  are necessary if want the  
 146 difference to be close to a Normal distribution. If we set  $\sigma^2 = p(1 - p)$  we  
 147 can rewrite the Central Limit Theorem as

$$\mathbb{P}(|\hat{p} - p| > \epsilon) \leq 2e^{-n\epsilon^2/(2\sigma^2)}.$$

148

149 **Chernoff Bound** Since  $\sigma^2 = p(1 - p) < 1/4$  we have from CLT that

$$\mathbb{P}\left(\left|\frac{1}{n} \sum_i A_i - p\right| > \epsilon\right) \leq 2e^{-2n\epsilon^2}.$$

150 An easy way to remember the Chernoff bound is that if we want the average  
 151 of  $n$  random variables to be  $\epsilon$ -close to their expected value with probability at  
 152 least  $1 - \delta$ , then we need

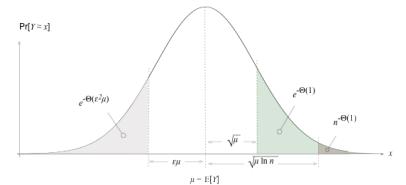
$$n = \Omega\left(\frac{1}{\epsilon^2} \log \frac{1}{\delta}\right)$$

153 samples.

154 Concentration of measure is an exciting area of probability theory and  
 155 similar results can be obtained for other distributions, other functions than averaging  
 156 of random variables  $A_1, \dots, A_n$  etc. Popular inequalities are Markov's  
 157 Inequality, Chebyshev's Inequality and Chernoff Bounds (and Hoeffding's  
 158 Inequality as an important special case). They are written in terms of increasing  
 159 tightness, but also of increasing assumptions of what we need to know  
 160 in order compute them. You can read a very good introduction to this topic  
 161 at <https://terrytao.wordpress.com/2010/01/03/254a-notes-1-concentration-of-measure/>.

163 In general, Markov's inequality only needs the expectation, Chebyshev's  
 164 Inequality needs the variance too, while Chernoff bounds usually need the

▲ This picture makes it easy to remember concentration inequalities for an  $n$ -dimensional Gaussian random variable  $Y$ .



❓ Do you see any patterns in the Chernoff bound with sample complexity in PAC-learning?

165 whole moment generating function. They are all applications of Markov's In-  
 166 equality on higher order statistics. The value of Chernoff bounds is increasingly  
 167 more important when we talk about distributions of few sufficient statistics,  
 168 like the Bernoulli distribution (or any exponential distribution).

### 169 13.3 Uniform convergence

170 We now lift the assumption that Nature's labeling function  $c \in \mathcal{C}$ . After all,  
 171 even if there exists such a true deterministic  $c$  we can never be sure that it is  
 172 inside  $\mathcal{F}$ , say the class of neural networks of a specific architecture that we are  
 173 using. This model is called the Agnostic PAC-Learning model.

174 We will stay within the confines of Empirical Risk Minimization  
 175 where we are provided with some samples where we output the hypothesis  
 176 with the smallest training error

$$\hat{R}(f) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{\{f(x^i) \neq y^i\}} \quad \text{minimizing this gives } f_{\text{ERM}} \in \mathcal{F}.$$

177 The population risk is

$$R(f) = \mathbb{E}_{(x,y) \sim P} [\mathbf{1}_{\{f_{\text{ERM}}(x) \neq y\}}] \quad \text{minimizing this gives } f^* \in \mathcal{F}.$$

178 Observe that  $f^*$  is *not* the Bayes optimal predictor that we saw in the bias-  
 179 variance tradeoff. This is because the former is restricted to the hypothesis  
 180 class  $\mathcal{F}$  while the latter has no such restriction to lie in  $\mathcal{F}$ , it is simply the  
 181 optimal hypothesis that minimizes the population risk.

Our goal while computing a *generalization bound* is to ask the following question: if we obtain an ERM hypothesis  $f_{\text{ERM}}$  with a good training error, then does this also mean that the population risk of the best hypothesis in the class  $f^*$  is small?

182 The above question is central, answering it in the affirmative ensures that  
 183 we are using a correct hypothesis class (say neural architecture) and that the  
 184 error on the training dataset is a good indicator of the performance on the  
 185 entire distribution. This involves the following two steps.

186 1. First, we need to make sure that the difference

$$|\hat{R}(f_{\text{ERM}}) - R(f_{\text{ERM}})| \rightarrow 0, \quad n \rightarrow \infty.$$

187 This is easy, it is akin to the concentration of measure we saw in the  
 188 previous section.

189 2. Second, we need to ensure that

$$\hat{R}(f_{\text{ERM}}) \approx R(f^*)$$

190 with high probability for every training dataset of  $n$  samples using which  
 191  $f_{\text{ERM}}$  is computed. If this is true, it tells us something about the ERM  
 192 procedure itself, i.e., it tells us whether minimizing the empirical risk

193      $\hat{R}(f)$  is a good thing if we want to build a classifier that works well on  
 194     the population.

195     This is difficult to do, after all  $f_{\text{ERM}}$  and  $f^*$  are totally different hypoth-  
 196     esis. Vapnik set up a powerful construction to do this. He showed that  
 197     a *sufficient* condition to achieve the above is that for all hypotheses in  
 198      $\mathcal{F}$ , the empirical risk and population risk are similar. This is known as  
 199     uniform convergence.

200     Let us now develop the two points above. Since data are drawn iid, we can  
 201     use the Chernoff bound to get that

$$\forall f \in \mathcal{F}, \mathbb{P} \left( |\hat{R}(f) - R(f)| > \epsilon \right) \leq 2e^{-2n\epsilon^2}.$$

202     If the hypothesis class is finite  $\mathcal{F}$ , we can use the union bound to show that for  
 203     any hypothesis, the training error and population risk are close.

$$\begin{aligned} & \mathbb{P} \left( \exists f \in \mathcal{F} : |\hat{R}(f) - R(f)| > \epsilon \right) \\ & \leq \sum_{f \in \mathcal{F}} \mathbb{P} \left( |\hat{R}(f) - R(f)| > \epsilon \right) \\ & \leq |\mathcal{F}| 2e^{-2n\epsilon^2}. \end{aligned}$$

204     If we want this above probability of a bad event to be less than  $\delta$  we  
 205     therefore need

$$n \geq \frac{1}{2\epsilon^2} \log \frac{2|\mathcal{F}|}{\delta} \quad (13.1)$$

206     training data. Notice how this bound changed from the Monotone Boolean  
 207     function example: we need  $\mathcal{O}(1/\epsilon)$  times more samples to get the uniform  
 208     convergence result.

209     Suppose we had a classifier  $f$  with 2% gap ( $\epsilon = 0.02$ ) between the training  
 210     error  $\hat{R}(f)$  and the validation error (which is a proxy for the population risk  
 211      $R(f)$ ), if we want to reduce this gap by half to 1% ( $\epsilon = 0.01$ ), we need 4 times  
 212     as many training data. We could also reduce this gap by fitting a classifier with  
 213     small  $|\mathcal{F}|$  but in this case, both the training and validation error will increase  
 214     even if their gap decreases.

215     Next, we need a relation between the population risk of  $f_{\text{ERM}}$  and the best  
 216     possible predictor  $f^* \mathcal{F}$  in our hypothesis class. Observe that

$$\begin{aligned} R(f_{\text{ERM}}) & \leq \hat{R}(f_{\text{ERM}}) + \epsilon && \text{(Chernoff bound on } f_{\text{ERM}}) \\ & \leq \hat{R}(f^*) + \epsilon && (f_{\text{ERM}} \text{ has the smallest training error}) \\ & \leq R(f^*) + 2\epsilon && \text{(Chernoff bound on } f^*). \end{aligned}$$

217     The two Chernoff bound inequalities hold with probability at least  $1 - \delta$  so  
 218     the final inequality

$$R(f_{\text{ERM}}) \leq R(f^*) + 2\epsilon$$

219     holds with probability at least  $1 - 2\delta$ . Substitute this in (13.1) to get

$$R(f_{\text{ERM}}) \leq R(f^*) + 2\sqrt{\frac{1}{2n} \log \frac{|\mathcal{F}|}{\delta}} \quad (13.2)$$

220     with probability  $1 - \delta$ . A result of this kind is called a Vapnik-Chervonenkis  
 221     (VC) bound or a PAC bound.

222 Let us consider our monotone Boolean formulae example again. Since  
 223  $|\mathcal{F}| = 2^d$ , if the input dimension is  $d = 1000$  and we set  $\delta = 10^{-3}$ , the VC-  
 224 bound predicts the following. In this case, we should imagine running ERM to  
 225 pick the best hypothesis  $f_{\text{ERM}}$ , not the elimination algorithm we discussed in  
 226 the section on monotone Boolean formulae.

- 227 1. With  $n = 1000$  data, we have  $R(f_{\text{ERM}}) \leq R(f^*) + 1.41$ . This is  
 228 vacuous/non-informative since the population risk is an expectation of  
 229 indicator variables and should therefore be less than 1.
- 230 2. With  $n = 10^5$ , we have  $R(f_{\text{ERM}}) \leq R(f^*) + 0.44$ . This is informative,  
 231 it means that the population risk of the classifier obtained by ERM is  
 232 within 44% of the population risk of the best classifier  $f^*$  in that class.  
 233 Of course it is only meaningful if  $f^*$  generalizes well, i.e., if  $R(f^*)$  is  
 234 small. This will happen if the hypothesis class  $\mathcal{F}$  is large enough.
- 235 3. With  $n = 10^6$ , we have  $R(f_{\text{ERM}}) \leq R(f^*) + 0.04$ .

### 236 13.4 Vapnik-Chernovenkis (VC) dimension

237 In the above section, the concept/hypothesis class was assumed to be finite  
 238  $|\mathcal{C}| < \infty$ . The union bound of course breaks if this is not the case. Notice that  
 239 once we pick a neural architecture (hypothesis class), the number of possible  
 240 models (hypotheses), each with different weight vectors, is infinite. Observe  
 241 that in the monotone Boolean formulae example, the algorithm  $L$  was using  
 242 the training data to eliminate hypothesis from  $\mathcal{C}$ , this is not going to work  
 243 if  $\mathcal{C}$  is not finite. It is therefore a natural question whether we can still learn a  
 244 hypothesis class with a finite number of training data.

245 Vladimir Vapnik and Alexey Chernovenkis (?) developed the so-called  
 246 VC-theory to answer the above question. Technically, VC-theory transcends  
 247 PAC-Learning but we will discuss only one aspect of it within the confinements  
 248 of the PAC framework. VC-theory assigns a “complexity” to each hypothesis  
 249  $f \in \mathcal{C}$ .

250 **Shattering a set of inputs** We say that the set of inputs  $D = \{x^1, \dots, x^n\}$   
 251 is *shattered* by the concept class  $\mathcal{C}$ , if we can achieve every possible labeling  
 252 out of the  $2^n$  labellings using some concept  $c \in \mathcal{C}$ . The size of the largest set  
 253  $D$  that can be shattered by  $\mathcal{C}$  is called the VC-dimension of the class  $\mathcal{C}$ . It is  
 254 a measure of the complexity/expressiveness of the class; it counts how many  
 255 different classifiers the class can express.

256 If we find a configuration of  $n$  inputs such that when we assign *any* labels  
 257 to these data, we can still find a hypothesis in  $\mathcal{C}$  that can realize this labeling,  
 258 then

$$\text{VC}(\mathcal{C}) \geq n.$$

259 On the other hand, if for every possible configuration of  $n + 1$  inputs, we can  
 260 always find a labeling such that no hypothesis in  $\mathcal{C}$  can realize this labeling,  
 261 then

$$n \leq \text{VC}(\mathcal{C}).$$

262 If we find some  $n$  for which both of the above statements are true, then

$$\text{VC}(\mathcal{C}) = n.$$

263 Some examples.

- 264 •  $d$ -dim Linear Threshold Functions: VC-dim =  $d + 1$ .

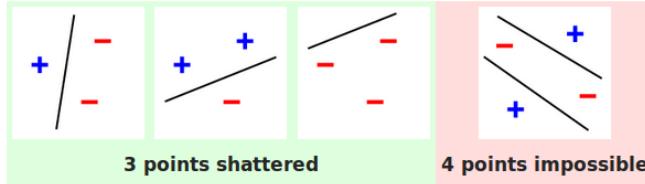


Figure 13.1:  $d=2$ : See that for the lower bound, we found some configuration of the 3 points, such that a linear threshold function always separates the points consistently with the labels; for any possible labeling. 3 such labellings are shown, convince yourselves that it can be done for all 8 cases. Observe that we cannot do the same for 4 points. In the figure above one such unrealizable configuration is given (With the “XOR” labeling). To prove the upper bound we need to talk about ANY configuration though. See that the only other case for 4 points, is that one point is inside the convex hull generated from the other 3. Find the labeling that cannot be obtained with linear classifiers in this case.

- 265 • 2 dimensional axis aligned rectangles: VC-dim = 4 (exercise)

- 266 • Monotone Boolean Formulae: VC-dim =  $n$  (exercise).

- 267 • If the hypothesis class is finite, then

$$\text{VC}(\mathcal{F}) \leq \log |\mathcal{F}|.$$

- 268 • If  $x \in \mathbb{R}$  and our concept class includes classifiers of the form

$$\text{sign}(\sin(wx))$$

269 where  $w$  is a learned parameter, then

$$\text{VC} = \infty.$$

- 270 • For a neural network with  $p$  weights and sign activation function

$$\text{VC} = \mathcal{O}(p \log p).$$

It is a deep result that if the VC-dimension of concept class is finite  $V = \text{VC}(\mathcal{F}) < \infty$ , then this class has the uniform convergence property (for any  $f \in \mathcal{F}$ , the empirical and population error are close). Therefore, we can learn this concept class agnostically (without worrying about whether Nature’s labeling function  $c$  is in our hypothesis class  $\mathcal{F}$  or not) in the PAC framework with

$$n = \Omega\left(\frac{V}{\epsilon^2} \log \frac{V}{\epsilon} + \frac{1}{\epsilon^2} \log \frac{1}{\delta}\right)$$

training data. If a hypothesis class has infinite VC-dimension, then it is not PAC-learnable and it also does not have the uniform convergence property.

271      The above result written in another form looks as follows. For a (finite or  
272 infinite) hypothesis class  $\mathcal{F}$  with finite VC-dimension  $V = \text{VC}(\mathcal{F})$

$$R(f_{\text{ERM}}) \leq R(f^*) + 2\sqrt{\frac{1}{n}(2V - \log \delta)} \quad (13.3)$$

273 with probability at least  $1 - \delta$ . This is an important expression to remember:  
274 the number of samples  $n$  required to learn a concept class scales linearly with  
275 the VC-dimension  $V$ . A more refined version of this bound looks like

$$R(f_{\text{ERM}}) \leq R(f^*) + 2\sqrt{\frac{1}{n}\left(V\left(\log\frac{2n}{V} + 1\right) + \log\frac{4}{\delta}\right)}. \quad (13.4)$$

276 **Bounds on the VC-dimension of deep neural networks** For general clas-  
277 sifiers, it is typically difficult to compute the VC dimension. One instead finds  
278 upper and lower bounds for the VC dimension to be used in inequalities of the  
279 form (13.4). Bounds on the VC-dimension of deep network architectures are  
280 available (?). With  $p$  weights and  $L$  layers, an essentially tight VC-dimension  
281 looks like

$$\Omega\left(p L \log \frac{p}{L}\right) = \text{VC}(\mathcal{F}) = \mathcal{O}(p L \log p)$$

282 for deep networks with ReLU nonlinearities.

283 This bound is not entirely useful in the VC-theory however. For instance,  
284 the ALL-CNN network you used in your homework with  $p \approx 10^6$  and  $L = 10$   
285 has  $\text{VC} \approx 10^8$ . If we use the coarse VC-bound in (13.3) with  $n = 50,000$   
286 samples, we have

$$R(f_{\text{ERM}}) \leq R(f^*) + 40$$

287 which is a vacuous generalization bound. However, remember that this is  
288 simply an *upper bound* on the generalization error of ERM. It is clear from  
289 empirical results in the literature (including your homework problems) that  
290 deep networks indeed generalize well to new data outside the training set and  
291 that means  $R(f_{\text{ERM}})$  is small.

292 The gap in applying VC-theory to deep networks therefore likely stems  
293 from the need for uniform convergence: we may not need that the empirical and  
294 population risk are close for *all* hypotheses in the class. If we only have uniform  
295 convergence within a small subset  $F \subset \mathcal{F}$  and if  $\text{VC}(F) \ll \text{VC}(\mathcal{F})$  and if the  
296 training algorithms like SGD always find ERM minimizers  $f_{\text{ERM}} \in F$ , then  
297 VC-theory/PAC-Learning do predict that deep networks will generalize well.  
298 Understanding this is the subject of a large body of ongoing research.