Learning Theory

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Contents

Unlike unsupervised learning, which comes in many different shapes and forms (anomaly detection, feature extraction, density estimation, dimensionality reduction, etc.), supervised learning comes in a much cleaner format. In supervised learning, we consider an input space $\mathcal{X}$ and an output space $\mathcal{Y}$. We assume that there exists some unknown measure $\mathbb{P}$ over $\mathcal{X} \times \mathcal{Y}$, making this some probability space. We then assume that some data $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}$ is generated sampled *independently and identically (iid)* from $\mathbb{P}$. Now this assumption is quite strong and is almost always not the case, as different data can be correlated, but we will relax this assumption later. Let's formally construct this from the bottom up.

1. We start off with a general probability space $(\Omega, \mathcal{F}, \mathbb{P})$. This is our model of the world and everything that we are interested in.
2. A measurable function $X : \Omega \to \mathcal{X}$ extracts a set of features, which we call the **covariates** and induces a probability measure on $\mathcal{X}$, say $\mathbb{P}_X$.
3. Another measurable function $Y : \Omega \to \mathcal{Y}$ extracts another set of features called the **labels** and induces another probability measure on $\mathcal{Y}$, the **label set**, say $\mathbb{P}_Y$.
4. At this point the function $X \times Y$ is all we are interested in, and we throw away Ω since we only care about the distribution over $\mathcal{X} \times \mathcal{Y}$.
5. We model the generation of data from Ω by sampling N samples from $\mathbb{P}_{X \times Y}$, which we assume to be iid (this assumption will be relaxed later). This gives us the **dataset**

$$\mathcal{D} = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^N$$

Now our goal is to construct a function $f : \mathcal{X} \to \mathcal{Y}$ that predicts Y from X, but we want to define some measure of how good our function is. We can use a loss function L to talk about this.

Definition 0.1 (Risk)

The **risk**, or **expected risk**, of function f is defined as

$$R(f) = \mathbb{E}_{X \times Y}[L(Y, f(X))] = \int_{\mathcal{X} \times \mathcal{Y}} L(y, f(x))\, d\mathbb{P}(x, y) \tag{1}$$

Clearly, we don't know what this risk is since we don't know the true measure $\mathbb{P}$, so we try to approximate it with the *empirical risk*.

Definition 0.2 (Empirical Risk)

The **empirical risk** of function f is defined as

$$\hat{R}_n(f) = \frac{1}{n} \sum_{i=1}^{n} L(y^{(i)}, f(x^{(i)})) \tag{2}$$

Now it would be great if minimizing the empirical risk—which is all we have—allows us to approximate the true risk with high probability. Note that there are two stages of estimates here.

1. First is that this is an *approximation*. We must justify whether the empirical risk is actually a good approximation of the true risk. There are many theorems—some simple and others convoluted—that provides results on this.
2. Second, this approximation occurs with *high probability*. This can be dealt with using concentration of measure.

This regime is known as *probably approximately correct (PAC) learning*, and with asymptotic analysis, we can prove this with some assumptions.

Definition 0.3 (Generalize)

A function f is said to **generalize** if

$$\lim_{n \to +\infty} \hat{R}_n(f) = R(f) \tag{3}$$

A final point is to consider how one even chooses the correct loss function L. This can be analyzed with *statistical decision theory*.

1 Function Spaces

Now that we've defined the risk and empirical risk, the true function that we want to find is the one that minimizes the empirical risk.

$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \hat{R}(f) \tag{4}$$

However, this depends on the function space $\mathcal{F}$ that we are minimizing over. If we chose f to be the space of all functions, then we just interpolate (fit perfectly over) the data[1], which is not good since we're **overfitting**. This is a problem especially in nonparametric supervised learning, and there are generally two ways to deal with this. The first is to use *localization*, which deals with local smoothing methods. The second is with **regularization**. The third is to restrict our class of functions to a smaller set. Perhaps we assume that nature is somewhat smooth and so naturally we want to work with smooth functions. There are two ways that we define smoothness, through Holder spaces that focus on local smoothness and Sobolev spaces that focus on global smoothness.

Definition 1.1 (L^p Space)

The $L^p(\mu)$ space is the normed vector space of all functions from $f : \mathcal{X} \to \mathbb{R}$ such that

$$||f||_p = \left(\int |f(x)|^p \, d\mu \right)^{1/p} < \infty \tag{5}$$

Theorem 1.1 (Countable Basis)

You can construct a countable orthonormal basis in $L^2(\mu)$ space.

There are a lot of well known orthonormal bases. For example, the Fourier basis, Legendre polynomials, Hermite polynomials, or wavelets. Therefore, every function can be expressed as a linear combination of this basis, and you can calculate coefficients by taking the inner product with the basis functions.

$$f(x) = \sum_{i=1}^{\infty} \alpha_i \phi_i(x) \text{ and } \alpha_i = \langle f, \phi_i \rangle \tag{6}$$

When working with function classes, we tend to divide them into two broad categories.

Definition 1.2 (Parametric Models)

A **parametric model** is a set of functions $\mathcal{M}_{\boldsymbol{\theta}}$ that can be parameterized by a finite-dimensional vector. The elements of this model are hypotheses functions $h_{\boldsymbol{\theta}}$, with the subscript used to emphasize that its parameters are $\boldsymbol{\theta}$. We have the flexibility to choose any form of h that we want, and that is ultimately a model assumption that we are making.

Example 1.1 (Examples of Parametric Models)

1. If we assume $h : \mathbb{R}^D \to \mathbb{R}$ to be linear, then h lives in the dual of $\mathbb{R}^D$, which we know to be D-dimensional.
2. If we assume h to be affine, then this just adds one more dimension.
3. If we assume $h : \mathbb{R} \to \mathbb{R}$ to be a kth degree polynomial, then g can be parameterized by a $k+1$ dimensional θ.

However, parametric models may be limited in the way that we are assuming some form about the data. For certain forms of data, where we may have domain knowledge, it is reasonable to use parametric models,

[1] unless there were two different values of Y for the same X

but there are cases when we will have absolutely no idea what the underlying distribution is. For example, think of classifying a $3 \times N \times N$ image as a cat or a dog. There is some underlying distribution in the space $[255]^{3N^2} \times \{\text{cat}, \text{dog}\}$, but we have absolutely no idea how to parameterize this. Should it be a linear model or something else? This is when nonparametric models come in. They are not restricted by the assumptions concerning the nature of the population from which the sample is drawn.

Definition 1.3 (Nonparametric Models)

Nonparametric models are ones that cannot be expressed in a finite set of parameters. They may be countably or uncountably infinite.

1.1 Holder Spaces

Holder spaces are used whenever we want to talk about local smoothness (and just as important, it is just a convenient assumption to be able to prove many things). For example, when we want to talk about local smoothing methods for regression and classification, talking about this smoothing is not quite possible if we don't have certain assumptions on the function. To make theory easier, we assume that the function has basic smoothness properties and this property is Holder smoothness. But note that these are ultimately assumptions.

Definition 1.4 (Holder Space)

For some $\beta \in \mathbb{N}$ and $L \in \mathbb{R}^+$, the $H(\beta, L)$ **Holder space** is the set of all functions $f : \mathcal{X} \subset \mathbb{R} \to \mathbb{R}$ such that

$$|f^{(\beta-1)}(y) - f^{(\beta-1)}(x)| \leq L||y - x|| \tag{7}$$

for all x, y. If we want $\mathcal{X}$ to be d-dimensional, then we want to bound the higher order total derivatives, and so $H(\beta, L)$ becomes all functions $f : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}$ such that

$$|D^{\mathbf{s}} f(x) - D^{\mathbf{s}} f(x)| \leq L\|y - x\|, \qquad D^{\mathbf{s}} = \frac{\partial^{|\mathbf{s}|}}{\partial x_1^{s_1} \dots \partial x_d^{s_d}} \tag{8}$$

for all $x, y \in \mathcal{X}$, and for all $\mathbf{s} = (s_1, \dots, s_d) \in \mathbb{N}^d$ with $|\mathbf{s}| \coloneqq \sum_{i=1}^d s_i = \beta - 1$.

The higher β is, the more smoothness we're demanding. If $\beta = 1$, then this reduces to the set of all Lipschitz functions. It is most common to assume that $\beta = 2$, which means that the derivative is Lipschitz. This is not rigorously true, but by dividing both sides by $||y - x||$ and taking the limit to 0, we can say that it implies that there exists some finite second derivative bounded by L.

1.2 Sobelov Spaces

In minimax estimation, suppose you wanted to get the minimax rate in L^2. Then you would be computing an integral that looks something like

$$\int (\hat{f} \cdot f)^2 \tag{9}$$

This is saying something about the integral of the whole function, so it's natural that people would use some notion of smoothness that involves the integral. This is what a Sobelov space is, and it is more of a global measure since we are integrating it across the whole space.

Definition 1.5 (Sobolev Space)

Given some compact set, say $[0, 1]$, the **Sobelov space** $W_{m,p}$ is the space of all functions

$$W_{m,p} \coloneqq \{f \in L^p([0, 1]) \mid D^m f \in L^p([0, 1])\} \tag{10}$$

So m tells us how many derivatives we want well behaved and p tells us under which norm are the derivatives well behaved. Almost always, we will assume $p = 2$. This is basically saying that of we take mth derivative, square it, and then integrate it, then it is finite. If the function was very wiggly, then say its third derivative might blow up when squared, and the integral would be infinite.

Note that this is slightly stronger than the usual definition of Sobolev spaces since we requiring the derivative rather than the weak derivative. There is also a related definition of a Sobelov ellipsoid that we'll be working with.

Definition 1.6 (Sobelov Ellipsoid)

Let $\theta = (\theta_1, \theta_2, \dots)$ be a sequence of real numbers. Then the set

$$\Theta_m = \left\{ \theta \mid \sum_{j=1}^{\infty} a_j^2 \theta_j^2 < C^2 \right\} \tag{11}$$

where $a_j^2 = (\pi \cdot j)^{2m}$. Note that since a_j is exploding, to stay finite the θ_j must be decaying.

This is useful because of the following theorem.

Theorem 1.2 (Conditions for Function being in Sobelov Space)

Given a function $f \in L^2(\mu)$ expanded in some orthonormal basis ϕ_j, then $f \in W_{m,2}$ if and only if the sequence of coefficients $(\alpha_j)_j$ is in the Sobelov ellipsoid.

Proof.

Therefore, checking whether a function is in the Sobelov space is equal to checking whether its coefficients in a basis die off fast enough to be in the Sobelov ellipsoid.

1.3 Reproducing Kernel Hilbert Spaces

Now let's talk about reproducing kernel Hilbert spaces (RKHS), and we provide some motivation. The problem with general Hilbert spaces is that they can contain a lot of unsmooth functions. Also, convergence in norm doesn't imply pointwise convergence. For example, take the function

$$f_n : \mathbb{R} \to \mathbb{R}, \qquad f_n(x) = \begin{cases} n & \text{if } 0 \leq x \leq \frac{1}{n} \\ 0 & \text{else} \end{cases} \tag{12}$$

This converges in norm but not pointwise, and the problem lies in the value at $f(0)$, which creates a "spiky" function. We might propose that a class of well-behaved functions shouldn't contain functions like this, and this is basically an RKHS. It gives you a nice class of functions that have good statistical properties but also are easy to compute with.

Definition 1.7 (Mercer Kernels)

A **Mercer kernel** is a function $K : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ that is

1. nonnegative,
2. symmetric, and
3. positive semidefinite in the sense that for any collection $x_1, \dots, x_n$ of arbitrary size n,

$$\sum_i \sum_j c_i c_j K(x_i, x_j) \geq 0 \tag{13}$$

for any choice of $c_1, \dots, c_n$. This is equivalent to saying that the matrix $\mathbb{K}$ formed by evaluating these kernels at the pairs of points is positive semi-definite.

Example 1.2 (Gaussian Kernel)

The Gaussian kernel is defined

$$K(x,y) = \exp\left(-\frac{||x-y||^2}{\sigma^2}\right) \tag{14}$$

This is indeed a kernel since it is obviously nonnegative and symmetric.

Now this kernel should tell us roughly how similar two points x and y are, and specifying which kernel to use is an art. For now, let's assume that a kernel is given, and using this kernel, we want to build a function space. For this, we need Mercer's theorem.

Theorem 1.3 (Mercer's Theorem)

If we have a Mercer kernel K that is continuous and bounded, i.e. $\sup_{x,y} K(x,y) < \infty$, then we can define a new linear operator T_K

$$T_K f(x) = \int K(x,y)f(y)\,dy = \iint K(x,y)f(x)f(y)\,dx\,dy \tag{15}$$

The theorem states that

1. there exists an orthonormal basis $\{\phi_i\}_{i=1}^{\infty}$ of continuous eigenfunctions of T_K
2. the corresponding set of eigenvalues $\{\lambda_i\}$ is nonnegative and the sum is bounded

$$\sum_i \lambda_i < \infty, \tag{16}$$

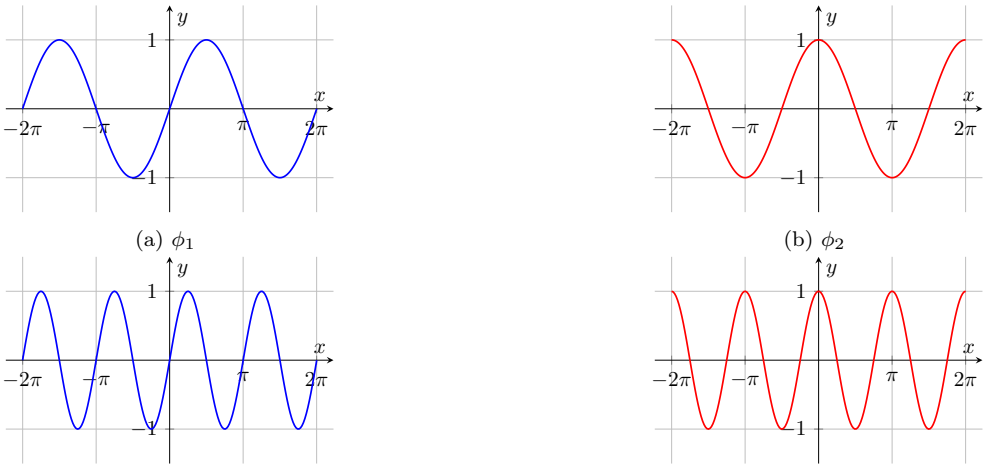
3. and we can write the kernel as a sum of the eigenfunctions where convergence is absolute and uniform.

$$K(x,y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x)\phi_i(y) \tag{17}$$

These ϕ_i's are the implicit high-dimensional features.

Proof.

What do these eigenfunctions ϕ_i look like? Well, they tend to look like functions that tend to get wigglier and wigglier as i increases, indicating that λ_i must decrease in such a way that it still keeps the function smooth.



(a) ϕ_1 (b) ϕ_2

(c) ϕ_3 (d) ϕ_4

Figure 1: The fourier basis as the eigenbases.

Now, we can fix the first term in the kernel and it will be function of the second term $K_x(\cdot) = K(x, \cdot)$. We do this for all $x \in \mathbb{R}$, which form the basis of our RKHS, and it consists of all functions that are finite linear combinations of these K_x's. This creates a vector space, and we can add a well-defined inner product. Finally, this inner product induces a norm which can be used to complete this inner product space into a Hilbert space.

Definition 1.8 (Reproducing Kernel Hilbert Space)

Given a kernel K, the **reproducing kernel Hilbert space (RKHS)** is defined as the completion of the vector space consisting of functions $f : \mathcal{X} \to \mathbb{R}$ of the form

$$f = \sum_{i=1}^{n} \alpha_i K_{x_i}(x) \tag{18}$$

for all number of combinations $n \in \mathbb{N}$,[a] for all choices of centers $x_1, \dots, x_n \in \mathcal{X}$, and for all coefficients $\alpha_1, \dots, \alpha_n \in \mathbb{R}$. The completion[b] is with respect to the inner product

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j K(x_i, x_j) \tag{19}$$

[a] Note it must be finite.
[b] The completion allows us to define for countable sums as well by taking limits.

Proof.

We know that a completion of a vector space is a vector space. So it remains to show that $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is a well-defined inner product. It follows from the positive semidefiniteness and symmetry of K that $\langle f, f \rangle \geq 0$ with $\langle f, f \rangle = 0 \iff f = 0$ and $\langle f, g \rangle = \langle g, f \rangle$. Bilinearity is also easy to prove.

It turns out that the norm of an RKHS tends to be a measure of the smoothness, which isn't obvious at first. Wigglier functions tend to have bigger norms.

Another nice property is that since K_x is itself in the RKHS, we can take the inner product of f and K_x, which just gives us back the evaluation of f at x.

Theorem 1.4 (Reproducing Property of RKHS)

An RKHS satisfies the **reproducing property**, which means that taking the inner product of a function f and a kernel K_x gives you the evaluation of f at x.

$$\langle f, K_x \rangle_{\mathcal{H}} = f(x) \tag{20}$$

and therefore it also means that $\langle K_x, K_x \rangle_{\mathcal{H}} = K(x, x)$. This also means that K_x is the evaluation functional in the dual space of $\mathcal{H}$ and this evaluation functional δ_x is continuous, which is not generally true in L^p spaces.

Proof.

We can evaluate from the inner product

$$f = \sum_i \alpha_i K_{x_i} \implies \langle f, K_x \rangle_K = \sum_i \alpha_i \langle K_{x_i}, K_x \rangle_K = \sum_i \alpha_i K(x_i, x) = f(x) \tag{21}$$

This reproducing property tends to be very useful, especially in the corollary below.

Corollary 1.1 (Convergence in RKHS)

Convergence in norm implies pointwise convergence in RKHS.

Proof.

Given that $f_n \to f$ in norm, we have that $||f_n - f|| \to 0$. Then for all points $x \in \mathcal{X}$, by Cauchy Schwartz we have

$$|f_n(x) - f(x)| = |\langle f_n - f, K_x \rangle_{\mathcal{H}}| \leq ||f_n - f|| \cdot ||K_x|| \to 0 \tag{22}$$

An alternative method is to take the evaluation functional $\delta_x f = f(x)$. Then, for a sequence $f_n \to f$ in norm

$$\delta_x f_n = \langle f_n, K_x \rangle \to \langle f, f_x \rangle = f(x) = \delta_x f \tag{23}$$

and so $f_n \to f$ implies $\delta_x f_x \to \delta_x f$.

Theorem 1.5 (Moore-Aronszajn)

Any positive definite function K is a reproducing kernel for some RKHS.

Proof.

We won't be too rigorous about this since this is not a functional analysis course. Assume that we have a positive definite kernel $K : X \times X \to \mathbb{R}$, where X is some measurable set, and we will show how to make a RKHS $\mathcal{H}_k$ such that K is the reproducing kernel on $\mathcal{H}$. It turns out that $\mathcal{H}_k$ is unique up to isomorphism. Since X exists, let us first define the set $S = \{k_x \mid x \in X\}$ such that $k_x(y) \coloneqq K(x, y)$. Now let us define the vector space V to be the span of S. Therefore, each element $v \in V$ can be written as

$$v = \sum_i \alpha_i k_{x_i}$$

Now we want to define an inner product on V. By expanding out the vectors w.r.t. the basis and the

properties of bilinearity, we have

$$\langle k_x, k_y \rangle_V = \left\langle \sum_i \alpha_i k_{x_i}, \sum_i \beta_i k_{y_i} \right\rangle = \sum_{i,j} \alpha_i \beta_j K(x_i, y_j)$$

At this point, V is not necessarily complete, but we can force it to be complete by taking the limits of all Cauchy sequences and adding them to V. In order to complete the construction, we need to ensure that K is continuous and doesn't diverge, i.e.

$$\iint K^2(x,y)\,dx\,dy < +\infty$$

which is a property known as finite trace.[a]

[a] Too much to write down here at this point, but for further information look at *thearticlehere*.

Now at first glance, this abstract construction makes it hard to determine what kind of functions there are in a RKHS generated by some kernel. Conversely, given some RKHS, it's not always easy to know which kernel it came from.

Example 1.3 (Fourier Basis)

Let us take the vector space of all real functions f for which its Fourier transform is supported on some finite interval $[-a, a]$. This is a RKHS with the kernel function

$$K(x,y) = \frac{\sin(a(y-x))}{a(y-x)} \tag{24}$$

with the inner product $\langle f, g \rangle = \int f(x)g(x)\,dx$.

Example 1.4 (Some Sobelov Spaces are RKHS)

Let us take the Sobelov space $W_{1,2}$ of all functions $f : [0,1] \to \mathbb{R}$ satisfying

$$\int (f'(x))^2\,dx < \infty \tag{25}$$

This is a RKHS with the kernel function

$$K(x,y) = \begin{cases} 1 + xy + \frac{xy^2}{2} - \frac{y^3}{6} & \text{if } 0 \le y \le x \le 1 \\ 1 + xy + \frac{x^2 y}{2} - \frac{x^3}{6} & \text{if } 0 \le x \le y \le 1 \end{cases} \tag{26}$$

The last two examples should show you that it's not easy to know what the elements of a RKHS look like for a given kernel. Let's try to build some intuition for this. A consequence of Mercer's theorem is that it gives us a conceptually easier way to think of functions f. We can either think of it in the finite kernel expansion—as defined in the RKHS—or as an infinite linear combination of its orthonormal eigenbasis.

$$f(x) = \sum_{i=1}^{n} \alpha_i K_{x_i}(x), \qquad f(x) = \sum_{j=1}^{\infty} \lambda_j \phi_j(x) \tag{27}$$

Conceptually, the basis expansion is nicer since it appeals to traditional linear algebra in that vectors are a linear combination of basis vectors. But when doing computation, the finite sum of the kernel expansion is nicer. In fact, when you talk about feature maps (e.g. in support vector machines), you're really just creating the map from $x \in \mathcal{X}$ into the infinite dimensional vector space

$$x \mapsto \Phi(x) = \left(\sqrt{\lambda_1}\phi_1(x), \sqrt{\lambda_2}\phi_2(x), \dots\right) \tag{28}$$

Therefore, you can either just work with x in the RKHS or work with the features Φ in a higher dimensional Euclidean space. The inner product between two functions is equal to the inner product between their feature maps.

$$\langle f, g \rangle = \sum_i \frac{\alpha_i \beta_i}{\lambda_i} \tag{29}$$

With this eigenbasis expansion, f, g must satisfy some smoothness constraints, and since the λ_i's are getting smaller, the α_i and β_i must die off quickly, making the sum finite. But we're never going to be actually computing this way since it's much easier to compute with the kernel expansion.

Theorem 1.6 (Representer Theorem)

Now later, when we get to kernel methods, we will see that the whole point of working in RKHS is that we know that the minimizer of the regularized loss has the form above by the representer theorem.

It turns out that even though we are working in an infinite-dimensional space, we only have to optimize over the observed data, and so this becomes an finite-dimensional optimization.

2 Concentration of Measure

Concentration of measure is a tool used to prove a lot of theorems in statistical machine learning. I have another series of notes on this, but we'll stick to the key points.

Theorem 2.1 (Hoeffding's Inequality)

Given $X_1, \dots, X_n$ are iid random variables with $a \leq X_i \leq b$, then for any $\epsilon > 0$,

$$\mathbb{P}\left(\left| \frac{1}{n} \sum_{i=1}^{n} X_i - \mathbb{E}[X] \right| \geq \epsilon \right) \leq 2 \exp\left(- \frac{2n\epsilon^2}{(b-a)^2} \right) \tag{30}$$

Proof.

Theorem 2.2 (Bernstein's Inequality)

Let $X_1, \dots, X_n$ be independent Rademacher random variables. Then for every $\epsilon > 0$,

$$\mathbb{P}\left(\left| \frac{1}{n} \sum_{i=1}^{n} X_i \right| > \varepsilon \right) \leq 2 \exp\left(- \frac{n\varepsilon^2}{2(1 + \frac{\varepsilon}{3})} \right) \tag{31}$$

Definition 2.1 (Subgaussian Random Variables)

A random variable X is **subgasussian** if

$$\mathbb{E}[e^{\lambda X}] \leq e^{\frac{\lambda^2 \sigma^2}{2}} \tag{32}$$

Gaussians and bounded random variables are subgaussian.

Lemma 2.1 (Bound on Subgaussian Random Variables)

Given a set of iid subgaussian random variables $X_1, \dots, X_n$

$$\mathbb{E}\big[\max_{1 \leq i \leq d} X_i \big] \leq \sigma \sqrt{2 \log d} \tag{33}$$

Use Hoeffding to show this.

$$\mathbb{P}(|\hat{R}(f) - R(f)| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \tag{34}$$

In 705 in CMU course.

3 Complexity

Therefore, if we apply it to some binary classifier $f : \mathcal{X} \to \{0, 1\}$, then we can say that the probability that the empirical risk deviates from the true risk is exponentially small.

$$\mathbb{P}(|\hat{R}(f) - R(f)| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \tag{35}$$

But when we do empirical risk minimization (ERM), we not given a classifier, but we must *choose* it. So given our space of classifiers f, we can plot the true risk and the noisy empirical risk. The equation above states that at any given point the probability of it deviating by more than ϵ is exponentially small. But we want something stronger: we want to bound the probability of the supremum of the difference over the whole class $\mathcal{F}$.

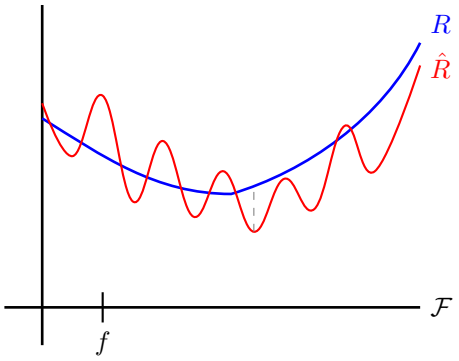


Figure 2: True risk of functions over $\mathcal{F}$ and its noisy empirical risk. We want to bound the maximum deviation of these two over the whole class.

By taking the supremum, this bound comes at a cost in the form of a coefficient term C.

$$\mathbb{P}\Big(\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \geq \epsilon\Big) \leq Ce^{-2n\epsilon^2} \tag{36}$$

This constant C—and the bound—will depend on how *complex* the function class $\mathcal{F}$ is, and to measure this complexity, we introduce some definitions.

3.1 Rademacher Complexity

Definition 3.1 (Rademacher Complexity)

Given **Rademacher random variables** $\sigma_1, \dots, \sigma_n$ with $\mathbb{P}(\sigma_i = 1) = \mathbb{P}(\sigma_i = -1) = \frac{1}{2}$, the **Rademacher complexity** of a function class $\mathcal{F}$ is defined

$$\text{Rad}_n(\mathcal{F}) = \mathbb{E}\left[\sup_{f \in \mathcal{F}} \left|\frac{1}{n}\sum_{i=1}^{n} \sigma_i f(Z_i)\right|\right] \tag{37}$$

where the expectation is across the random σ_i's and the Z_i's, which are independent.

To get some intuition of what this is, let's consider a function class of a single function f. Then, the sup disappears and the term inside the absolute value sign becomes a 0-mean random variable. Now if we have a very complex function class $\mathcal{F}$ with a lot of "wiggly" functions, then this value should be large. In this case, imagine a game where you pick generate some random variables σ_i and the Z_i. Then, I pick a function that maximizes this value. How can I do that? If I can find a function f that matches the sign of the σ_i's ($+1$ or -1) at each of the values of Z_i, then this would be maximized.

(a) One round of the game.

(b) Another round of the game.

Figure 3: Given the 5 random points Z_i chosen on the horizontal axis and their directions given by σ_i, we would like to find a function $f \in \mathcal{F}$ that interpolates the points.

Therefore, if I have a sufficiently complex class, then I can pick a function that tracks your σ_i's. Another way of looking at it is given noise variables σ and Z, we're looking at the correlation between σ and $f(Z)$. If we can maximize this correlation, then this is a complex class.

This is the most natural way of defining the complexity of the class, and in some cases it can be explicitly computed. However, in most cases it cannot be, but it can be bounded be something that is computable, like the VC dimension.

Lemma 3.1 (Bigger Class, Bigger Complexity)

If $\mathcal{F} \subset \mathcal{G}$, then $\text{Rad}_n(\mathcal{F}) \leq \text{Rad}_n(\mathcal{G})$.

Lemma 3.2 (Convex Hull)

If $\mathcal{F}$ is a convex set, then $\text{Rad}_n(\mathcal{F}) = \text{Rad}_n(\text{conv}(\mathcal{F}))$, where $\text{conv}(\mathcal{F})$ is the convex hull of $\mathcal{F}$.

This lemma is quite useful since if we have a certain finite set of functions, then their convex hull can encompass quite a bit, and we can also easily compute that convex hull's Rademacher complexity. Since the extremes haven't changed, the complexity doesn't change, and this might suggest that the Rademacher complexity is a good measure.

Lemma 3.3 (Change of Complexity with Lipschitz Functions)

Consider a L-Lipschitz function g with $g(0) = 0$ and consider the class $\mathcal{F}$, then we can bound the class of functions $g \circ \mathcal{F} = \{g \circ f \mid f \in \mathcal{F}\}$.

$$\text{Rad}_n(g \circ \mathcal{F}) \leq 2L\text{Rad}_n(\mathcal{F}) \tag{38}$$

This constant multiplicative bound is also useful.

3.2 Shattering Numbers and VC Dimension

Definition 3.2 (Projection of Function Class onto Points)

Given a binary function class $\mathcal{F}$ with functions $f : \mathcal{X} \to \{0, 1\}$, let us denote the projection of $\mathcal{F}$ onto a set of points $z_1, \dots, z_n \in \mathcal{X}$ to be

$$\mathcal{F}_z = \mathcal{F}_{z_1,\dots,z_n} = \{(f(z_1), \dots, f(z_n)) \mid f \in \mathcal{F}\} \subset \{0, 1\}^n \tag{39}$$

This projection determines the set of all possible binary labels that can be perfectly classified by some function f.

Definition 3.3 (Shattering Number)

The **shattering number** of $\mathcal{F}$ is defined

$$s_n(\mathcal{F}) = s(\mathcal{F}, n) = \sup_{z_1,\dots,z_n} |\mathcal{F}_{z_1,\dots,z_n}| \tag{40}$$

In other words, given the points z_j, how many different labels (out of the 2^n possible ones) can we put on the z_j so that there exists a function $f \in \mathcal{F}$ that can perfectly classify the z_j's?

The highest number that this can be is 2^n, since this is the number of possible binary vectors of length n.

Definition 3.4 (Shattering a Set)

Given a set of n points $z_1, \dots, z_n$, we say that the function class $\mathcal{F}$ **shatters** this set if $\mathcal{F}_{z_1,\dots,z_n} = |2^n|$. That is, for *every* one of the 2^n labels on these points, there exists a function in $\mathcal{F}$ that can perfectly classify them.

Therefore, if $\mathcal{F}$ shatters a set, the function class is in a sense too powerful to use on the dataset, since no matter what labels we put on the data, there exists a perfect function that interpolates it.

Example 3.1 (Binary Functions)

Consider the function class $\mathcal{F}$ of all binary functions of the form

$$f(x) = \begin{cases} 1 & \text{if } x > t \\ 0 & \text{if } x \leq t \end{cases} \tag{41}$$

Then, the projection of $\mathcal{F}$ onto some $n = 3$ points is the set

$$\{(0,0,0), (0,0,1), (0,1,1), (1,1,1)\} \tag{42}$$

and this is true no matter how I pick the z_1, z_2, z_3, and so the Shattering number is $s_3(\mathcal{F}) = 4$.

What is great about the shattering number is that it can be used to upper bound the Rademacher complexity. Often times, we do not know the Rademacher complexity but know the shattering number.

Theorem 3.1 (Bound of Rademacher Complexity with Shattering Number)

The Rademacher complexity of a binary function class $\mathcal{F}$ is bounded by

$$\text{Rad}_n(\mathcal{F}) \leq \sqrt{\frac{2 \log s_n(\mathcal{F})}{n}} \tag{43}$$

Proof.

Given the projection $\mathcal{F}_{z_1,\dots,z_n}$, we can use the law of iterated expectations on the Rademacher complexity.

$$\text{Rad}_n(\mathcal{F}) = \mathbb{E}\left[\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^n \sigma_i f(Z_i) \right| \right] \tag{44}$$

$$= \mathbb{E}_Z \left[\mathbb{E}_\sigma \left[\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^n \sigma_i f(Z_i) \right| \;\middle|\; Z_1, \dots Z_n \right] \right] \tag{45}$$

Note that in the inner expectation, since $f(Z_i)$ is now fixed, then are bounding a linear combination of a bunch of σ_i's, which are subgaussian. Using the bound above, we can reduce it to

$$\mathbb{E}_Z\left[\sqrt{\frac{2\log|F_{z_1,\dots,z_n}|}{n}}\right] \leq \sqrt{\frac{2\log s_n(\mathcal{F})}{n}} \leq \sqrt{\frac{2d\log n}{n}} \tag{46}$$

However, this is not the best possible bound, and in cases such as K means clustering in high dimensions, this bound can be tightened.

3.3 VC Dimension

We know that the shattering number is bounded above by 2^n. For $n = 1$, it is reasonable that it achieves this bound, but as n grows, the Shattering number may die off. The point at which it dies off is precisely the VC dimension.

Definition 3.5 (VC Dimension)

The **VC dimension** is the largest n number of points that can be shattered by the function class without misclassification [VC71].

$$n^{\text{VC}} := \sup_n\{s_n(\mathcal{F}) = 2^n\} \tag{47}$$

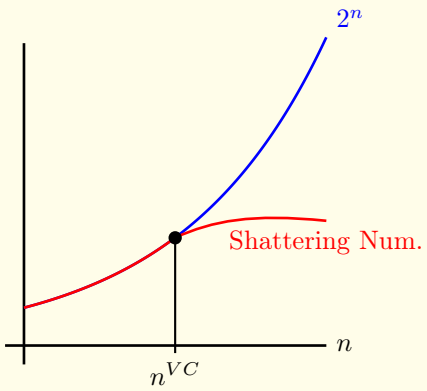


Figure 4: The Shattering number of $\mathcal{F}$ will grow exponentially until it reaches the VC dimension, at which point it will grow polynomially. The point at which it "dies off" is the VC dimension.

It turns out that there are very interesting properties about the VC dimension. One such fact is Sauer's lemma, which states that if the VC dimension is finite, then the rate of growth of the shattering number suddenly changes from exponential 2^n to polynomial n^{VC}, and this is what makes a lot of machine learning work.

Lemma 3.4 (Sauer–Shelah Lemma)

Now we move onto the big VC theorem which now bounds the supremum of the difference between the empirical risk and the true risk. To prove this, we need a few tricks, the first being the symmetrization trick using ghost samples.

Lemma 3.5 (Symmetrization Lemma)

Given a set of random variables $Z_1, \dots, Z_n$ and a function class $\mathcal{F}$, we can define ghost samples $Z_1', \dots, Z_n'$ that are iid copies of $Z_1, \dots, Z_n$. Then, we can bound the Rademacher complexity of the function class $\mathcal{F}$ by

$$\mathbb{P}\left(\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \geq \epsilon \right) \leq 2\mathbb{P}\left(\sup_{f \in \mathcal{F}} |\hat{R}(f) - \hat{R}'(f)| \geq \epsilon/2 \right) \tag{48}$$

where $\hat{R}, \hat{R}'$ is the empirical risk over the original and ghost samples, respectively.

Proof.

Assume that we have a function f that achieves this minimum. By the triangle inequality,

$$|\hat{R}(f) - R(f)| > t \text{ and } |\hat{R}'(f) - R(f)| < \frac{t}{2} \implies |\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2} \tag{49}$$

We write this again as an indicator function.

$$\mathbb{1}(|\hat{R}(f) - R(f)| > t, |\hat{R}'(f) - R(f)| < \frac{t}{2}) \implies \mathbb{1}(|\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2}) \tag{50}$$

and since the samples and the ghost samples are independent, we can take the probability over the ghost samples to get

$$\mathbb{1}(|\hat{R}(f) - R(f)| > t)\, \mathbb{P}_{Z'}(|\hat{R}'(f) - R(f)| < \frac{t}{2}) \implies \mathbb{P}_{Z'}(|\hat{R}(f) - \hat{R}'(f)| > \frac{t}{2}) \tag{51}$$

and the rest of the proof can be found online.

The reason we want this is that it removes the $R(f)$, which is some unknown true mean that can be hard to deal with since it takes infinite values. It's easier to work with two empirical risks than deal with the true risk.

Theorem 3.2 (VC Theorem)

Given a binary function class $\mathcal{F}$, we have

$$\mathbb{P}\left(\sup_{f \in \mathcal{F}} |\hat{R}(f) - R(f)| \geq \epsilon \right) \leq 2S(\mathcal{F}, n) e^{-n\epsilon^2/8} \approx n^d e^{-n\epsilon^2/8} \tag{52}$$

You can see that the exponential term is from Hoeffding but there is an extra cost of taking the supremum over the whole function class, which is the shattering number.

Proof.

Given $Z_1, \dots, Z_n \sim \mathbb{P}$, we take a new set of random variables $Z_1', \dots, Z_n'$ that are iid copies of $Z_1, \dots, Z_n$, called *ghost samples*.

Therefore, for some classes of sets with finite VC dimension, the shattering term will grow polynomially in n but the exponential term decays faster, which is what makes this work. That's why as n grows, we can get a good bound on the supremum of this difference.

Theorem 3.3 ()

With probability $\geq 1-\delta$, we have

$$\sup_{f\in\mathcal{F}} |\hat{R}(f) - R(f)| \leq 2\text{Rad}_n(\mathcal{F}) + \sqrt{\frac{\log(2/\delta)}{2n}} \tag{53}$$

4 Decision Theory

How can we choose our loss functions? There are two ways of doing this, either through model assumptions or with domain knowledge. When talking about model assumptions, we assume that the residual distribution is of certain form, and the maximum likelihood formulation leads to a certain loss function. For example, assuming that the residuals are normally distributed leads to the squared loss or Laplacian residuals leads to the absolute value loss. These are just modeling assumptions, and if there are no specific assumptions, we are lost. The other way is through domain expertise which allows us to construct our own loss functions. Fortunately, there is a deeper theory behind the choice of loss functions, known as decision theory, which allows us to define loss functions from the get go rather than assume distributions taking particular forms.[2]

Definition 4.1 (Misclassification Loss)

The **misclassification loss** is defined as

$$L(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ 1 & \text{if } y \neq \hat{y} \end{cases} \tag{54}$$

Example 4.1 (Misclassification Risk)

Substituting the misclassification loss function into the risk gives the **misclassification risk**.

$$R(f) = \mathbb{E}[\mathbb{1}_{\{Y \neq f(X)\}}] = \mathbb{P}(Y \neq f(X)) \tag{55}$$

and therefore our empirical risk is

$$\hat{R}(f) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{y^{(i)} \neq f(x^{(i)})\}} \tag{56}$$

which is just the number of misclassifications over the total number of samples.

However, depending on the context, the loss for misclassification one one label can be quite different from that of another label. Consider the medical example where you're trying to detect cancer. Falsely detecting a non-cancer patient as having cancer is not as bad as falsely detecting a cancer patient as not having cancer.

Definition 4.2 (Weighted Misclassification Loss)

The **loss matrix** K defines the loss that we incur when predicting the ith class on a sample with true label j.

$$L(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ K_{ij} & \text{if } y = i \neq j = \hat{y} \end{cases} \tag{57}$$

Definition 4.3 (Squared Loss)

The **squared loss** is defined as

$$L(y, \hat{y}) = (y - \hat{y})^2 \tag{58}$$

[2] Credits to Edric for telling me this.

Example 4.2 (Mean Squared Risk)

Substituting the squared loss function into the risk gives the **mean squared risk**.

$$R(f) = \mathbb{E}[(Y - f(X))^2] \tag{59}$$

and therefore our empirical risk is

$$\hat{R}(f) = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - f(x^{(i)})^2 \tag{60}$$

Definition 4.4 (Absolute Loss)

The **absolute loss** is defined as

$$L(y, \hat{y}) = |y - \hat{y}| \tag{61}$$

5 Minimax Theory

Bibliography

[VC71] V. N. Vapnik and A. Ya. Chervonenkis. On the uniform convergence of relative frequencies of events to their probabilities. *Theory of Probability & Its Applications*, 16(2):264–280, 1971.