Guarantees for Machine Learning FS 2023

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Contents

Disclaimer

This note is mainly based on Prof. Fanny Yang's slides and the textbook (High-Dimensional Statistics: A Non-Asymptotic Viewpoint by Martin J. Wainwright). This note is mainly adapted from Tao Sun's note in 2021.

1 Introduction (Lec. 1)

1.1 Stats. Perspective of Supervised ML

Suppose that we have training data (x_n, y_n), we select a $\hat{f}_n \in \mathcal{F}$ to fit this training data, which means that there's an algorithm $\mathcal{A} : (\mathcal{X} \times \mathcal{Y})^n \to \mathcal{F}$, which would result in predicted $\hat{y}$. An example (x_i, y_i) is randomly chosen (i.i.d.) by probability $\mathbb{P} \to (\mathcal{X}, \mathcal{Y}) \sim \mathbb{P}$.

We want to know if $\hat{f}_n$ is a good model estimator. We could use **pointwise** loss $l((\mathcal{X}, \mathcal{Y}), \hat{f}_n)$. Ex 1. $l((\mathcal{X}, \mathcal{Y}), \hat{f}_n) = (\hat{f}_n(\mathcal{X}) - \mathcal{Y})^2$ for regression.

1.2 The Well-specified Case

Given a collection of n samples $\{x_i, y_i\}_{i=1}^n$ sampled from a fixed distribution $\mathbb{P}$. Let f^* be the "true" estimator that minimizes some loss $\ell(x, y; f)$, i.e., $f^* := \arg\min_{f \in \mathcal{F}} \mathbb{E}_{x,y} \ell(x, y; f)$.

Def. 1 (Risk) The estimation of losses is called *risk*:

- Empirical risk:

$$R_n(f) := \frac{1}{n} \sum_{i=1}^{n} \ell((x_i, y_i); f)$$

- Population risk:

$$R(f) := \mathbb{E}_{x,y \sim \mathbb{P}} \ell(x, y; f)$$

Remark: Please note that the notation in our course is slightly different from the MW Chapter 4, where it uses a more burdensome notation as $R(f, f^*)$. Here, the f^* is omitted since it is fixed in a problem.

Def. 2 (Excess risk) Q: For classification, we dont know if $R(\hat{f}_n) = 20\%$ is bad or good. It depends on how hard task is. Therefore we should compare population risk with the best possible function if we knew the full distribution, i.e. evaluate the **excess risk**. The excess risk is defined as

$$\mathcal{E}_n(\hat{f}_n, f^*) := R(\hat{f}_n) - R(f^*) \leq \mathbf{UB}(n, \mathcal{F}, f^*).$$

Questions we'd like to answer: 1) Does **UB** $\to 0$ as $n \to \infty$ 2) If I collect twice as many training sample, how much does $\mathcal{E}_R(n)$ decrease. We here decompose the risk into several terms.

Thm. 1 (Risk decomposition) The excess risk $R(\hat{f}_n)) - R(f^*)$ can be decomposed into

$$= \underbrace{R(\hat{f}_n) - R_n(\hat{f}_n)}_{T_1} + \underbrace{R_n(\hat{f}_n) - R_n(f^*)}_{T_3} + \underbrace{R_n(f^*) - R(f^*)}_{T_2}$$

We observe that by optimality, the second term is smaller than zero. Then we just bound T_1 and T_2.

Remark: The following figure illustrate the risk decomposition. In the figure, the upper and lower layers represent the empirical risk and the population risk, respectively.

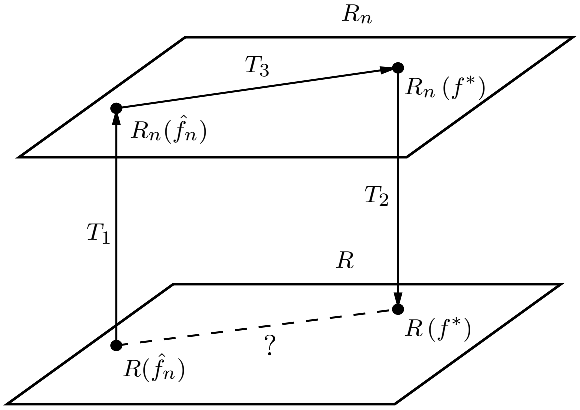


Figure: Risk decomposition (well-specified)

1.3 The Mis-specification Case

We call the problem mis-specification, when $f^* \notin \mathcal{F}$.

Thm. 2 (Bias-variance trade-off) The excess risk $R(\hat{f}) - R(f^*)$ can be decomposed into

$$R(\hat{f}_n) - R\left(f^\star\right) = \underbrace{R(\hat{f}_n) - R\left(f^{\star,\mathcal{F}}\right)}_{\text{"Variance"}} + \underbrace{R\left(f^{\star,\mathcal{F}}\right) - R\left(f^\star\right)}_{\text{"Bias" = "approx error"}}$$

where $f^{\star,\mathcal{F}} = \arg\min_{f \in \mathcal{F}} R(f)$.

Remark: The following figure provides some insights.

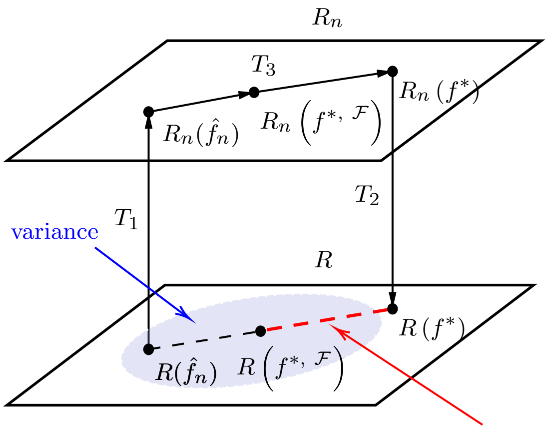


Figure: Bias and variance under mis-specification

2 Concentration bounds (Ch. 2)

2.1 Classical bounds

The most basic tail bound is Markov's inequality.

Thm. 3 (Markov's inequality) For a random non-negative variable X with finite mean,

$$P(X \geq t) \leq \frac{\mathbb{E}X}{t}, \qquad \forall t > 0.$$

Proof. Using the non-negativity of X and the definition of expectation,

$$\mathbb{E}X = \int_0^\infty xf(x)\ \mathrm{d}x = \int_0^t xf(x)\ \mathrm{d}x + \int_t^\infty xf(x)\ \mathrm{d}x$$
$$\geq \int_t^\infty xf(x)\ \mathrm{d}x \geq t\int_a^\infty f(x)\ \mathrm{d}x = tP(X \geq t).$$

□

Thm. 4 (Chebyshev's inequality) For a random variable X with finite k-th order center momentum,

$$P(|X-\mu| \geq t) = P(|X-\mu|^k \geq t^k)$$
$$\leq \frac{\mathbb{E}|X-\mu|^k}{t^k}, \qquad \forall t > 0.$$

Proof. Replacing X with $|X-\mu|^k$ in Markov's inequality. □

Method. 1 (Chernoff bound) Apply Markov's inequality to random variable $Y = e^{\lambda(X-\mu)}$ $(0 \leq \lambda \leq b)$, we get

$$P(X-\mu \geq t) = P(e^{\lambda(X-\mu)} \geq e^{\lambda t}) \leq \frac{\mathbb{E}e^{\lambda(X-\mu)}}{e^{\lambda t}}.$$

Then, optimizing λ to get a tighter bound,

$$\log P(X-\mu \geq t) \leq \inf_\lambda \left(\log \mathbb{E}e^{\lambda(X-\mu)} - \lambda t\right).$$

Chernoff bound will be used in achieving tail bounds of the sub-Gaussian and sub-exponential distribution.

2.2 Sub-Gaussian and Hoeffding bounds

Def. 3 (Sub-Gaussian) A random variable X with mean $\mathbb{E}(X) = \mu$ is sub-Gaussian with parameter if one of following holds:

- MGF condition:

$$\mathbb{E}e^{\lambda(X-\mu)} \leq e^{\frac{\lambda^2\sigma^2}{2}}, \quad \forall \lambda \in \mathbb{R}.$$

- Tail bound condition ($Z \sim \mathcal{N}(0,\sigma^2)$):

$$P(|X-\mu| \geq t) \leq cP(|Z-\mu| \geq t), \quad \exists c > 0, \forall t \geq 0.$$

For simplicity, we denote the sub-Gaussian random variable X with mean μ and parameter σ^2 as $X \sim SG(\mu, \sigma^2)$.

Prop. 1 (Sub-Gaussian tail bound) For $X \sim SG(\mu, \sigma^2)$,

$$P(X-\mu \geq t) \leq e^{-\frac{t^2}{2\sigma^2}}, \quad \forall t \in \mathbb{R}.$$

Proof. Applying Chernoff bound on $e^{\lambda(X-\mu)}$, we have

$$\log P(X-\mu \geq t) \leq \inf_{\lambda>0}\left(\log \mathbb{E}e^{\lambda(X-\mu)} - \lambda t\right)$$
$$\leq \inf_{\lambda>0}\left(\frac{\sigma^2\lambda^2}{2} - \lambda t\right) = -\frac{t^2}{2\sigma^2}.$$

Taking exponential on both sides gives the desired form. □
Example:

1. Gaussians $\mathcal{N}(\mu,\sigma^2)$ are σ-sub-Gaussian 2. Bounded variables are also sub-Gaussian.

Prop. 2 (Hoeffding inequality bound) For $X \sim SG(\mu, \sigma^2)$,

$$\mathbb{P}(\frac{1}{n}\sum_{i=1}^n X_i - \mu \geq t) \leq e^{-n\frac{t^2}{2\sigma^2}}, \quad \forall t \in \mathbb{R}.$$

Proof.

$$\mathbb{E}e^{\lambda\frac{1}{n}(\sum_{i=1}^n X_i - \mu)} = \prod_{i=1}^n \mathbb{E}e^{\frac{\lambda}{n}(X_i - \mathbb{E}(X))}$$

.
We have

$$\mathbb{E}e^{\lambda(X-\mu)} \leq e^{\frac{\lambda^2\sigma^2}{2}}, \quad \forall \lambda \in \mathbb{R}.$$
$$\prod_{i=1}^n \mathbb{E}e^{\frac{\lambda}{n}(X_i-\mathbb{E}(X))} \leq \prod_{i=1}^n e^{\frac{\lambda^2\sigma^2}{2n^2}} = e^{\frac{\lambda^2\sigma^2}{2n}}$$

. Therefore it serves $SG(\mu, \frac{\sigma}{\sqrt{n}})$. Then we substitute into sub-Gaussian tail bound and we have:

$$\mathbb{P}(\frac{1}{n}\sum_{i=1}^n X_i - \mu \geq t) \leq e^{-\frac{t^2}{2(\frac{\sigma}{\sqrt{n}})^2}} = e^{-n\frac{t^2}{2\sigma^2}}$$

□

Prop. 3 (Sum of sub-Gaussian RVs) For $X_1 \sim SG(\mu_1, \sigma_1^2)$, $X_2 \sim SG(\mu_2, \sigma_2^2)$,

$$X_1 + X_2 \sim SG(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2).$$

Prop. 4 (Sub-Gaussian for bounded RV) For a RV $X \in [a,b]$ almost surely, X is a sub-Gaussian with parameter at most $\sigma = \frac{b-a}{2}$.

Proof. Define function $\phi(\lambda) = \log \mathbb{E}e^{\lambda x}$. It is easy to show that $\phi(0) = 0$ and $\phi'(0) = \mathbb{E}X := \mu$. The second derivative is

$$\phi''(\lambda) = \mathbb{E}_\lambda[X^2] - \mathbb{E}_\lambda[X]^2, \quad \text{where } \mathbb{E}_\lambda[X] = \frac{\mathbb{E}f(X)e^{\lambda X}}{\mathbb{E}e^{\lambda X}}$$

Taking a Taylor expansion of $\phi(\lambda)$ at $\lambda = 0$,

$$\phi(\lambda) = \phi(0) + \lambda\phi'(0) + \frac{\lambda^2}{2}\phi''(\epsilon)$$
$$\leq \lambda\mu + \frac{\lambda^2}{2} - \frac{(b-a)^2}{4}.$$

□

Thm. 5 (Hoeffding bound) For n independent sub-Gaussian random variables $X_i \in SG(\mu_i, \sigma_i^2), i = [n]$,

$$P\left(\sum_{i=1}^n (X_i - \mu_i) \geq t\right) \leq e^{-\frac{t^2}{2\sum_{i=1}^n \sigma_i^2}}$$

Proof. Using the sub-Gaussian tail bound (Prop. 1) and the property of sum of Sub-Gaussian RVs (Prop. 3). □

Thm. 6 (Sub-Gaussian maxima) For a sequence of sub-Gaussian RVs $\{X_i\}_{i=1}^n$, $X_i \sim SG(0,\sigma^2)$, the following bounds hold,

$$\mathbb{E}\max_{i=1,\dots,n} X_i \le \sqrt{2\sigma^2\log n}$$
$$\mathbb{E}\max_{i=1,\dots,n} |X|_i \le \sqrt{2\sigma^2\log 2n}$$

Remark: This bound is frequently used in deriving other bounds.

Proof. Let $f(x)=e^{\lambda x}$ $(\lambda>0)$, we have

$$\begin{aligned} e^{\lambda\mathbb{E}[\max_i X_i]} &\le \mathbb{E}\left[e^{\lambda\max_i X_i}\right] && (f(x) \text{ is convex})\\ &= \mathbb{E}\left[\max_i e^{\lambda X_i}\right] && (f(x) \text{ is mono-increasing})\\ &\le \sum_{i=1}^n \mathbb{E}\left[e^{\lambda X_i}\right] \le ne^{\sigma^2\lambda^2/2} \end{aligned}$$

Therefore,

$$\mathbb{E}[\max_i X_i] \le \frac{\log n}{\lambda} + \frac{\lambda\sigma^2}{2}, \quad \forall\lambda>0.$$

Using Chernoff bound, we get

$$\mathbb{E}[\max_i X_i] \le \inf_{\lambda>0}\frac{\log n}{\lambda} + \frac{\lambda\sigma^2}{2} = \sqrt{2\sigma^2\log n},$$

The second inequality can be proved by using the fact that

$$\max_i |X_i| = \max\{X_1,\cdots,X_n,(-X_1).\cdots,(-X_n)\}.$$

□

2.3 Sub-exponential and Bernstein bounds

Def. 4 (Sub-exponential) A random variable X with mean μ is sub-exponential with parameter (v,α) if one of following holds:

- MGF condition:

$$\mathbb{E}e^{\lambda(X-\mu)} \le e^{\frac{\lambda^2v^2}{2}}, \quad \forall|\lambda|<\frac{1}{\alpha}.$$

- Tail bound condition:

$$P(|X-\mu|\ge t) \le c_1e^{-c_2t}, \quad \exists c_1,c_2>0, \forall t\ge 0.$$

Thm. 7 (Bernstein-type bound) For any random variable satisfying the Bernstein condition $\left|\mathbb{E}\left[(X-\mu)^k\right]\right| \le \frac{1}{2}k!\sigma^2b^{k-2}$, we have,

$$P(|X-\mu|\ge t) \le 2e^{-\frac{t^2}{2(\sigma^2+bt)}}$$

Remark: For bounded RV, this bound is more tighter compared with Hoeffding bound for sub-Gaussian with σ when $\sigma << b$.

Proof. Using Taylor expansion of the the MGF of sub-exponential RV, we have

$$\begin{aligned} \mathbb{E}\left[e^{\lambda(X-\mu)}\right] &\le 1+\frac{\lambda^2\sigma^2}{2}+\sum_{k=3}^\infty \lambda^k\frac{\mathbb{E}\left[(X-\mu)^k\right]}{k!}\\ &\le 1+\frac{\lambda^2\sigma^2}{2}+\frac{\lambda^2\sigma^2}{2}\sum_{k=3}^\infty(|\lambda|b)^{k-2}\\ &\le 1+\frac{\lambda^2\sigma^2/2}{1-b|\lambda|} \le e^{\frac{\lambda^2\sigma^2/2}{1-b|\lambda|}} \end{aligned}$$

Then, based on Chernoff bound, we get

$$\begin{aligned} \log P(X-\mu\ge t) &\le \inf_\lambda\left(\log\mathbb{E}e^{\lambda(X-\mu)}-\lambda t\right)\\ &\le \inf_\lambda\left(\frac{\lambda^2\sigma^2/2}{1-b|\lambda|}-\lambda t\right) = -\frac{t^2}{2(\sigma^2+bt)}. \end{aligned}$$

This gives the one-side bound. The two-side version can be obtained with additional factor of 2. □

2.4 Martingale-based Methods

Def. 5 (Martingale) A sequence of RVs $Y_1,Y_2,\cdots$ is said to be a martingale with respect to another sequence of RVs $X_1,X_2,\dots$ if for all n,

$$\mathbb{E}|Y_n|<\infty \quad \text{and} \quad \mathbb{E}[Y_{n+1}\mid X_1,\dots,X_n]=Y_n.$$

Def. 6 (Doob martingale difference) For a function $g_n:\mathcal{X}\to\mathbb{R}$ on independent RV $X_i\in\mathcal{X}$ and the σ-field $F_i=\sigma(X_1,\cdots,X_i)$, the Doob martingale difference $\{(D_i,F_i)\}_{i=1}^n$ is defined as

$$D_i := S_i - S_{i-1}, \quad \text{where } S_i := \mathbb{E}[g_n(X)\mid X_1,\cdots,X_i]$$

Here, we often define $S_0=\mathbb{E}[g_n(X)]$, so that we have the *telescoping decomposing*

$$S_n - S_0 = \sum_{i=1}^n D_i.$$

Thm. 8 (Azuma-Hoeffding) For a martingale difference sequence $\{(D_i,F_i)\}_{i=1}^n$, $D_i\mid F_{i-1}\in[a_i,b_i]$ almost surely for $i=[n]$, then

$$P\left(\sum_{i=1}^n D_i\ge t\right) \le e^{-\frac{2t^2}{\sum_{i=1}^n(b_i-a_i)^2}}$$

Proof. Since $D_i\mid F_{i-1}\in[a_i,b_i]$, we have

$$\mathbb{E}\left[e^{\lambda D_i}\mid F_{i-1}\right] \le e^{\frac{\lambda^2(b_i-a_i)^2}{8}}$$

To show the $\sum_{i=1}^n D_i$ is sub-Gaussian, we use the iterated expectation as,

$$\begin{aligned} \mathbb{E}\left[e^{\lambda\sum_{i=1}^n D_i}\right] &= \mathbb{E}_{D_1,\cdots,D_n}\left[e^{\lambda\sum_{i=1}^{n-1}D_i}\cdot\mathbb{E}_{D_n}\left[e^{\lambda D_n}\mid F_{n-1}\right]\right]\\ &= \mathbb{E}_{D_1,\cdots,D_{n-1}}\left[e^{\lambda\sum_{i=1}^{n-1}D_i}\right]\cdot\mathbb{E}_{D_n}\left[e^{\lambda D_n}\mid F_{n-1}\right]\\ &\le \mathbb{E}_{D_1,\cdots,D_{n-1}}\left[e^{\lambda\sum_{i=1}^{n-1}D_i}\right]e^{\frac{\lambda^2(b_n-a_n)^2}{8}} \end{aligned}$$

Using it recursively, we get $\mathbb{E}\left[e^{\lambda \sum_{i=1}^{n} D_i}\right] \leq e^{\frac{\lambda^2 \sum_{i=1}^{n}(b_i-a_i)^2}{8}}$. Then we can achieve the desired bound via Chernoff bound (similar to Prop. 1, sub-Gaussian tail bound). □

Thm. 9 (McDiarmid inequality) If $g_n(Z)$ satisfies the bounded difference condition, i.e. $|g_n(z) - g_n(z^{\setminus k})| \leq \sigma_k$, for a random vector Z with n independent entries, then

$$P(g_n(Z) - \mathbb{E}g_n(Z) \geq t) \leq e^{-\frac{2t^2}{\sum_{i=1}^{n}\sigma_i^2}}$$

where $z = (z_1, \cdots, z_k, \cdots, z_n)$, $z^{\setminus k} = (z_1, \cdots, z_k', \cdots, z_n)$.

Proof. First, please note that

$$g_n(Z) - \mathbb{E}g_n(Z) = S_n - S_0 = \sum_{i=1}^{n} D_i,$$

where $D_i = \mathbb{E}\left[g_n(Z) \mid Z_1, \ldots, Z_i\right] - \mathbb{E}\left[g_n(Z) \mid Z_1, \ldots, Z_{i-1}\right]$. Therefore, we can use the Azuma-Hoeffding inequality if we show that D_i is bounded.

$$\begin{aligned}
D_k &\leq \sup_z \mathbb{E}_{Z_{k+1:n}}\left[g_n\left(Z_{1:k-1}, z, Z_{k+1:n}\right)\right] \\
&\quad - \inf_z \mathbb{E}_{Z_{k+1:n}}\left[g_n\left(Z_{1:k-1}, z, Z_{k+1:n}\right)\right] \\
&\leq \sup_{z,z'} \Big| \mathbb{E}_{Z_{k+1:n}}\left[g_n\left(Z_{1:k-1}, z, Z_{k+1:n}\right)\right] \\
&\quad - \mathbb{E}_{Z_{k+1:n}}\left[g_n\left(Z_{1:k-1}, z', Z_{k+1:n}\right)\right] \Big| \\
&\leq \sigma_k
\end{aligned}$$

Then, we can plug it into the Azuma-Hoeffding inequality and conclude the proof. □

2.5 Functional bounds

Thm. 10 (Lipschitz functions) If $g : \mathbb{R}^n \to \mathbb{R}$ is L-Lipschitz function for vector z with edclidean norm, $z_i \sim \mathcal{N}(0, \sigma^2)$.

$$P(g(z) - \mathbb{E}g(z) \geq t) \leq e^{-\frac{ct^2}{L^2\sigma^2}}$$

3 Uniform Laws of Large Numbers (Ch. 4)

3.1 Motivation

Def. 7 (Glivenko-Cantelli class) We say $\mathcal{F}$ is Glivenko-Cantelli class if

$$\|P_n - P\|_{\mathcal{F}} := \sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} f(X_i) - \mathbb{E}f(X_i) \right| \longrightarrow 0,$$

in probability as $n \to 0$.

3.2 A uniform law via Rademacher complexity

Thm. 11 (Uniform law of large number) For b-uniformly bounded $\mathcal{F}$, we have

$$P\left(\sup_{f\in\mathcal{F}} R(f) - R_n(f) \geq 2\mathcal{R}_n(\mathcal{F}) + t\right) \leq e^{-\frac{nt^2}{2b^2}}.$$

Here, population risk is $R(f) = \mathbb{E}f(x)$ and empirical risk is $R_n(f) = \frac{1}{n}\sum_{i=1}^n f(x_i)$. The Rademacher complexity is

$$\mathcal{R}_n(\mathcal{F}) = \mathbb{E}_\epsilon \sup_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^n \epsilon_i h(z_i), \quad \epsilon_i \sim \text{Red}(\{-1,1\})$$

Proof. 1. **Concentration around mean**. Let's denote

$$g_n(x_{1:n}) := \sup_{f\in\mathcal{F}} R(f) - R_n(f) = \sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(x_i) - \mathbb{E}f(x).$$

Let $z = (x_1, \cdots, x_k, \cdots, x_n)$ and $z^{\backslash k} = (x_1, \cdots, x_k', \cdots, x_n)$,

$$\begin{aligned}
&\left|g_n(z) - g_n\left(z^{\backslash k}\right)\right| \\
=&\left|\sup_{h\in\mathcal{H}} \frac{1}{n}\sum_i \left[h(z_i) - \mathbb{E}h\right] - \sup_{\tilde{h}\in\mathcal{H}} \frac{1}{n}\sum_i \left[\tilde{h}\left(z_i^{\backslash k}\right) - \mathbb{E}\tilde{h}\right]\right| \\
\leq&\left|\sup_{h\in\mathcal{H}} \frac{\sum_i h(z_i) - h\left(z_i^{\backslash k}\right)}{n}\right| \leq \left|\sup_{h\in\mathcal{H}} \frac{h(x_k) - h(x_k')}{n}\right| \leq \frac{2b}{n},
\end{aligned}$$

which means g_n has Lipschitz property. Using McDiarmid inequality, $P\left(g_n(X) - \mathbb{E}g_n(X) \geq t\right) \leq e^{-\frac{nt^2}{2b^2}}$.

2. **Upper bound on mean**. Using symmetrization technique and the definition of Rademacher complexity, we have

$$\begin{aligned}
\mathbb{E}g_n(X) &= \mathbb{E}_X\left[\sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(x_i) - \mathbb{E}f(x)\right] \\
&\leq \mathbb{E}_{X,Y}\left[\sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n f(x_i) - f(y_i)\right] && \text{(symmetrize)} \\
&= \mathbb{E}_{X,Y,\epsilon}\left[\sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n \epsilon(f(x_i) - f(y_i))\right] && \text{(plug in } \epsilon) \\
&\leq 2\mathbb{E}_{X,\epsilon}\left[\sup_{f\in\mathcal{F}} \frac{1}{n}\sum_{i=1}^n \epsilon f(x_i)\right] = 2\mathcal{R}_n(\mathcal{F}).
\end{aligned}$$

Combining these two parts, we have the desired theorem that $P\left(g_n(X) - 2\mathcal{R}_n(\mathcal{F}) \geq t\right) \leq e^{-\frac{nt^2}{2b^2}}$. □

Thm. 12 (Uniform law - corollary) If $\mathcal{R}_n(\mathcal{F}) = o(1)$, then when $n \to \infty$, we have

$$\sup_{f\in\mathcal{F}} R(f) - R_n(f) \longrightarrow 0, \quad (a.s.)$$

In other words, $\mathcal{R}_n(\mathcal{F}) = o(1)$ implies that $\mathcal{F}$ is a Glivenko-Cantelli class.

Proof. Let $\mathcal{E}_n(\alpha)$ denote the event that $\sup_{f\in\mathcal{F}} R(f) - R_n(f) \geq \alpha$. The uniform law shows that

$$P\left(\mathcal{E}_n(2\mathcal{R}_n(\mathcal{H}) + t)\right) \leq e^{-\frac{nt^2}{2b^2}}.$$

Using union bound, $\forall t > 0$, we have,

$$\begin{aligned}
\sum_{n=1}^\infty P(\mathcal{E}_n(2t)) &\leq \sum_{n=1}^k P\left(\mathcal{E}_n(2t)\right) + \sum_{n=k+1}^\infty P\left(\mathcal{E}_n\left(2\mathcal{R}_n(\mathcal{H}) + t\right)\right) \\
&\leq \sum_{n=1}^k P\left(\mathcal{E}_n(2t)\right) + \sum_{n=k+1}^\infty e^{-\frac{nt^2}{2b^2}} < \infty.
\end{aligned}$$

The k is chosen such that when $n > k$, $\mathcal{R}_n(f) < \frac{t}{2}$. Such k must exist, since $\mathcal{R}_n(f) = o(1)$. Using the Borel-Cantalli lemma, we show that

$$P\left(\lim_{n\to\infty} \sup \mathcal{E}_n(2t)\right) = 0.$$

Considering that t can be arbitrarily small, we have

$$P\left(\lim_{n\to\infty} \sup_{f\in\mathcal{F}} R(f) - R_n(f) = 0\right) = 1.$$

□

3.3 Upper bounds on the Rademacher complexity

Def. 8 (Growth function) The growth function $N_\mathcal{H}$ for a hypothesis space $\mathcal{H}$ is defined as: $\forall m \in \mathbb{N}$,

$$N_\mathcal{H}(n) := \sup_{z_{1:n}\subseteq Z} \left|\{(h(z_1), \cdots, h(z_n)) \mid h \in \mathcal{H}\}\right|$$

Remark: Growth function measures the maximum number of distinct ways in which m points can be classified using hypotheses in $\mathcal{H}$.

Thm. 13 (Massart lemma) For a data set $z_{1:n} = \{z_1, \cdots, z_n\}$, the hypothesis $h : Z \to \{0,1\}$ and the hypothesis space $\mathcal{H}(z_{1:n}) := \{(h(z_1), \cdots, h(z_n)) \mid h \in \mathcal{H}\}$, we have

$$\mathcal{R}_n(\mathcal{H}) := \mathbb{E}_\epsilon\left[\sup_{h\in\mathcal{H}} \frac{1}{n}\sum_{i=1}^n \epsilon_i h(z_i)\right] \leq 2\sqrt{\frac{\log|\mathcal{H}(z_{1:n})|}{n}}$$

Remark: Using this result, we can now bound the Rademacher complexity in terms of the growth function.

Proof. First, we show that $\epsilon^T\theta$ is $\sqrt{n}$ sub-Gaussian. Using the independence of z, $\forall\lambda \in \mathbb{R}$, we have

$$\begin{aligned}
\mathbb{E}_\epsilon\left[\exp(\lambda\epsilon^\top\theta)\right] &= \mathbb{E}_\epsilon\left[\exp\left(\lambda\sum_{i=1}^n \epsilon_i\theta_i\right)\right] \\
&= \mathbb{E}_{\epsilon_1}\left[\exp\left(\lambda\epsilon_1\theta_1\right)\right] \cdots \mathbb{E}_{\epsilon_n}\left[\exp\left(\lambda\epsilon_n\theta_n\right)\right] \\
&\leq \exp\left(\frac{\lambda^2\theta_1^2}{2} + \cdots + \frac{\lambda^2\theta_n^2}{2}\right) \leq \exp\left(\frac{\lambda^2 n}{2}\right).
\end{aligned}$$

Next, using the Gaussian maxima, we get

$$\mathbb{E}\max_{\theta\in\mathbb{T}} \epsilon^T\theta \leq 2\sqrt{n\log\left|\mathcal{H}\left(z_1^n\right)\right|}$$

Then, we can get the intended results. □

Def. 9 (VC Dimension) The VC dimension of $\mathcal{H}$ is the biggest $n \in \mathbb{N}$ such that there exists n samples in $\mathcal{H}$ which can be arbitrarily scattered by a binary classifier, i.e.,

$$d_{VC} = \max_{n\in\mathbb{N}} n, \quad \text{s.t. } \exists z_{1:n} \in Z^n, \mathcal{H}(z_{1:n}) = \{0,1\}^n.$$

Here, $\mathcal{H}(z_{1:n}) := \{(h(z_1), \cdots, h(z_n)) \mid h \in \mathcal{H}\}$

Remark: Finite VC dimension can make $\mathcal{H}$ a Glivenko-Cantelli class.

Thm. 14 (Sauer-Shelah) For a space $\mathcal{H}$ with VC dimension d_{VC}, for any $z_1, \cdots, z_n$, we have growth function

$$N_{\mathcal{H}}(n) := \sup_{z_{1:n}\in Z^n} |\mathcal{H}(z_{1:n})| \le (n+1)^{d_{VC}}, \quad \forall n \ge d_{VC}$$

Proof. Proof by combination algebra. See the Chapter 4.3 for more details. □

Thm. 15 (Rademacher contraction) For any $\mathbb{T} \subseteq \mathbb{R}^n$ and $\ell : \mathbb{R}^n \to \mathbb{R}^n$ with univariate L-Lipschitz functions it holds that

$$\tilde{\mathcal{R}}_n(\ell \circ \mathbb{T}) \le L\tilde{\mathcal{R}}_n(\mathbb{T})$$

Proof. See the slides of Lecture 5. □

4 Non-uniform Learnability (Lec. 6-7)

4.1 Structural risk minimization (SRM)

Def. 10 (SRM) Say we have a nested family of function spaces $\mathcal{H}_1 \subset \mathcal{H}_2 \subset \cdots$, where $\mathcal{H} = \bigcup_k \mathcal{H}_k$. For each $\mathcal{H}_k$ define the event

$$E_{k,h} = \left\{ R(h) - R_n(h) \le c\sqrt{\frac{\log(1/\delta_k)}{n}} + 2\mathcal{R}_n(\mathcal{H}_k) \right\}.$$

Thm. 16 (Uniform law via the SRM) Define $k(h) = \min\{k \mid f \in \mathcal{H}_k\}$ which for each h finds the minimum set $\mathcal{H}_k$.
If $P(\bigcap_{h\in\mathcal{H}_k} E_{k,h}) \ge 1-\delta_k$ for each k and if $\sum_k \delta_k \le \delta$, with probability at least $1-\delta$,

$$\sup_{h\in\mathcal{H}} R(h) - R_n(h) \le c\sqrt{\frac{\log\left(1/\delta_{k(h)}\right)}{n}} + 2\mathcal{R}_n\left(\mathcal{H}_{k(h)}\right)$$

Proof. Observe that

$$A := \left\{ \sup_{h\in\mathcal{H}} R(h) - R_n(h) \le c\sqrt{\frac{\log\left(1/\delta_{k(h)}\right)}{n}} + 2\mathcal{R}_n\left(\mathcal{H}_{k(h)}\right) \right\}$$
$$= \cap_{h\in\mathcal{H}} \cap_{k:h\in\mathcal{H}_k} E_{k,h} = \cap_{k\in\mathbb{N}} \cap_{h\in\mathcal{H}_k} E_{k,h}$$

Then, we can use the union bound,

$$P(A) = 1 - P\left(\cup_{k\in\mathbb{N}} \cup_{h\in\mathcal{H}_k} E_{k,h}\right) \ge 1 - \sum_k \delta_k \ge 1-\delta,$$

which concludes the proof. □

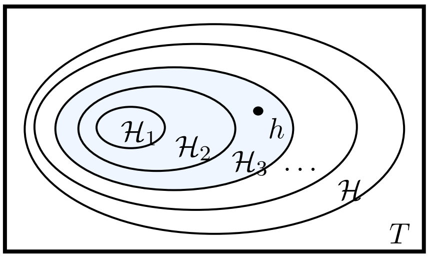


Figure: Demonstration of SRM when $k(h) = 3$.

4.2 Margin bound for linear classifiers

Def. 11 (Linear classifiers) Define the empirical risk

$$R_n^\gamma(f) = \frac{1}{n}\sum_{i=1}^n 1_{y_i f(x_i)\le\gamma},$$

and the population risk

$$R^\gamma(f) := \mathbb{E}_{X,Y} 1_{y_i f(x_i)\le\gamma}.$$

Thm. 17 (Rademacher complexity of L_2-bounded linear class) For a class of linear functions $\mathcal{F}_{B,2} = \{f(x) = \langle w, x\rangle : \|w\|_2 \le B\}$, we have

$$\mathcal{R}_n\left(\mathcal{F}_{B,2}\right) \le \frac{B\max_i \|x_i\|_2}{\sqrt{n}}$$

Proof. Using the definition of Rademacher complexity and Cauchy's inequality, we have

$$\begin{aligned}
n \cdot \mathcal{R}_n\left(\mathcal{F}_{B,2}\right) &= \mathbb{E}_\sigma \sup_{f\in\mathcal{F}_{B,2}} \sum_{i=1}^n \sigma_i f(x_i) \\
&= \mathbb{E}_\sigma \sup_{\|w\|_2\le B} \sum_{i=1}^n \sigma_i \langle w, x_i\rangle \\
&= \mathbb{E}_\sigma \sup_{\|w\|_2\le B} \left\langle w, \sum_{i=1}^n \sigma_i x_i \right\rangle \\
&\le B\mathbb{E}_\sigma \sqrt{\left\|\sum_{i=1}^n \sigma_i x_i\right\|_2^2} && \text{(Cauchy's)} \\
&\le B\sqrt{\mathbb{E}_\sigma \left\|\sum_{i=1}^n \sigma_i x_i\right\|_2^2} && \text{(Jensen's)}
\end{aligned}$$

Finally, since the Rademacher variables σ are independent, we have

$$\begin{aligned}
\mathbb{E}_\sigma \left\|\sum_{i=1}^m \sigma_i x_i\right\|_2^2 &= \mathbb{E}_\sigma \sum_{i,j} \sigma_i\sigma_j \langle x_i, x_j\rangle \\
&= \sum_{i\ne j} \langle x_i, x_j\rangle \mathbb{E}_\sigma\left[\sigma_i\sigma_j\right] + \sum_{i=1}^m \langle x_i, x_i\rangle \mathbb{E}_\sigma[\sigma_i^2] \\
&= \sum_{i=1}^m \|x_i\|_2^2 \le n \max_i \|x_i\|_2^2.
\end{aligned}$$

Plug into the previous inequality and we get the result. $\square$

Thm. 18 (Non-uniform margin bound) If the assumptions are valid for any fixed γ, with probability at least $1-\delta$, for any $f \in \mathcal{F}_B$, we have

$$R^0(f) = P(y \neq \text{sign}(f(x))) \leq R_n^\gamma(f) + \frac{2DB}{\gamma\sqrt{n}} + c\sqrt{\frac{\log(1/\delta)}{n}}$$

Proof. Please refer to Lec. 7 and Exercise class 1. $\square$

4.3 Margin bounds for SVM

Thm. 19 (Non-uniform margin bound for SVM) If the assumptions are valid for any fixed γ, with probability at least $1-\delta$, for any $f \in \mathcal{F}_B$, we have

$$P(y \neq \text{sign}(f(x))) \leq R_n^\gamma(f) + \frac{2D\|w^*\|_2}{\sqrt{n}} + c\sqrt{\frac{\log(1/\delta)}{n}}$$

Proof. Using the margin bound theorem (Thm. 18) with $\gamma = 1$ then yields the result. $\square$

Thm. 20 (Uniform margin bound for SVM)

$$\begin{aligned}\mathbb{P}(yf_{SVM}(x) < 0) \leq & \frac{2eD\|w_{SVM}\|_2}{\sqrt{n}} \\ & + c\sqrt{\frac{\log(1/\delta) + \log\left(4\log\|w_{SVM}\|_2\right)}{n}}\end{aligned}$$

Proof. Choose $B_k = e^k$ and the nested function space is $\mathcal{F}_{B_k} := \{w \mid \|w\| \leq B_k\}$. According to the Non-uniform margin bound for SVM (Thm. 19), let $\delta_k = \frac{\delta}{2k^2}$. Then $k(w) = \log\|w\|$ and thus $B_{k(w)} = \|w\|\, e$ and

$$\frac{1}{\delta_{k(w)}} = \frac{2(k(w))^2}{\delta} \leq \frac{2(2\log\|w\|)^2}{\delta}.$$

Plugging in the quantities yields the results with probability at

$$1 - \sum_{i=1}^{\infty}\delta_k = 1 - \delta\sum_{i=1}^{\infty}\frac{1}{2k^2} \geq 1-\delta,$$

which concludes the proof. $\square$

5 Metric Entropy (Ch. 5)

5.1 Covering and Packing

Def. 12 (Covering number) A δ-cover of a set $\mathbb{T}$ with a metric ρ is a set $\{\theta^1, \cdots, \theta^N\} \subset \mathbb{T}$, such that $\forall\theta \in \mathbb{T}, \exists i \in [N], \rho(\theta, \theta^i) \leq \delta$. The covering number $N(\delta; \mathbb{T})$ is the cardinality of the smallest δ-cover.

Def. 13 (Packing number) A δ-cover of a set $\mathbb{T}$ with a metric ρ is a set $\{\theta^1, \cdots, \theta^N\} \subset \mathbb{T}$, such that $\forall\theta \in \mathbb{T}, \exists i \in [N], \rho(\theta, \theta^i) \leq \delta$.
The covering number $N(\delta; \mathbb{T})$ is the cardinality of the smallest δ-cover.

Below are some common spaces' complexity.

Space	Rademacher C.	Gaussian C.
$B_1^d(1)$	1	$\sqrt{2\log d} \pm o(1)$
$B_2^d(1)$	$\sqrt{d}$	$\sqrt{d} - o(1)$
$B_q^d(1), q > 1$	-	$\sqrt{\frac{2}{\pi}}d^{1-1/q} \sim c_q d^{1-1/q}$

5.2 Metric entropy and sub-Gaussian processes

Def. 14 (sub-Gaussian processes) For zero-mean random variables $\{X_\theta, \theta \in \mathbb{T}\}$, we say it is a sub-Gaussian process with metric $\rho_X(\cdot,\cdot)$ on T if

$$\mathbb{E}[e^{\lambda(X_\theta - X_{\theta'})}] \leq e^{\frac{\lambda^2\rho_X^2(\theta,\theta')}{2}}, \quad \forall\lambda \in \mathbb{R} \text{ and } \theta, \theta' \in \mathbb{T}.$$

Remark: It can be shown that $X_\theta - X_{\theta'}$ is a sub-Gaussian RV with parameter $\sigma = \sup_{\theta,\theta'}\rho_X(\theta,\theta')$.

Thm. 21 (One-step discretization bound) For a zero-mean sub-Gaussian process $\{X_\theta, \theta \in \mathbb{T}\}$ with $\rho(\theta,\theta')$, we have an upper bound for any $\delta \in [0, \sigma]$,

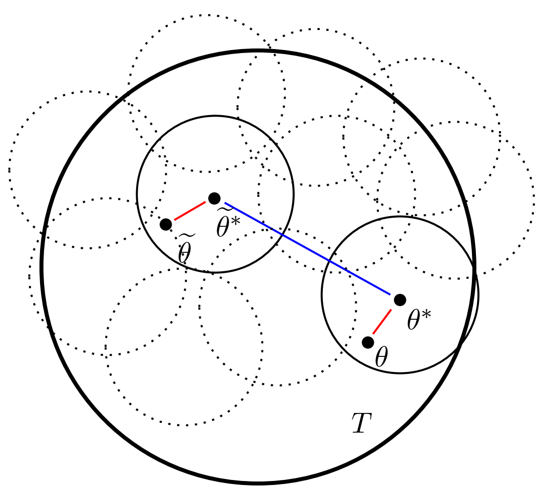
$$\mathbb{E}\sup_{\theta,\theta' \in \mathbb{T}} X_\theta - X_{\theta'} \leq 2\mathbb{E}\sup_{\substack{\theta,\theta' \in \mathbb{T} \\ \rho(\theta,\theta') \leq \delta}} (X_\theta - X_{\theta'}) + 4\sigma\sqrt{\log N(\delta)},$$

where $\sigma = \sup_{\theta,\theta' \in \mathbb{T}}\rho(\theta,\theta')$.

Proof. Let $\{\theta_1, \cdots, \theta_N\}$ be a σ-cover of T. For any $\theta \in \mathbb{T}$, we can find at least one θ^* in the cover, s.t. $\rho(\theta,\theta^*) \leq \delta$, (the same for $\widetilde{\theta}^*$), and hence,

$$\begin{aligned} X_\theta - X_{\widetilde{\theta}} &= X_\theta - X_{\theta^*} + X_{\theta^*} - X_{\widetilde{\theta}^*} + X_{\widetilde{\theta}^*} - X_{\widetilde{\theta}} \\ &\leq 2\sup_{\rho(\theta,\theta') \leq \delta}(X_\theta - X_{\theta'}) + \max_{i,j=1,\cdots,N}|X_{\theta_i} - X_{\theta_j}| \end{aligned}$$

Below is a figure to illustrate it.



Then, take the expectation on both sides. We use the sub-Gaussian maxima (Thm. 6) on $|X_{\theta_i} - X_{\theta_j}|$, which has parameter at most $\rho(\theta_i, \theta_j) \le \sigma$. Therefore,

$$\mathbb{E} \sup_{\theta,\theta' \in \mathbb{T}} X_\theta - X_{\theta'} \le 2\mathbb{E} \sup_{\substack{\theta,\theta' \in \mathbb{T} \\ \rho(\theta,\theta') \le \delta}} (X_\theta - X_{\theta'}) + 4\sigma\sqrt{\log N(\delta)}$$

$\square$

Thm. 22 (One-step discretization bound - corollary) Let $X_\theta = \frac{1}{n}\sum_{i=1}^n \epsilon_i \theta_i$, where ϵ are Rademacher RVs. Then $\{X_\theta, \theta \in \mathbb{T}\}$ is a sub-Gaussian process with $\rho(\theta, \theta') = \frac{\|\theta-\theta'\|_2}{\sqrt{n}}$. We have an upper bound as

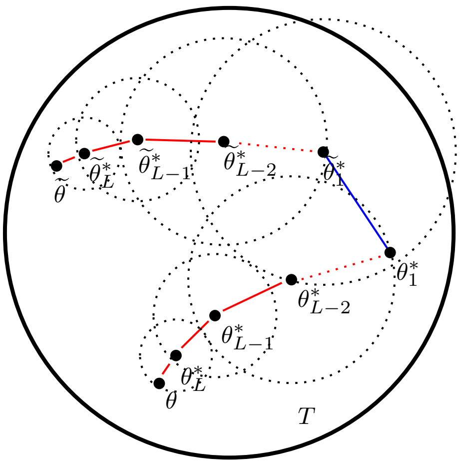
$$\mathcal{R}_n(T) \le \frac{1}{\sqrt{n}}\mathbb{E} \sup_{\theta,\theta' \in \mathbb{T}} X_\theta - X_{\theta'} \le \frac{2}{\sqrt{n}}[\delta\sqrt{n} + 2\sigma\sqrt{\log N(\delta}],$$

Remark: This provides a usage of sub-Gaussian process, to bound the Rademacher complexity.

Thm. 23 (Dudley's integral) Let $\{X_\theta, \theta \in \mathbb{T}\}$ be a zero-mean sub-Gaussian process with a metric ρ. Define $D = \sup_{\theta,\theta'} \rho(\theta, \theta')$.

$$\mathbb{E} \sup_{\theta,\theta'} X_\theta - X_{\theta'} \le 2\mathbb{E} \sup_{\rho(\theta,\theta')} X_\theta - X_{\theta'} + 16 \int_{\delta/4}^{D} \sqrt{\log N(t)}\mathrm{d}t.$$

Remark: The Dudley's integral (sometimes) achieves a tighter bound on the last term of $4\sigma\sqrt{\log N(\delta)}$ by chaining method.



Proof. Define $L = \log_2 \frac{D}{\delta}$ sets of δ_i-covers $\mathcal{C}_i$, where $\delta_i = \frac{1}{2^i}D$. Let $N(\delta_i)$ denote the covering number in $\mathcal{C}_i$.

$$\begin{aligned}
X_{\theta_L} - X_{\widetilde{\theta_L}} &\le X_{\theta_L} - X_{\theta^*_{L-1}} + X_{\theta^*_{L-1}} - X_{\tilde{\theta}^*_{L-1}} + X_{\tilde{\theta}^*_{L-1}} - X_{\widetilde{\theta_L}} \\
&= 2 \max_{\theta \in \mathcal{C}_L} X_\theta - X_{\theta^*_{L-1}} + \max_{\theta,\theta' \in \mathcal{C}_{L-1}} X_\theta - X_{\theta'} \\
&\cdots\cdots \\
&\le 2\sum_{i=2}^{L} \max_{\theta \in \mathcal{C}_i} X_\theta - X_{\theta^*_{i-1}} + \max_{\theta,\theta' \in \mathcal{C}_1} X_\theta - X_{\theta'}
\end{aligned}$$

Next, we use sub-Gaussian maxima,

$$\begin{aligned}
\mathbb{E} \max_{\theta \in \mathcal{C}_i} X_\theta - X_{\theta^*_{i-1}} &\le 2\delta_{i-1}\sqrt{\log|\mathcal{C}_i|} \le 2 \cdot \frac{D}{2^{i-1}}\sqrt{\log N\left(\frac{D}{2^{i-1}}\right)} \\
&\le 8\int_{D/2^{i-1}}^{D/2^i} \sqrt{\log N(t)}\mathrm{d}t
\end{aligned}$$

Putting things together, we get

$$\begin{aligned}
\mathbb{E} \max_{\theta,\tilde{\theta} \in \mathcal{C}_L} X_\theta - X_{\tilde{\theta}} &\le 16\sum_{i=2}^{L} \int_{\frac{D}{2^{i-1}}}^{\frac{D}{2^i}} \sqrt{\log N(t)}\mathrm{d}t + 2D\sqrt{\log N\left(\frac{D}{2}\right)} \\
&\le 16\int_{\delta/4}^{D} \sqrt{\log N_{\mathbb{T}}(t)}\mathrm{d}t
\end{aligned}$$

This gives the desired form. $\square$

6 Reproducing Kernel Hilbert Spaces (Ch. 12)

6.1 Basics of Hilbert space

Def. 15 (Hilbert spaces) A Hilbert space $\mathcal{H}$ is a complete inner product space. In a Hilbert space

- There endows an inner product: $\langle \cdot, \cdot \rangle_{\mathcal{H}}$,
- Every Cauchy sequence $(f_n)_{n=1}^\infty$ in $\mathcal{H}$ converges to some element $f^* \in \mathcal{H}$.

Thm. 24 (Riesz representation) Let L be a bounded linear functional on a Hilbert space $\mathcal{H}$. Then there exists a unique representer $g \in \mathcal{H}$ such that $L(f) = \langle f, g \rangle_{\mathcal{H}}$ for all $f \in H$.

Proof. Consider a null space $\mathrm{Null}(L) := \{h \mid L(h) = 0\}$. If $\mathrm{Null}(L) = H$, then $\mathrm{Null}(L)^\perp = \{0\}$, we take $g = 0$.
In a non-trivial case (i.e., $\mathrm{Null}(L)^\perp \ne \{0\}$), there exist a non-zero element $g \in \mathrm{Null}(L)^\perp$ such that $\|g\|_{\mathcal{H}} = L(g)$. Define $h := L(f)g - L(g)f$, then we note

$$L(h) = L(f)L(g) - L(g)L(f) = 0,$$

which means $h \in \mathrm{Null}(L)$. Therefore, we have $h \perp g$, i.e.,

$$0 = \langle h, g \rangle_{\mathcal{H}} = L(f)\|g\|^2_{\mathcal{H}} - L(g)\langle f, g \rangle_{\mathcal{H}}.$$

This implies $L(f) = \langle f, g \rangle_{\mathcal{H}}$. $\square$

6.2 Reproducing kernel Hilbert space

Def. 16 (Kernel function) Given a feature map $\phi : \mathcal{X} \to \mathcal{H}$ and the Hilbert space $\mathcal{H}$ that ϕ maps to, the kernel function is defined as

$$K(x, y) := \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}.$$

Def. 17 (RKHS - defined by kernel) A reproducing kernel Hilbert space is a Hilbert space $\mathcal{H}$ of functions $f : \mathcal{X} \to \mathbb{R}$ with a kernel function $K(\cdot, \cdot)$ that

- For any $x \in \mathcal{X}$, $K(\cdot, x) \in \mathcal{H}$,

Space	Kernel	Eigenfunctin
2-poly.	$K(x,z) = (1+xz)^2$	$\phi_j(x) = a_0^j + a_1^j x + a_2^j x^2$, const via eigen-decomposition.
1-Sobolev $W_2^1([0,1])$	$K(x,z) = \min\{x,z\}$	$\phi_j(t) = \sin \frac{(2j-1)\pi t}{2}, \mu_j = \left(\frac{2}{(2j-1)\pi}\right)^2$

- Satisfies the "reproducing property":

$$\langle f(\cdot), K(\cdot, x)\rangle_{\mathcal{H}} = f(x), \quad \forall f \in \mathcal{H}.$$

Thm. 25 (RKHS from kernel function) Given any positive semi-definite kernel function $K(\cdot,\cdot)$, there is a **unique** Hilbert space $\mathcal{H}$ in which the kernel $K(\cdot,\cdot)$ satisfies the reproducing property.
Given some data $\{x_i\}_{i=1}^n$, such Hilbert space $\mathcal{H}$ is

$$\mathcal{H} := \left\{ f(\cdot) = \sum_{i=1}^n \alpha_i K(\cdot, x_i) \;\middle|\; x_i \in \mathcal{X} \right\}$$

with the norm

$$\langle f, f'\rangle_{\mathcal{H}} := \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j' K(x_i, x_j)$$

Remark: For a fixed kernel function, there will be (infinitely) many feature maps, and thus many Hilbert spaces of the feature. But the Hilbert space that **satisfies the reproducing property** is unique!

Def. 18 (RKHS - defined by evaluation functional) A reproducing kernel Hilbert space is a Hilbert space $\mathcal{H}$ of functions $f : \mathcal{X} \to \mathbb{R}$ such that for each $x \in \mathcal{X}$, the evaluation functional $L_x : \mathcal{H} \to \mathbb{R}$ that performs the operation $L_x(f) = f(x)$ is bounded, i.e.,

$$f(x) = |L_x(f)| \le M \|f\|_{\mathcal{H}}, \quad \exists M < \infty, \forall f \in \mathcal{H}.$$

Proof. Let's prove the equivalence to the first definition.

When L_x is a bounded linear functional, the Riesz theorem shows that there exists a unique $R_x \in \mathcal{H}$ such that

$$L_x(f) = \langle f, R_x\rangle_{\mathcal{H}}.$$

Similarly, we can get a unique R_y based on y. The kernel is defined as $K(x,y) = \langle R_x, R_y\rangle_{\mathcal{H}}$. Next, we can verify that K is positive semidefinite.

$$\begin{aligned}\alpha^T K \alpha &= \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(x_i, x_j) = \langle \sum_{i=1}^n \alpha_i R_{x_i}, \sum_{j=1}^n \alpha_j R_{x_j}\rangle_{\mathcal{H}} \\ &= \left\| \sum_{i=1}^n \alpha_i R_{x_i} \right\|_{\mathcal{H}}^2 \ge 0.\end{aligned}$$

$\square$

6.3 Mercer's theorem and its consequences

Thm. 26 (Mercer's) For a continuous and PSD kernel function K that satisfies the Hilbert-Schmidt condition. Then there exist a sequence of eigenfunctions $(\phi_i)_{i=1}^\infty$ that form an orthonormal basis of $L^2(\mathcal{X}; P)$ and non-negative eigenvalues $(\mu_i)_{i=1}^\infty$ such that

$$T_K(\phi_i) = \mu_i \phi_i, \quad \forall i = 1, 2, \cdots \tag{6.1}$$

Moreover, the kernel function has the expansion

$$K(x,y) = \langle \Phi(x), \Phi(y)\rangle_{\ell^2(\mathbb{N})} := \sum_{i=1}^\infty \mu_i \phi_i(x) \phi_j(y)$$

7 Non-parametric Least Squares (Ch. 13)

7.1 Fixed design

Def. 19 (Least square regression) For a function f^* and data collection $\{(x_i, y_i)\}_{i=1}^n$, where $y_i = f^*(x_i) + \sigma w_i$, $w_i \sim \mathcal{N}0, 1$, the least-squares estimateor estimator is given by

$$\hat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2.$$

Prop. 5 (Basic inequality) In the non-parametric least squares, we have the optimality of $\hat{f}$, which means

$$\frac{1}{n} \sum_{i=1}^n \left(\hat{f}(x_i) - y_i\right)^2 \le \frac{1}{n} \sum_{i=1}^n \left(f^*(x_i) - y_i\right)^2$$

Or, equivalently,

$$\|f - f^*\|_n^2 \le \frac{2\sigma}{n} \sum_{i=1}^n w_i \left(f(x_i) - f^*(x_i)\right).$$

Proof. Let's prove the equivalence. Note that $y_i = f^*(x_i) + \sigma w_i$, we have

$$\begin{aligned}0 &\ge \frac{1}{n} \sum_{i=1}^n \left(\hat{f}(x_i) - y_i\right)^2 - \frac{1}{n} \sum_{i=1}^n \left(f^*(x_i) - y_i\right)^2 \\ &\ge \frac{1}{n} \sum_{i=1}^n \left((\hat{f}(x_i)^2 - f^*(x_i)^2) - 2y_i(\hat{f}(x_i) - f^*(x_i)) \right) \\ &\ge \frac{1}{n} \sum_{i=1}^n \left((\hat{f}(x_i) - f^*(x_i))^2 - 2\sigma w_i(\hat{f}(x_i) - f^*(x_i)) \right),\end{aligned}$$

which means

$$\frac{1}{n} \sum_{i=1}^n \left((\hat{f}(x_i) - f^*(x_i))^2 \right) \le \frac{2\sigma}{n} \sum_{i=1}^n \left(w_i(\hat{f}(x_i) - f^*(x_i)) \right).$$

$\square$

Def. 20 (Localized Gaussian complexity) If we restrict the radius of function space $\mathcal{F}$, i.e., $\|f\|_n \leq \delta$, we have the localized Gaussian complexity for $\mathcal{F}$,

$$\mathcal{G}_n(\delta; \mathcal{F}) := \mathbb{E}_{w \sim \mathcal{N}(0,1)} \left[\sup_{f \in \mathcal{F}, \|f\|_n \leq \delta} \frac{1}{n} \sum_{i=1}^{n} w_i f(x_i) \right]$$

Def. 21 (Critical radius) For a local Gaussian complexity $\mathcal{G}_n$ around f^* with radius δ, the radius δ is said to be *valid* if the following *critical inequality* satisfies,

$$\frac{\mathcal{G}_n(\delta; \mathcal{F}^*)}{\delta} \leq \frac{\delta}{2\sigma}$$

The smallest δ satisfies it is the *critical radius*, which must exist for any star-shaped function class $\mathcal{F}$.

Remark: One intuition is that the satisfaction of critical inequality means the optimality of $\hat{f}$. One example is that if we have the optimality of $\hat{f}$, i.e.,

$$\frac{1}{2n} \sum_{i=1}^{n} \left(y_i - \widehat{f}(x_i)\right)^2 \leq \frac{1}{2n} \sum_{i=1}^{n} \left(y_i - f^*(x_i)\right)^2$$

And let $\delta = \mathbb{E}\left\|\hat{f} - f^*\right\|_n$, then we can show the δ satisfies $\frac{1}{2}\delta^2 \leq \sigma \mathcal{G}_n(\delta; \mathcal{F}^*)$, which is equivalent to the critical inequality.

Thm. 27 (Risk decomposition) In the least-squares regression, where $y_i = f^*(x_i) + \sigma w_i, w_i \sim \mathcal{N}(0,1)$, we have risk decomposition

$$R(f) = \left(\mathbb{E}f(x) - \mathbb{E}f^*(x)\right)^2 + \operatorname{var}(f(x)) + \sigma^2$$

Proof. Using the fact $\operatorname{var}(x) = \mathbb{E}x^2 - (\mathbb{E}x)^2$ and the independence of y and $f(x)$, we have

$$\begin{aligned}
R(f) &= \mathbb{E}\left[(y - f(x))^2\right] \\
&= \mathbb{E}y^2 + \mathbb{E}f(x)^2 - 2\mathbb{E}yf(x) \qquad (y \text{ and } f(x) \text{ are indep.}) \\
&= \operatorname{var}(y) + (\mathbb{E}y)^2 + \operatorname{var}((f(x)) - (\mathbb{E}f(x))^2 + 2(\mathbb{E}y)(\mathbb{E}f(x)) \\
&= \operatorname{var}(y) + \operatorname{var}(f(x)) + (\mathbb{E}f(x) - \mathbb{E}y)^2 \\
&= \underbrace{\left(\mathbb{E}f(x) - \mathbb{E}f^*(x)\right)^2}_{\text{bias}^2} + \underbrace{\operatorname{var}(f(x))}_{\text{variance}} + \underbrace{\sigma^2}_{\text{irreducible noise}}.
\end{aligned}$$

If there is no variance in model, we can also get the decomposition as,

$$\begin{aligned}
R(f) &= \mathbb{E}\frac{1}{n}\sum_{i=1}^{n}(y_i - f(x_i))^2 \\
&= \mathbb{E}\frac{1}{n}\sum_{i=1}^{n}\left(f^*(x_i) + \sigma w_i - f(x_i)\right)^2 \\
&= \mathbb{E}\frac{1}{n}\sum_{i=1}^{n}\left(f^*(x_i) - f(x_i)\right)^2 + \mathbb{E}\frac{1}{n}\sum_{i=1}^{n}\sigma^2 w^2 \\
&\quad + 2\mathbb{E}\frac{1}{n}\sum_{i=1}^{n} w\left(f^*(x_i) - f(x_i)\right) \\
&= \|f - f^*\|_n^2 + \sigma^2
\end{aligned}$$

$\square$

Thm. 28 (Prediction error bound) If $\mathcal{F}^*$ is star-shaped, then for any δ satisfies the critical inequality and $t \geq \delta$, the non-parametric least square estimate $\hat{f}_n$ satisfies

$$P\left(\left\|\hat{f}_n - f^*\right\|_n^2 \geq 16t\delta_n\right) \leq \exp\left(-\frac{nt\delta_n}{2\sigma^2}\right),$$

which also means for some constant c,

$$\mathbb{E}\left\|\hat{f}_n - f^*\right\|_n^2 \leq c\left(\delta_n^2 + \frac{\sigma^2}{n}\right).$$

Remark: This theorem links the local Gaussian complexity to the error bounds.

Proof. Let $\hat{\Delta} = f - f^*$, and thus $\|\hat{\Delta}\| = \|f - f^*\|_n^2$. Our goal is to show for any $\|\hat{\Delta}\|_n \geq \sqrt{t}\delta_n$,

$$\|\hat{\Delta}\|_n^2 \leq \frac{2\sigma}{n}\sum_{i=1}^n w_i \hat{\Delta}(x_i) \overset{(i)}{\leq} 4\|\hat{\Delta}\|_n \sqrt{t}\delta_n$$

with probability $1 - e^{-\frac{nt\delta_n^2}{2\sigma^2}}$. The theorem follows from rearranging terms. We organize the proof in multiple steps.

For a given scalar $u \geq \delta_n$, define the event

$$\mathcal{A}(u) := \left\{\exists g \in \mathcal{F}^* \cap \{\|g\|_n \geq u\} \;\middle|\; \left|\frac{\sigma}{n}\sum_{i=1}^n \tilde{w}_i g(x_i)\right| \geq 2u\|g\|_n\right\}$$

$\square$

Thm. 29 (Bounds via metric entropy) Any $\delta \in (0, \sigma]$ such that

$$\frac{16}{\sqrt{n}}\int_{\frac{\delta^2}{4\sigma}}^{\delta} \sqrt{\log N_n\left(t; \mathbb{B}_n\left(\delta; F^*\right)\right)}dt \leq \frac{\delta^2}{4\sigma}$$

satisfies the critical inequality.

7.2 Error bounds for RKHS

Def. 22 (R-restrained space) The function space inside the radius R is

$$\mathcal{F}_R := \{f \in \mathcal{F} \mid \|f\|_{\mathcal{F}} \leq R\}$$

Thm. 30 (Localized Gaussian complexity for RKHS) Let an RKHS $\mathcal{F}$ with kernel function $K(\cdot,\cdot)$. Defining $\hat{\mu}_j$ as eigenvalues of the kernel matrix K, we have the local Gaussian complexity bounded by

$$\mathcal{G}_n\left(\delta; \mathcal{F}_R\right) \leq \sqrt{\frac{R+1}{n}}\sqrt{\sum_{j=1}^n \min\left\{\delta^2, \hat{\mu}_j\right\}}$$

Note that the localized Gaussian complexity is computed under $\|f\|_{\mathcal{F}} \leq R, \|f\|_n \leq \delta$.

Thm. 31 (Prediction error for norm-bounded RKHS) When $\lambda_n \geq 2\delta_{n;R}^2$ there is universal constants c_0, c_1, c_3 such that

$$P\left(\left\|\widehat{f}_{\lambda_n} - f^\star\right\|_n^2 \geq cR^2\left(\delta_{n;R}^2 + \lambda_n\right)\right) \leq c_0 e^{-c_1\frac{nR^2\delta_{n:R}^2}{\sigma^2}}$$

7.3 Random design

WIP...