Lecture 2: Concentration without Independence

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1 Martingale-based Methods

1.1 Martingale

• **Definition** (*Martingale*) [Resnick, 2013] Let $\{X_n, n \geq 0\}$ be a stochastic process on (Ω, \mathscr{F}) and $\{\mathscr{F}_n, n \geq 0\}$ be a *filtration*; that is, $\{\mathscr{F}_n, n \geq 0\}$ is an *increasing sub* σ -fields of \mathscr{F}

$$\mathscr{F}_0 \subset \mathscr{F}_1 \subset \mathscr{F}_2 \subset \ldots \subset \mathscr{F}$$
.

Then $\{(X_n, \mathscr{F}_n), n \geq 0\}$ is a martingale (mg) if

- 1. X_n is **adapted** in the sense that for each $n, X_n \in \mathscr{F}_n$; that is, X_n is \mathscr{F}_n -measurable.
- 2. $X_n \in L_1$; that is $\mathbb{E}[|X_n|] < \infty$ for $n \ge 0$.
- 3. For $0 \le m < n$

$$\mathbb{E}\left[X_n \mid \mathscr{F}_m\right] = X_m, \quad \text{a.s.} \tag{1}$$

If the equality of (1) is replaced by \geq ; that is, things are getting better on the average:

$$\mathbb{E}\left[X_n \mid \mathscr{F}_m\right] \ge X_m, \quad \text{a.s.} \tag{2}$$

then $\{X_n\}$ is called a <u>sub-martingale (submg)</u> while if things are getting worse on the average

$$\mathbb{E}\left[X_n \mid \mathscr{F}_m\right] \le X_m, \quad \text{a.s.} \tag{3}$$

 ${X_n}$ is called a *super-martingale* (*supermg*).

- Remark $\{X_n\}$ is martingale if it is both a sub and supermartingale. $\{X_n\}$ is a supermartingale if and only if $\{-X_n\}$ is a submartingale.
- Remark If $\{X_n\}$ is a martingale, then $\mathbb{E}[X_n]$ is constant. In the case of a submartingale, the mean increases and for a supermartingale, the mean decreases.
- Proposition 1.1 [Resnick, 2013] If $\{(X_n, \mathscr{F}_n), n \geq 0\}$ is a (sub, super) martingale, then

$$\{(X_n, \sigma(X_0, X_1, \dots, X_n)), n \ge 0\}$$

is also a (sub, super) martingale.

- Definition (Martingale Differences). [Resnick, 2013] $\{(d_j, \mathcal{B}_j), j \geq 0\}$ is a <u>(sub, super) martingale difference sequence</u> or a (sub, super) fair sequence if
 - 1. For $j \geq 0$, $\mathscr{B}_j \subset \mathscr{B}_{j+1}$.
 - 2. For $j \geq 0$, $d_j \in L_1$, $d_j \in \mathcal{B}_j$; that is, d_j is absolutely integrable and \mathcal{B}_j -measurable.
 - 3. For $j \geq 0$,

$$\mathbb{E}[d_{j+1}|\mathcal{B}_j] = 0,$$
 (martingale difference / fair sequence);
 $\geq 0,$ (submartingale difference / subfair sequence);
 $< 0,$ (supmartingale difference / supfair sequence)

• Proposition 1.2 (Construction of Martingale From Martingale Difference)[Resnick, 2013]

If $\{(d_j, \mathcal{B}_j), j \geq 0\}$ is (sub, super) martingale difference sequence, and

$$X_n = \sum_{j=0}^n d_j,$$

then $\{(X_n, \mathcal{B}_n), n \geq 0\}$ is a (sub, super) martingale.

• Proposition 1.3 (Construction of Martingale Difference From Martingale) [Resnick, 2013]

Suppose $\{(X_n, \mathcal{B}_n), n \geq 0\}$ is a **(sub, super) martingale**. Define

$$d_0 := X_0 - \mathbb{E}[X_0]$$

 $d_j := X_j - X_{j-1}, \quad j \ge 1.$

Then $\{(d_j, \mathcal{B}_j), j \geq 0\}$ is a (sub, super) martingale difference sequence.

• Proposition 1.4 (Orthogonality of Martingale Differences). [Resnick, 2013] If $\{(X_n, \mathcal{B}_n), n \geq 0\}$ is a martingale where X_n can be decomposed as

$$X_n = \sum_{j=0}^n d_j,$$

 d_j is \mathscr{B}_j -measurable and $\mathbb{E}[d_j^2] < \infty$ for $j \geq 0$, then $\{d_j\}$ are **orthogonal**:

$$\mathbb{E}\left[d_i\,d_j\right] = 0 \quad i \neq j.$$

Proof: This is an easy verification: If j > i, then

$$\mathbb{E} [d_i d_j] = \mathbb{E} [\mathbb{E} [d_i d_j | \mathscr{B}_i]]$$
$$= \mathbb{E} [d_i \mathbb{E} [d_j | \mathscr{B}_i]] = 0. \quad \blacksquare$$

A consequence is that

$$\mathbb{E}\left[X_n^2\right] = \mathbb{E}\left[\sum_{i=1}^n d_i^2\right] + 2\sum_{0 \le i < j \le n} \mathbb{E}\left[d_i d_j\right] = \mathbb{E}\left[\sum_{i=1}^n d_i^2\right],$$

which is **non-decreasing**. From this, it seems likely (and turns out to be true) that $\{X_n^2\}$ is a **sub-martingale**.

• Example (Smoothing as Martingale) Suppose $X \in L_1$ and $\{\mathscr{B}_n, n \geq 0\}$ is an increasing family of sub σ -algebra of \mathscr{B} . Define for $n \geq 0$

$$X_n := \mathbb{E}\left[X|\mathscr{B}_n\right].$$

Then (X_n, \mathcal{B}_n) is a *martingale*. From this result, we see that $\{(d_n, \mathcal{B}_n), n \geq 0\}$ is a *martingale difference sequence* when

$$d_n := \mathbb{E}\left[X|\mathscr{B}_n\right] - \mathbb{E}\left[X|\mathscr{B}_{n-1}\right], \quad n \ge 1. \tag{4}$$

Proof: See that

$$\mathbb{E}\left[X_{n+1}|\mathscr{B}_n\right] = \mathbb{E}\left[\mathbb{E}\left[X|\mathscr{B}_{n+1}\right]|\mathscr{B}_n\right]$$

$$= \mathbb{E}\left[X|\mathscr{B}_n\right] \qquad \text{(Smoothing property of conditional expectation)}$$

$$= X_n \quad \blacksquare$$

 $\bullet \ {\bf Example} \ ({\it Sums} \ of \ Independent \ Random \ Variables) \\$

Suppose that $\{Z_n, n \geq 0\}$ is an *independent* sequence of integrable random variables satisfying for $n \geq 0$, $\mathbb{E}[Z_n] = 0$. Set

$$X_0 := 0,$$

$$X_n := \sum_{i=1}^n Z_i, \quad n \ge 1$$

$$\mathscr{B}_n := \sigma(Z_0, \dots, Z_n).$$

Then $\{(X_n, \mathcal{B}_n), n \geq 0\}$ is a martingale since $\{(Z_n, \mathcal{B}_n), n \geq 0\}$ is a martingale difference sequence.

• Example (*Likelihood Ratios*).

Suppose $\{Y_n, n \geq 0\}$ are *independent identically distributed* random variables and suppose the true density of Y_n is f_0 (The word "density" can be understood with respect to some fixed reference measure μ .) Let f_1 be some other probability density. For simplicity suppose $f_0(y) > 0$, for all y. For $n \geq 0$, define the likelihood ratio

$$X_n := \frac{\prod_{i=0}^n f_1(Y_i)}{\prod_{i=0}^n f_0(Y_i)}$$
$$\mathscr{B}_n := \sigma(Y_0, \dots, Y_n)$$

Then (X_n, \mathcal{B}_n) is a **martingale**.

Proof: See that

$$\mathbb{E}\left[X_{n+1}|\mathscr{B}_{n}\right] = \mathbb{E}\left[\left(\frac{\prod_{i=0}^{n} f_{1}(Y_{i})}{\prod_{i=0}^{n} f_{0}(Y_{i})}\right) \frac{f_{1}(Y_{n+1})}{f_{0}(Y_{n+1})} \mid Y_{0}, \dots, Y_{n}\right]$$

$$= X_{n} \mathbb{E}\left[\frac{f_{1}(Y_{n+1})}{f_{0}(Y_{n+1})} \mid Y_{0}, \dots, Y_{n}\right]$$

$$= X_{n} \mathbb{E}\left[\frac{f_{1}(Y_{n+1})}{f_{0}(Y_{n+1})}\right] \quad \text{(by independence)}$$

$$:= X_{n} \int \frac{f_{1}(y_{n+1})}{f_{0}(y_{n+1})} f_{0}(y_{n+1}) d\mu(y_{n+1}) = X_{n}.$$

1.2 Bernstein Inequality for Martingale Difference Sequence

• Proposition 1.5 (Bernstein Inequality, Martingale Difference Sequence Version)
[Wainwright, 2019]

Let $\{(D_k, \mathcal{B}_k), k \geq 1\}$ be a martingale difference sequence, and suppose that

$$\mathbb{E}\left[\exp\left(\lambda D_{k}\right) \middle| \mathscr{B}_{k-1}\right] \leq \exp\left(\frac{\lambda^{2} \nu_{k}^{2}}{2}\right)$$

almost surely for any $|\lambda| < 1/\alpha_k$. Then the following hold:

1. The sum $\sum_{k=1}^{n} D_k$ is **sub-exponential** with **parameters** $\left(\sqrt{\sum_{k=1}^{n} \nu_k^2}, \alpha_*\right)$ where $\alpha_* := \max_{k=1,...,n} \alpha_k$. That is, for any $|\lambda| < 1/\alpha_*$,

$$\mathbb{E}\left[\exp\left\{\lambda\left(\sum_{k=1}^{n}D_{k}\right)\right\}\right] \leq \exp\left(\frac{\lambda^{2}\sum_{k=1}^{n}\nu_{k}^{2}}{2}\right)$$

2. The sum satisfies the concentration inequality

$$\mathbb{P}\left\{\left|\sum_{k=1}^{n} D_{k}\right| \geq t\right\} \leq \begin{cases}
2\exp\left(-\frac{t^{2}}{2\sum_{k=1}^{n} \nu_{k}^{2}}\right) & \text{if } 0 \leq t \leq \frac{\sum_{k=1}^{n} \nu_{k}^{2}}{\alpha_{*}} \\
2\exp\left(-\frac{t}{\alpha_{*}}\right) & \text{if } t > \frac{\sum_{k=1}^{n} \nu_{k}^{2}}{\alpha_{*}}.
\end{cases}$$
(5)

Proof: We follow the standard approach of controlling the moment generating function of $\sum_{k=1}^{n} D_k$, and then applying the Chernoff bound. For any scalar λ such that $|\lambda| < 1/\alpha_*$, conditioning on \mathcal{B}_{n-1} and applying iterated expectation yields

$$\mathbb{E}\left[\exp\left\{\lambda\left(\sum_{k=1}^{n}D_{k}\right)\right\}\right] = \mathbb{E}\left[\exp\left\{\lambda\left(\sum_{k=1}^{n-1}D_{k}\right)\right\}\mathbb{E}\left[\exp\left\{\lambda D_{n}\right\} \mid \mathcal{B}_{n-1}\right]\right]$$

$$\leq \mathbb{E}\left[\exp\left\{\lambda\left(\sum_{k=1}^{n-1}D_{k}\right)\right\}\right]\exp\left(\frac{\lambda^{2}\nu_{k}^{2}}{2}\right),$$

where the inequality follows from the stated assumption on D_n . Iterating this procedure yields the bound $\mathbb{E}\left[\exp\left\{\lambda\left(\sum_{k=1}^n D_k\right)\right\}\right] \leq \exp\left(\frac{\lambda^2\sum_{k=1}^n \nu_k^2}{2}\right)$, valid for all $|\lambda| < 1/\alpha_*$. By definition, we conclude that $\sum_{k=1}^n D_k$ is sub-exponential with parameters $\left(\sqrt{\sum_{k=1}^n \nu_k^2}, \alpha_*\right)$, as claimed. The tail bound (5) follows by properties of sub-exponential distribution.

• Remark This result is a generalization of the Bernstein's inequality when $\{D_k\}$ are independent sub-exponential distributed random variables.

The proof used the property of conditional expectation

$$\mathbb{E}\left[\mathbb{E}\left[X|\mathscr{B}_{n}\right]\right] = \mathbb{E}\left[X\right], \quad \mathbb{E}\left[h(X)g(Y)|Y\right] \stackrel{a.s.}{=} h(X)\mathbb{E}\left[g(Y)|Y\right]$$

1.3 Azuma-Hoeffding Inequality

• Corollary 1.6 (Azuma-Hoeffding Inequality, Martingale Difference) [Wainwright, 2019] Let $\{(D_k, \mathcal{B}_k), k \geq 1\}$ be a martingale difference sequence for which there are constants $\{(a_k, b_k)\}_{k=1}^n$ such that $D_k \in [a_k, b_k]$ almost surely for all $k = 1, \ldots, n$. Then, for all $t \geq 0$,

$$\mathbb{P}\left\{ \left| \sum_{k=1}^{n} D_k \right| \ge t \right\} \le 2 \exp\left(-\frac{2t^2}{\sum_{k=1}^{n} (b_k - a_k)^2}\right) \tag{6}$$

1.4 McDiarmid's Inequality

• An important application of Azuma-Hoeffding Inequality concerns functions that satisfy a bounded difference property.

Definition (Functions with Bounded Difference Property)

Given vectors $x, x' \in \mathcal{X}^n$ and an index $k \in \{1, 2, ..., n\}$, we define a new vector $x^{(-k)} \in \mathcal{X}^n$ via

$$x_j^{(-k)} = \begin{cases} x_j & j \neq k \\ x_k' & j = k \end{cases}$$

With this notation, we say that $f: \mathcal{X}^n \to \mathbb{R}$ satisfies <u>the bounded difference inequality</u> with parameters (L_1, \ldots, L_n) if, for each index $k = 1, 2, \ldots, n$,

$$\left| f(x) - f(x^{(-k)}) \right| \le L_k, \quad \text{for all } x, x' \in \mathcal{X}^n.$$
 (7)

• Corollary 1.7 (McDiarmid's Inequality / Bounded Differences Inequality)[Wainwright, 2019]

Suppose that f satisfies **the bounded difference property** (7) with parameters (L_1, \ldots, L_n) and that the random vector $X = (X_1, X_2, \ldots, X_n)$ has **independent** components. Then

$$\mathbb{P}\left\{|f(X) - \mathbb{E}\left[f(X)\right]| \ge t\right\} \le 2\exp\left(-\frac{2t^2}{\sum_{k=1}^n L_k^2}\right). \tag{8}$$

Proof: Consider the associated martingale difference sequence

$$D_k := \mathbb{E}\left[f(X)|X_1,\ldots,X_k| - \mathbb{E}\left[f(X)|X_1,\ldots,X_{k-1}|\right]\right].$$

We claim that D_k lies in an interval of length at most L_k almost surely. In order to prove this claim, define the random variables

$$A_k := \inf_{x} \left\{ \mathbb{E} \left[f(X) | X_1, \dots, X_{k-1}, x \right] \right\} - \mathbb{E} \left[f(X) | X_1, \dots, X_{k-1} \right]$$

$$B_k := \sup \left\{ \mathbb{E} \left[f(X) | X_1, \dots, X_{k-1}, x \right] \right\} - \mathbb{E} \left[f(X) | X_1, \dots, X_{k-1} \right].$$

On one hand, we have

$$D_k - A_k = \mathbb{E}[f(X)|X_1, \dots, X_k] - \inf_{x \in \mathbb{R}} \{\mathbb{E}[f(X)|X_1, \dots, X_{k-1}, x]\},$$

so that $D_k \geq A_k$ almost surely. A similar argument shows that $D_k \leq B_k$ almost surely. We now need to show that $B_k - A_k \leq L_k$ almost surely. Observe that by the independence of $\{X_k\}_{k=1}^n$, we have

$$\mathbb{E}[f(X) | x_1, \dots, x_k] = \mathbb{E}_{(k+1)}[f(x_1, \dots, x_k, X_{k+1}, \dots, X_n)], \text{ for any } (x_1, \dots, x_k),$$

where $\mathbb{E}_{(k+1)}[\cdot]$ denote the expectation over (X_{k+1},\ldots,X_n) . Consequently, we have

$$B_{k} - A_{k} = \sup_{x} \mathbb{E}_{(k+1)} \left[f(X_{1}, \dots, X_{k-1}, x, X_{k+1}, \dots, X_{n}) \right]$$

$$- \inf_{x} \mathbb{E}_{(k+1)} \left[f(X_{1}, \dots, X_{k-1}, x, X_{k+1}, \dots, X_{n}) \right]$$

$$\leq \sup_{x,y} \left\{ \mathbb{E}_{(k+1)} \left[f(X_{1:k-1}, x, X_{k+1:n}) \right] - \mathbb{E}_{(k+1)} \left[f(X_{1:k-1}, y, X_{k+1:n}) \right] \right\}$$

$$< L_{k},$$

using the bounded differences assumption. Thus, the variable D_k lies within an interval of length L_k at most surely, so that the claim follows as a corollary of the Azuma-Hoeffding inequality.

1.5 Applications

• Example (*U-Statistics*) [Wainwright, 2019] Let $g: \mathbb{R}^2 \to \mathbb{R}$ be a *symmetric function* of its arguments. Given an i.i.d. sequence $\{X_k, k \geq 1\}$, of random variables, the quantity

$$U := \frac{1}{\binom{n}{2}} \sum_{j < k} g(X_j, X_k) \tag{9}$$

is known as a *pairwise U-statistic*. For instance, if g(s,t) = |s-t|, then U is an *unbiased* estimator of the mean absolute pairwise deviation $\mathbb{E}[|X_1X_2|]$. Note that, while U is **not** a sum of independent random variables, the dependence is relatively weak, and this fact can be revealed by a martingale analysis.

If g is bounded (say $||g||_{\infty} \leq b$), then the Bounded Difference Inequality can be used to establish the concentration of U around its mean. Viewing U as a function $f(x) = f(x_1, \ldots, x_n)$, for any given coordinate k, we have

$$\left| f(x) - f(x^{(-k)}) \right| \le \frac{1}{\binom{n}{2}} \sum_{j \neq k} \left| g(x_j, x_k) - g(x_j, x_k') \right|$$
$$\le \frac{(n-1)2b}{\binom{n}{2}} = \frac{4b}{n},$$

so that the bounded differences property holds with parameter $L_k = \frac{4b}{n}$ in each coordinate. Thus, we conclude that

$$\mathbb{P}\left\{|U - \mathbb{E}\left[U\right]| \ge t\right\} \le 2\exp\left(-\frac{n\,t^2}{8b^2}\right),$$

This tail inequality implies that U is a consistent estimate of $\mathbb{E}[U]$, and also yields finite sample bounds on its quality as an estimator. Similar techniques can be used to obtain tail bounds on U-statistics of higher order, involving sums over k-tuples of variables.

• Example (Clique Number in Erdös-Rényi Random Graphs) [Wainwright, 2019] Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be an undirected graph, where $\mathcal{V} = \{1, \ldots, d\}$ is the vertex set and $\mathcal{E} = \{(i, j), i, j \in \mathcal{V}\}$ is the undirected edge set. A graph clique C is a subset of vertices such that $(i, j) \in \mathcal{E}$ for all $i, j \in C$. The clique number $C(\mathcal{G})$ of the graph is the cardinality of the largest clique. Note that $C(\mathcal{G}) \in [1, d]$. When the edges \mathcal{E} of the graph are drawn according to some random process, then the clique number $C(\mathcal{G})$ is a random variable, and we can study its concentration around its mean $\mathbb{E}[C(\mathcal{G})]$.

The Erdös-Rényi ensemble of random graphs is one of the most well-studied models: it is defined by a parameter $p \in (0,1)$ that specifies the probability with which each edge (i,j) is included in the graph, independently across all $\binom{d}{2}$ edges. More formally, for each i < j, let us introduce a Bernoulli edge-indicator variable $X_{i,j}$ with parameter p, where $X_{i,j} = 1$ means that edge (i,j) is included in the graph, and $X_{i,j} = 0$ means that it is not included.

Note that the $\binom{d}{2}$ -dimensional random vector $Z := \{X_{i,j}\}_{i < j}$ specifies the edge set; thus, we may view the clique number $C(\mathcal{G})$ as a function $Z \to f(Z)$. Based on definition in Section 2.3, we see that f(Z) is a **configuration function** with property of "being in a clique".

Let Z' denote a vector in which a *single coordinate* of Z has been changed, and let \mathcal{G}' and \mathcal{G} be the associated graphs. It is easy to see that $C(\mathcal{G}')$ can differ from $C(\mathcal{G})$ by at most 1, so that

$$\left| f(Z) - f(Z') \right| \le 1,$$

Thus, the function $C(\mathcal{G}) = f(Z)$ satisfies the bounded difference property in each coordinate with parameter L = 1, so that

$$\mathbb{P}\left\{\frac{1}{n}\left|C(\mathcal{G}) - \mathbb{E}\left[C(\mathcal{G})\right]\right| \ge \delta\right\} \le 2\exp\left(-2n\delta^2\right).$$

Consequently, we see that the clique number of an $Erd\ddot{o}s$ - $R\acute{e}nyi\ random\ graph$ is $very\ sharply\ concentrated\ around\ its\ expectation.$

• Example (Rademacher Complexity) [Wainwright, 2019] Let $\{\epsilon_k\}_{k=1}^n$ be an i.i.d. sequence of Rademacher variables (i.e., taking the values $\{-1,+1\}$ equiprobably). Given a collection of vectors $\mathcal{A} \subset \mathbb{R}^n$, define the random variable

$$Z := \sup_{a \in \mathcal{A}} \sum_{k=1}^{n} \epsilon_k a_k = \sup_{a \in \mathcal{A}} \langle a, \epsilon \rangle.$$
 (10)

The random variable Z measures the size of A in a certain sense, and its expectation

$$\mathfrak{R}(\mathcal{A}) := \mathbb{E}\left[Z(\mathcal{A})\right] \tag{11}$$

is known as the Rademacher complexity of the set A.

Let us now show how the bounded difference inequality can be used to establish that Z(A) is **sub-Gaussian**. Viewing Z(A) as a function $(\epsilon_1, \ldots, \epsilon_n) \to f(\epsilon_1, \ldots, \epsilon_n)$, we need to bound the maximum change when coordinate k is changed. Given two Rademacher vectors $\epsilon, \epsilon' \in \{-1, +1\}^n$, recall our definition of the modified vector $\epsilon^{(-k)}$. Since

$$f(\epsilon^{(-k)}) \ge \langle a, \epsilon^{(-k)} \rangle$$
, for any $a \in \mathcal{A}$,

we have

$$\langle a, \epsilon \rangle - f(\epsilon^{(-k)}) \le \langle a, \epsilon - \epsilon^{(-k)} \rangle = a_k(\epsilon_k - \epsilon'_k) \le 2 |a_k|.$$

Taking the supremum over A on both sides, we obtain the inequality

$$f(\epsilon) - f(\epsilon^{(-k)}) \le 2 \sup_{a \in \mathcal{A}} |a_k|.$$

Since the same argument applies with the roles of ϵ and $\epsilon^{(-k)}$ reversed, we conclude that f satisfies the bounded difference inequality in coordinate k with parameter $L_k := 2 \sup_{a \in \mathcal{A}} |a_k|$.

Consequently, the bounded difference inequality implies that the random variable $Z(\mathcal{A})$ is sub-Gaussian with parameter at most $2\sqrt{\sum_{k=1}^n\sup_{a\in\mathcal{A}}a_k^2}$. This sub-Gaussian parameter can be reduced to the (potentially much) smaller quantity $\sqrt{\sup_{a\in\mathcal{A}}\sum_{k=1}^na_k^2}$ using alternative techniques.

2 Bounding Variance

2.1 The Efron-Stein Inequality

• **Remark** Let X be a random variable with finite variance Var(X). By Chebyshev's Inequality, for any t > 0, we have

$$\mathbb{P}\left\{|X - \mathbb{E}\left[X\right]| \ge t\right\} \le \frac{\operatorname{Var}(X)}{t^2}.$$

Thus, we can obtain the tail probability by bounding the variance Var(X).

• Remark (Variance of Independence Random Variables)
Let $X_n = \sum_{i=1}^n Z_i$ be the sum of independent real-valued random variables Z_1, \ldots, Z_n .
Then we have

$$\mathbb{E}\left[\left(X_n - \mathbb{E}\left[X_n\right]\right)^2\right] = \sum_{i=1}^n \mathbb{E}\left[\left(Z_i - \mathbb{E}\left[Z_i\right]\right)^2\right]$$
$$\Rightarrow \operatorname{Var}(X_n) = \sum_{i=1}^n \operatorname{Var}(Z_i).$$

• Remark (Variance of Smoothing Martingale Difference Sequence) Suppose $X \in L_1$ and $\{\mathscr{B}_n, n \geq 0\}$ is an increasing family of sub σ -algebra of \mathscr{B} formed by

$$\mathscr{B}_n := \sigma(Z_1,\ldots,Z_n)$$
.

For $n \geq 1$, define

$$\begin{aligned} d_0 &:= \mathbb{E} \left[X \right] \\ d_n &:= \mathbb{E} \left[X | \mathscr{B}_n \right] - \mathbb{E} \left[X | \mathscr{B}_{n-1} \right] \\ &= \mathbb{E} \left[X | Z_1, \dots, Z_n \right] - \mathbb{E} \left[X | Z_1, \dots, Z_{n-1} \right]. \end{aligned}$$

From (4) we see that (d_n, \mathcal{B}_n) is a martingale difference sequence. By orthogonality of martingale difference, we see that

$$\mathbb{E}\left[d_i \, d_i\right] = 0 \quad i \neq j.$$

Therefore, based on the decomposition

$$X - EX = \sum_{i=1}^{n} d_i$$

we have

$$\operatorname{Var}(X) = \mathbb{E}\left[\left(\sum_{i=1}^{n} d_{i}\right)^{2}\right] = \sum_{i=1}^{n} \mathbb{E}\left[d_{i}^{2}\right] + 2\sum_{i>j} \mathbb{E}\left[d_{i} d_{j}\right]$$
$$= \sum_{i=1}^{n} \mathbb{E}\left[d_{i}^{2}\right]. \tag{12}$$

• Remark (Variance of General Functions of Independent Random Variables)

Then above formula (12) holds when $X = f(Z_1, ..., Z_n)$ for general function $f: \mathbb{R}^n \to \mathbb{R}$ with n independent random variables $(Z_1, ..., Z_n)$. By Fubini's theorem,

$$\mathbb{E}[X|Z_1, \dots, Z_i] = \int_{\mathcal{Z}^{n-i}} f(Z_1, \dots, Z_i, z_{i+1}, \dots, z_n) \ d\mu_{i+1}(z_{i+1}) \dots d\mu_n(z_n)$$

where μ_j is the probability distribution of Z_j for $j \geq 1$.

Let $Z_{(-i)} := (Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$ be all random variables (Z_1, \ldots, Z_n) except for Z_i . Denote $\mathbb{E}_{(-i)}[\cdot]$ as the conditional expectation of X given $Z_{(-i)}$

$$\mathbb{E}_{(-i)}[X] := \mathbb{E}[X|Z_1, \dots, Z_{i-1}, Z_{i+1}, \dots, Z_n]$$
$$= \int_{\mathcal{Z}} f(Z_1, \dots, Z_{i-1}, z_i, Z_{i+1}, \dots, Z_n) \ d\mu_i(z_i).$$

Then, again by Fubini's theorem (smoothing properties of conditional expectation),

$$\mathbb{E}\left[\mathbb{E}_{(-i)}\left[X\right]|Z_1,\ldots,Z_i\right] = \mathbb{E}\left[X|Z_1,\ldots,Z_{i-1}\right] \tag{13}$$

• Proposition 2.1 (Efron-Stein Inequality) [Boucheron et al., 2013] Let Z_1, \ldots, Z_n be independent random variables and let X = f(Z) be a square-integrable function of $Z = (Z_1, \ldots, Z_n)$. Then

$$Var(X) \le \sum_{i=1}^{n} \mathbb{E}\left[\left(X - \mathbb{E}_{(-i)}\left[X\right]\right)^{2}\right] := \nu. \tag{14}$$

Moreover, if Z'_1, \ldots, Z'_n are **independent** copies of Z_1, \ldots, Z_n and if we define, for every $i = 1, \ldots, n$,

$$X'_{i} := f(Z_{1}, \ldots, Z_{i-1}, Z'_{i}, Z_{i+1}, \ldots, Z_{n}),$$

then

$$\nu = \frac{1}{2} \sum_{i=1}^{n} \mathbb{E} \left[\left(X - X_{i}' \right)^{2} \right] = \sum_{i=1}^{n} \mathbb{E} \left[\left(X - X_{i}' \right)_{+}^{2} \right] = \sum_{i=1}^{n} \mathbb{E} \left[\left(X - X_{i}' \right)_{-}^{2} \right]$$

where $x_{+} = \max\{x, 0\}$ and $x_{-} = \max\{-x, 0\}$ denote the **positive** and **negative** parts of a real number x. Also,

$$\nu = \inf_{X_i} \sum_{i=1}^n \mathbb{E}\left[(X - X_i)^2 \right],$$

where the infimum is taken over the class of all $Z_{(-i)}$ -measurable and square-integrable variables X_i , i = 1, ..., n.

Proof: We begin with the proof of the first statement. Note that, using (13), we may write

$$d_{i} := \mathbb{E}\left[X|Z_{1}, \dots, Z_{i}\right] - \mathbb{E}\left[X|Z_{1}, \dots, Z_{i-1}\right]$$

$$= \mathbb{E}\left[X|Z_{1}, \dots, Z_{i}\right] - \mathbb{E}\left[\mathbb{E}_{(-i)}\left[X\right]|Z_{1}, \dots, Z_{i}\right]$$

$$= \mathbb{E}\left[X - \mathbb{E}_{(-i)}\left[X\right]|Z_{1}, \dots, Z_{i}\right].$$

By Jensen's inequality used conditionally,

$$d_i^2 \leq \mathbb{E}\left[\left(X - \mathbb{E}_{(-i)}\left[X\right]\right)^2 | Z_1, \dots, Z_i\right]$$

Using (12) $\operatorname{Var}(X) = \sum_{i=1}^n \mathbb{E}\left[d_i^2\right]$, we have

$$\operatorname{Var}(X) \leq \sum_{i=1}^{n} \mathbb{E}\left[\mathbb{E}\left[\left(X - \mathbb{E}_{(-i)}\left[X\right]\right)^{2} | Z_{1}, \dots, Z_{i}\right]\right] = \sum_{i=1}^{n} \mathbb{E}\left[\left(X - \mathbb{E}_{(-i)}\left[X\right]\right)^{2}\right],$$

we obtain the desired inequality.

To prove the identities for ν , denote by $\operatorname{Var}_{(-i)}$ the *conditional variance operator* conditioned on $Z_{(-i)} := (Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$. Then we may write ν as

$$\nu = \sum_{i=1}^{n} \mathbb{E} \left[\operatorname{Var}_{(-i)}(X) \right].$$

Now note that one may simply use (conditionally) the elementary fact that if X and Y are independent and identically distributed real-valued random variables, then

$$\operatorname{Var}(X) = \frac{1}{2} \mathbb{E}\left[(X - Y)^2 \right].$$

Since conditionally on $Z_{(-i)}$, X'_i is an independent copy of X, we may write

$$\operatorname{Var}_{(i)}(X) = \frac{1}{2} \mathbb{E}_{(-i)} \left[\left(X - X_i' \right)^2 \right] = \sum_{i=1}^n \mathbb{E}_{(-i)} \left[\left(X - X_i' \right)_+^2 \right] = \sum_{i=1}^n \mathbb{E}_{(-i)} \left[\left(X - X_i' \right)_-^2 \right],$$

where we used the fact that the conditional distributions of X and X'_i are identical.

The last identity is obtained by recalling that, for any real-valued random variable X,

$$\operatorname{Var}(X) = \inf_{a \in \mathbb{R}} \mathbb{E}\left[(X - a)^2 \right].$$

Using this fact conditionally, we have, for every i = 1, ..., n,

$$\operatorname{Var}_{(-i)}(X) = \inf_{X_i} \mathbb{E}_{(-i)} \left[(X - X_i)^2 \right].$$

Note that this infimum is achieved whenever $X_i = \mathbb{E}_{(-i)}[X]$.

• Example (*The Jackknife Estimate*)

We should note here that the Efron-Stein inequality was first motivated by the study of the so-called *jackknife estimate* of *statistics*.

To describe this estimate, assume that Z_1, \ldots, Z_n are i.i.d. random variables and one wishes to estimate a functional θ of the distribution of the Z_i by a function $X = f(Z_1, \ldots, Z_n)$ of the data. The quality of the estimate is often measured by its bias $\mathbb{E}[X] - \theta$ and its variance $\operatorname{Var}(X)$. Since the distribution of the Z_i 's is unknown, one needs to estimate the bias and variance from the same sample. The jackknife estimate of the bias is defined by

$$(n-1)\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}-X\right) \tag{15}$$

where X_i is an appropriately defined function of $Z_{(-i)} := (Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$. $Z_{(-i)}$ is often called **the** *i*-**th jackknife sample** while X_i is the so-called **jackknife replication** of X. In an analogous way, **the jackknife estimate** of the **variance** is defined by

$$\sum_{i=1}^{n} (X - X_i)^2 \tag{16}$$

Using this language, the Efron-Stein inequality simply states that the jackknife estimate of the variance is <u>always positively biased</u>. In fact, this is how Efron and Stein originally formulated their inequality.

• Remark Observe that in the case when $X = \sum_{i=1}^{n} Z_i$ is a sum of independent random variables (with finite variance), then the Efron-Stein inequality becomes an equality. Thus, the bound in the Efron-Stein inequality is, in a sense, not improvable.

2.2 Functions with Bounded Differences

• Remark Recall that a function $f: \mathcal{X}^n \to \mathbb{R}$ satisfies the bounded difference inequality with parameters (L_1, \ldots, L_n) if, for each index $k = 1, 2, \ldots, n$,

$$\left| f(z) - f(z^{(-k)}) \right| \le L_k$$
, for all $z, z' \in \mathcal{X}^n$.

where

$$z_j^{(-k)} = \begin{cases} z_j & j \neq k \\ z_k' & j = k \end{cases}$$

• Corollary 2.2 [Boucheron et al., 2013] If f has the **bounded differences property** with parameters (L_1, \ldots, L_n) , then

$$Var(f(Z)) \leq \frac{1}{4} \sum_{i=1}^{n} L_i^2.$$

Proof: From the Efron-Stein inequality,

$$\operatorname{Var}(f(Z)) \leq \sum_{i=1}^{n} \mathbb{E}\left[\operatorname{Var}_{(-i)}(f(Z))\right]$$
$$= \inf_{X_i} \sum_{i=1}^{n} \mathbb{E}_{(-i)}\left[\left(f(Z) - X_i\right)^2\right]$$

where the infimum is taken over the class of all $Z_{(-i)}$ -measurable and square-integrable variables X_i . Here we choose

$$X_{i} = \frac{1}{2} \left(\sup_{z'_{i}} f(Z_{1:i-1}, z'_{i}, Z_{i+1:n}) - \inf_{z'_{i}} f(Z_{1:i-1}, z'_{i}, Z_{i+1:n}) \right)$$

Hence

$$(f(Z) - X_i)^2 \le \frac{1}{4}L_i^2,$$

and the proposition follows.

2.3 Self-Bounding Functions

• Another simple property which is satisfied for many important examples is the so-called self-bounding property.

Definition (Self-Bounding Property)

A nonnegative function $f: \mathcal{X}^n \to [0, \infty)$ has the <u>self-bounding property</u> if there exist functions $f_i: \mathcal{X}^{n-1} \to \mathbb{R}$ such that for all $z_1, \ldots, z_n \in \overline{\mathcal{X}}$ and all $i = 1, \ldots, n$,

$$0 \le f(z_1, \dots, z_n) - f_i(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_n) \le 1$$
(17)

and also

$$\sum_{i=1}^{n} \left(f(z_1, \dots, z_n) - f_i(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_n) \right) \le f(z_1, \dots, z_n). \tag{18}$$

• Remark Clearly if f has the self-bounding property,

$$\sum_{i=1}^{n} \left(f(z_1, \dots, z_n) - f_i(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_n) \right)^2 \le f(z_1, \dots, z_n)$$
(19)

Taking expectation on both sides, we have the following inequality

• Corollary 2.3 [Boucheron et al., 2013] If f has the self-bounding property, then

$$Var(f(Z)) \leq \mathbb{E}[f(Z)].$$

• Remark (*Relative Stability*) [Boucheron et al., 2013] A sequence of nonnegative random variables $(Z_n)_{n\in\mathbb{N}}$ is said to be *relatively stable* if

$$\frac{Z_n}{\mathbb{E}\left[Z_n\right]} \stackrel{\mathbb{P}}{\to} 1.$$

This property guarantees that the random fluctuations of Z_n around its expectation are of negligible size when compared to the expectation, and therefore most information about the size of Z_n is given by $\mathbb{E}[Z_n]$.

Bounding the variance of Z_n by its expected value implies, in many cases, the relative stability of $(Z_n)_{n\in\mathbb{N}}$. If Z_n has the self-bounding property, then, by Chebyshev's inequality, for all $\epsilon > 0$,

$$\mathbb{P}\left\{ \left| \frac{Z_n}{\mathbb{E}\left[Z_n\right]} - 1 \right| > \epsilon \right\} \le \frac{\operatorname{Var}(Z_n)}{\epsilon^2(\mathbb{E}\left[Z_n\right])^2} \le \frac{1}{\epsilon^2 \mathbb{E}\left[Z_n\right]}.$$

Thus, for relative stability, it suffices to have $\mathbb{E}[Z_n] \to \infty$.

• An important class of functions satisfying the self-bounding property consists of the so-called configuration functions.

Definition (Configuration Function)

Assume that we have a property Π defined over the union of finite products of a set \mathcal{X} , that is, a sequence of sets

$$\Pi_1 \subset \mathcal{X}, \ \Pi_2 \subset \mathcal{X} \times \mathcal{X}, \ \dots, \ \Pi_n \subset \mathcal{X}^n.$$

We say that $(z_1, \ldots, z_m) \in \mathcal{X}^m$ satisfies the property Π if $(z_1, \ldots, z_m) \in \Pi_m$.

We assume that Π is **hereditary** in the sense that if (z_1, \ldots, z_m) satisfies Π then so does any sub-sequence $\{\overline{z_{i_1}, \ldots, z_{i_k}}\}$ of (z_1, \ldots, z_m) .

The function f that maps any vector $z = (z_1, \ldots, z_n)$ to **the size** of a **largest sub-sequence** satisfying Π is **the configuration function** associated with property Π .

• Corollary 2.4 [Boucheron et al., 2013]

Let f be a configuration function, and let $X = f(Z_1, ..., Z_n)$, where $Z_1, ..., Z_n$ are independent random variables. Then

$$Var(f(Z)) \leq \mathbb{E}[f(Z)].$$

Proof: It suffices to show that any configuration function is self-bounding. Let $X_i := f(Z_{(-i)}) = f(Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$. By definition of configuration function, the condition $0 \le X - X_i \le 1$ is trivially satisfied.

On the other hand, assume that X = k and let $\{Z_{i_1}, \ldots, Z_{i_k}\} \subset \{Z_1, \ldots, Z_n\}$ be a subsequence of cardinality k such that $f_k(Z_{i_1}, \ldots, Z_{i_k}) = k$. (Note that by the definition of a configuration function such a sub-sequence exists.) Clearly, if the index i is such that $i \notin \{i_1, \ldots, i_k\}$ then $X = X_i$, and therefore

$$\sum_{i=1}^{n} (X - X_i) \le X$$

is also satisfied, which concludes the proof.

• Example (*VC Dimension*)

Let \mathcal{H} be an arbitrary collection of subsets of \mathcal{X} , and let $x = (x_1, \ldots, x_n)$ be a vector of n points of \mathcal{X} . Define the **trace** of \mathcal{H} on x by

$$\operatorname{tr}(x) = \{A \cap \{x_1, \dots, x_n\} : A \in \mathcal{H}\}.$$

The shatter coefficient, (or Vapnik-Chervonenkis growth function) of \mathcal{H} in x is $\tau_{\mathcal{H}}(x) = |\operatorname{tr}(x)|$, the size of the trace. $\tau_{\mathcal{H}}(x)$ is the number of different subsets of the n-point set $\{x_1, \ldots, x_n\}$ generated by intersecting it with elements of \mathcal{H} . A subset $\{x_{i_1}, \ldots, x_{i_k}\}$ of $\{x_1, \ldots, x_n\}$ is said to be **shattered** if $2^k = T(x_{i_1}, \ldots, x_{i_k})$.

The VC dimension D(x) of \mathcal{H} (with respect to x) is the cardinality k of the largest shattered subset of x. From the definition it is obvious that f(x) = D(x) is a **configuration function** (associated with the property of "shatteredness") and therefore if X_1, \ldots, X_n are independent random variables, then

$$Var(D(X)) \le \mathbb{E}[D(X)].$$

2.4 Applications

2.4.1 Kernel Density Estimation

• Example (Kernel Density Estimation)

Let Z_1, \ldots, Z_n be i.i.d. samples drawn according to some (unknown) density ϕ on the real line. The density is estimated by the kernel estimate

$$\phi_n(z) = \frac{1}{n h_n} \sum_{i=1}^n K\left(\frac{z - Z_i}{h_n}\right),\,$$

where $h_n > 0$ is a *smoothing parameter*, and K is a nonnegative function with $\int K(z) = 1$. The performance of the estimate is typically measured by **the** L_1 **error**:

$$X(n) := f(Z_1, ..., Z_n) = \int |\phi(z) - \phi_n(z)| dz.$$

It is easy to see that

$$\left| f(z_1, \dots, z_n) - f_i(z_1, \dots, z_{i-1}, z_i', z_{i+1}, \dots, z_n) \right| \le \frac{1}{nh_n} \int \left| K\left(\frac{z - z_i}{h_n}\right) - K\left(\frac{z - z_i'}{h_n}\right) \right| dz$$

$$\le \frac{2}{n},$$

so without further work we obtain

$$\operatorname{Var}(X(n)) \le \frac{1}{n}$$

It is known that for every ϕ , $\sqrt{n}\mathbb{E}[X(n)] \to \infty$, which implies, by Chebyshev's inequality, that for every $\epsilon > 0$

$$\mathbb{P}\left\{\left|\frac{X(n)}{\mathbb{E}\left[X(n)\right]} - 1\right| > \epsilon\right\} = \mathbb{P}\left\{\left|X(n) - \mathbb{E}\left[X(n)\right]\right| > \epsilon \mathbb{E}\left[X(n)\right]\right\} \le \frac{\mathrm{Var}(X(n))}{\epsilon^2(\mathbb{E}\left[X(n)\right])^2} \to 0$$

as $n \to \infty$. That is, $\frac{X(n)}{\mathbb{E}[X(n)]} \to 1$ in probability, or in other words, X(n) is relatively stable. This means that the random L_1 -error essentially behaves like its expected value.

By bounded difference inequality, we have

$$\mathbb{P}\left\{|X(n) - \mathbb{E}\left[X(n)\right]| \ge t\right\} \le 2\exp\left(-\frac{nt^2}{2}\right) \quad \blacksquare$$

2.4.2 Convex Poincaré Inequality

• Theorem 2.5 (Convex Poincaré Inequality) [Boucheron et al., 2013] Let Z_1, \ldots, Z_n be independent random variables taking values in the interval [0,1] and let $f:[0,1]^n \to \mathbb{R}$ be a separately convex function whose partial derivatives exist; that is, for every $i=1,\ldots,n$ and fixed $z_1,\ldots,z_{i-1},z_{i+1},\ldots,z_n$, f is a convex function of its i-th variable. Then $f(Z)=f(Z_1,\ldots,Z_n)$ satisfies

$$Var(f(Z)) \le \mathbb{E}\left[\|\nabla f(Z)\|_2^2\right].$$
 (20)

Proof: The proof is an easy consequence of the Efron-Stein inequality, because it suffices to bound the random variable $\sum_{i=1}^{n} (X - X_i)^2$ where $X_i := \inf_{z'_i} f(Z_1, \dots, Z_{i-1}, z_i, Z_{i+1}, \dots, Z_n)$. Denote by Z'_i the value of z'_i for which the minimum is achieved. This is guaranteed by **continuity** and the **compactness** of the domain of f. Then, writing $\bar{Z}_{(i)} = (Z_1, \dots, Z_{i-1}, Z'_i, Z_{i+1}, \dots, Z_n)$, we have

$$\sum_{i=1}^{n} (X - X_i)^2 = \sum_{i=1}^{n} (f(Z) - f(\bar{Z}_{(i)}))^2$$

$$\leq \sum_{i=1}^{n} \left(\frac{\partial f}{\partial z_i}(Z)\right)^2 (Z - \bar{Z}_{(i)})^2 \quad (\text{ by separate convexity})$$

$$\leq \sum_{i=1}^{n} \left(\frac{\partial f}{\partial z_i}(Z)\right)^2 = \|\nabla f(Z)\|_2^2. \quad \blacksquare$$

• Remark (Dimension-Free Concentration)

Note that the convex Poincaré inequality provides a dimension-free concentration for an arbitrary sub-Gaussian distribution given that f is separately convex.

2.4.3 Gaussian Poincaré Inequality

• Theorem 2.6 (Gaussian Poincaré Inequality) [Boucheron et al., 2013] Let $Z = (Z_1, ..., Z_n)$ be a vector of i.i.d. standard Gaussian random variables (i.e. Z is a Gaussian vector with zero mean vector and identity covariance matrix). Let $f : \mathbb{R}^n \to \mathbb{R}$ be any continuously differentiable function. Then

$$Var(f(Z)) \le \mathbb{E}\left[\|\nabla f(Z)\|_2^2\right].$$
 (21)

Proof: We may assume that $\mathbb{E}\left[\|\nabla f(Z)\|_2^2\right] < \infty$, since otherwise the inequality is trivial.

The proof is based on a double use of the Efron-Stein inequality. A first straightforward use of it reveals that it suffices to prove the theorem when the dimension n equals 1. Thus, the problem reduces to show that

$$\operatorname{Var}(f(Z)) \le \mathbb{E}\left[(f'(Z))^2 \right],\tag{22}$$

where $f: \mathbb{R} \to \mathbb{R}$ is any continuously differentiable function on the real line and Z is a standard normal random variable.

- 1. First, notice that it suffices to prove this inequality when f has a **compact support** and is **twice continuously differentiable**.
- 2. Now let $\epsilon_1, \ldots, \epsilon_n$ be independent Rademacher random variables and introduce

$$S_n := \frac{1}{\sqrt{n}} \sum_{j=1}^n \epsilon_j.$$

Since for every i

$$\operatorname{Var}_{(-i)}(f(S_n)) = \frac{1}{4} \left(f\left(S_n + \frac{1+\epsilon_i}{\sqrt{n}}\right) - f\left(S_n - \frac{1+\epsilon_i}{\sqrt{n}}\right) \right)^2,$$

applying the Efron-Stein inequality again, we obtain

$$\operatorname{Var}(f(S_n)) \le \frac{1}{4} \sum_{i=1}^n \mathbb{E}\left[\left(f\left(S_n + \frac{1+\epsilon_i}{\sqrt{n}}\right) - f\left(S_n - \frac{1+\epsilon_i}{\sqrt{n}}\right) \right)^2 \right]$$
 (23)

The central limit theorem implies that S_n converges in distribution to Z, where Z has the standard normal law. Hence $Var(f(S_n))$ converges to Var(f(Z)).

3. Let K denote the supremum of the absolute value of the second derivative of f. Taylor's theorem implies that, for every i,

$$\left| f\left(S_n + \frac{1+\epsilon_i}{\sqrt{n}}\right) - f\left(S_n - \frac{1+\epsilon_i}{\sqrt{n}}\right) \right| \le \frac{2}{\sqrt{n}} \left| f'(S_n) \right| + \frac{2K}{n}$$

and therefore

$$\frac{n}{4}\left(f\left(S_n + \frac{1+\epsilon_i}{\sqrt{n}}\right) - f\left(S_n - \frac{1+\epsilon_i}{\sqrt{n}}\right)\right)^2 \le \left(f'(S_n)\right)^2 + \frac{2K}{\sqrt{n}}\left|f'(S_n)\right| + \frac{K^2}{n}$$

This and the central limit theorem imply that

$$\limsup_{n \to \infty} \frac{1}{4} \sum_{i=1}^{n} \mathbb{E} \left[\left(f \left(S_n + \frac{1 + \epsilon_i}{\sqrt{n}} \right) - f \left(S_n - \frac{1 + \epsilon_i}{\sqrt{n}} \right) \right)^2 \right] = \mathbb{E} \left[(f'(Z))^2 \right],$$

which means that (23) leads to (22) by letting n go to infinity.

• Remark (Lipschitz Function of Gaussian Vector)

A straightforward consequence of the Gaussian Poincaré inequality is that, whenever $f: \mathbb{R}^n \to \mathbb{R}$ is L-**Lipschitz**, that is, for all $x, y \in \mathbb{R}^n$,

$$|f(x) - f(y)| < L ||x - y||$$

and Z is a **standard Gaussian** random vector, then

$$Var(f(Z)) \le L. \tag{24}$$

Note that this is independent from the dimensionality of function domain.

2.5 A Proof of the Efron-Stein Inequality Based on Duality

• Proposition 2.7 (Variational Principle for Variance Estimator) [Boucheron et al., 2013]

If Y is a real-valued square-integrable random variable $(Y \in L^2 \text{ in short})$, then

$$Var(Y) = \sup_{T \in L^2} (2Cov(Y, T) - Var(T)). \tag{25}$$

Proof: since $Var(YT) \ge 0$, and

$$Var(Y) \ge 2Cov(Y,T) - Var(T)$$

and since this inequality becomes an equality whenever T = Y, the duality formula follows.

• Remark Let X = f(Z) for $Z = (Z_1, ..., Z_n)$ and define $\mathbb{E}_i[X] := \mathbb{E}[f(Z)|Z_1, ..., Z_i]$. Then consider the telescoping sum

$$(f(Z))^2 - (\mathbb{E}[f(Z)])^2 = \sum_{i=1}^n ((\mathbb{E}_i[f(Z)])^2 - (\mathbb{E}_{i-1}[f(Z)])^2),$$

which leads to

$$Var(f(Z)) = \mathbb{E}\left[(f(Z))^2 \right] - (\mathbb{E}\left[f(Z) \right])^2 = \sum_{i=1}^n \mathbb{E}\left[(\mathbb{E}_i \left[f(Z) \right])^2 - (\mathbb{E}_{i-1} \left[f(Z) \right])^2 \right]$$

Note that $f(Z) - \mathbb{E}\left[f(Z)\right] = \sum_{i=1}^{n} \left(\mathbb{E}_{i}\left[f(Z)\right] - \mathbb{E}_{i-1}\left[f(Z)\right]\right)$

$$\operatorname{Var}(f(Z)) = \mathbb{E}\left[(f(Z) - \mathbb{E}\left[f(Z) \right])^2 \right] = \sum_{i=1}^n \mathbb{E}\left[(\mathbb{E}_i \left[f(Z) \right] - \mathbb{E}_{i-1} \left[f(Z) \right])^2 \right]$$

Thus

$$\sum_{i=1}^{n} \mathbb{E}\left[\left(\mathbb{E}_{i} \left[f(Z) \right] - \mathbb{E}_{i-1} \left[f(Z) \right] \right)^{2} \right] = \sum_{i=1}^{n} \mathbb{E}\left[\left(\mathbb{E}_{i} \left[f(Z) \right] \right)^{2} - \left(\mathbb{E}_{i-1} \left[f(Z) \right] \right)^{2} \right]$$

Similarly to our first proof of the Efron-Stein inequality, the independence of the variables X_1, \ldots, X_n is used by noting that

$$\mathbb{E}_{(-i)}\left[\mathbb{E}_i\left[f(Z)\right]\right] = \mathbb{E}_{i-1}\left[f(Z)\right]$$

and therefore

$$\sum_{i=1}^{n} \mathbb{E}\left[(\mathbb{E}_{i} \left[f(Z) \right])^{2} - (\mathbb{E}_{i-1} \left[f(Z) \right])^{2} \right] = \mathbb{E}\left[\operatorname{Var}_{(-i)}(\mathbb{E}_{i} \left[f(Z) \right]) \right]$$

In other words, we have proven the following alternative formulation (using *independence* but without using the orthogonality structure of the martingale differences):

$$\operatorname{Var}(f(Z)) = \sum_{i=1}^{n} \mathbb{E}\left[\operatorname{Var}_{(-i)}(\mathbb{E}_{i}\left[f(Z)\right])\right]. \tag{26}$$

It remains to commute the $Var_{(-i)}$ and \mathbb{E}_i operators and this is precisely the step where we use a duality argument.

• Lemma 2.8 [Boucheron et al., 2013] For every i = 1, ..., n,

$$\mathbb{E}\left[Var_{(-i)}(\mathbb{E}_i\left[f(Z)\right])\right] \leq \mathbb{E}\left[Var_{(-i)}(f(Z))\right].$$

Proof: Applying the duality formula of (25) conditionally on $Z_{(-i)}$, we show that for any square-integrable variable T,

$$2Cov_{(-i)}(f(Z), T) - Var_{(-i)}(T) \le Var_{(-i)}(f(Z))$$
 (27)

But if we take T to be (Z_1, \ldots, Z_i) -measurable, then

$$\mathbb{E}\left[\operatorname{Cov}_{(-i)}(f(Z),T)\right] = \mathbb{E}\left[f(Z)\left(T - \mathbb{E}_{i}\left[T\right]\right)\right]$$
$$= \mathbb{E}\left[\mathbb{E}_{i}\left[f(Z)\right]\left(T - \mathbb{E}_{i}\left[T\right]\right)\right]$$
$$= \mathbb{E}\left[\operatorname{Cov}_{(-i)}(\mathbb{E}_{i}\left[f(Z)\right],T\right].$$

Hence, choosing $T = \mathbb{E}_i [f(Z)]$ leads to

$$\mathbb{E}\left[\operatorname{Cov}_{(-i)}(f(Z), \mathbb{E}_i[f(Z)])\right] = \mathbb{E}\left[\operatorname{Var}_{(-i)}(\mathbb{E}_i[f(Z)])\right]$$

and therefore, by (27),

$$\mathbb{E}\left[\operatorname{Var}_{(-i)}(\mathbb{E}_i\left[f(Z)\right])\right] \leq \mathbb{E}\left[\operatorname{Var}_{(-i)}(f(Z))\right] \quad \blacksquare$$

• Remark Combining Lemma above with the decomposition (26) leads to

$$\operatorname{Var}(f(Z)) \le \sum_{i=1}^{n} \mathbb{E}\left[\operatorname{Var}_{(-i)}(f(Z))\right]$$
(28)

which is equivalent to the EfronStein inequality.

2.6 Exponential Tail Bounds via the Efron-Stein Inequality

• Remark (Assumption) [Boucheron et al., 2013] Suppose $Z := (Z_1, \ldots, Z_n)$ are independent random variables and X := f(Z). X_i is the *i-th Jackknife replication* of X, which is a function of $Z_{(-i)} := (Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n)$, the *i-th Jackknife sample*.

Assume that there exists a positive constant ν such that

$$\sum_{i=1}^{n} (X - X_i)_+^2 \le \nu \tag{29}$$

holds almost surely. Define, for any $\alpha \in (0,1)$, the α -quantile of X := f(Z) by

$$Q_{\alpha} = \inf \left\{ \alpha : \mathbb{P} \left\{ X \le x \right\} \ge \alpha \right\}.$$

In particular, we denote the **median** of Z by $Med(Z) = Q_{1/2}$.

• Remark (Clipping of Function)

The trick is to use the Efron-Stein inequality for the random variable $g_{a,b}(Z) = g_{a,b}(Z_1, \ldots, Z_n)$ where $b \geq a$ and the function $g_{a,b} : \mathcal{X}^n \to \mathbb{R}$ is defined as

$$g_{a,b}(z) = \begin{cases} b & \text{if } f(z) \ge b \\ f(z) & \text{if } a < f(z) < b \\ a & \text{if } f(z) \le a \end{cases}$$

It is the clipping of function f(z) taking values within [a, b], i.e. $g_{a,b}(z) = \max\{a, \min\{f(z), b\}\}$.

• Remark (Bounding Variance of $g_{a,b}(Z)$)

First observe that if $a \ge \text{Med}(X)$, then $\mathbb{E}[g_{a,b}(Z)] \le (a+b)/2$ and therefore the lower bound of the variance is

$$\operatorname{Var}(g_{a,b}(Z)) \ge \frac{(b-a)^2}{4} \mathbb{P}\{g_{a,b}(Z) = b\} = \frac{(b-a)^2}{4} \mathbb{P}\{f(Z) \ge b\}.$$

On the other hand, we may use the Efron-Stein inequality to obtain an upper bound for the variance of $g_{a,b}(Z)$. To this end, observe that if $f(z) \leq a$ then

$$g_{a,b}(\bar{z}^{(i)}) \ge g_{a,b}(z),$$

for

$$\bar{z}^{(i)} := (z_1, \dots, z_{i-1}, z'_i, z_{i+1}, \dots, z_n)$$

and so

$$\begin{split} \sum_{i=1}^{n} \mathbb{E} \left[\left(g_{a,b}(Z) - g_{a,b}(\bar{Z}^{(i)}) \right)^{2} \right] &= 2 \sum_{i=1}^{n} \mathbb{E} \left[\left(g_{a,b}(Z) - g_{a,b}(\bar{Z}^{(i)}) \right)_{+}^{2} \right] \\ &\leq 2 \sum_{i=1}^{n} \mathbb{E} \left[\mathbb{1} \left\{ f(Z) > a \right\} \left(g_{a,b}(Z) - g_{a,b}(\bar{Z}^{(i)}) \right)_{+}^{2} \right] \\ &\leq 2 \nu \mathbb{P} \left\{ f(Z) > a \right\}, \end{split}$$

where, in the last step, we used the fact that condition (29) implies that

$$\sum_{i=1}^{n} \left(g_{a,b}(Z) - g_{a,b}(\bar{Z}^{(i)}) \right)_{+}^{2} \le \sum_{i=1}^{n} \left(f(Z) - f(\bar{Z}^{(i)}) \right)_{+}^{2} \le \nu.$$

Comparing the obtained upper and lower bounds for $Var(g_{a,b}(Z))$, we get

$$b-a \leq \sqrt{8\nu \frac{\mathbb{P}\left\{f(Z) > a\right\}}{\mathbb{P}\left\{f(Z) \geq b\right\}}}.$$

• Remark (Bounding the Distance between Quantiles of f(Z))

To this end, let $0 < \delta < \gamma \le 1/2$ and choose $a = Q_{1-\gamma}$ and $b = Q_{1-\delta}$. Then $\mathbb{P}\{f(Z) > a\} \le \gamma$ and $\mathbb{P}\{f(Z) \ge b\} \ge \delta$ and therefore the distance between any two quantiles of X = f(Z) (to the *right* of the median) can be *bounded* as

$$b - a = Q_{1 - \delta} - Q_{1 - \gamma} \le \sqrt{\frac{8\nu\gamma}{\delta}}$$

It is instructive to choose $\gamma = 2^{-k}$ and $\delta = 2^{-(k+1)}$ for some integer $k \geq 1$. Then, denoting $a_k = Q_{1-2^{-k}}$, we get

$$a_{k+1} - a_k \le 4\sqrt{\nu},$$

so the difference between consecutive quantiles corresponding to exponentially decreasing tail probabilities is bounded by a constant. In particular, by summing this inequality for $k = 1, \ldots, m$, we have

$$a_{m+1} \le \operatorname{Med}(f(Z)) + 4m\sqrt{\nu}$$

which implies that for all t > 0,

$$\mathbb{P}\left\{f(Z) > \operatorname{Med}(f(Z)) + t\right\} \le 2^{-\frac{t}{4\sqrt{\nu}}}.$$
(30)

• Remark (Bounding the Deviations from Mean instead of Median of f(Z))
An alternative route to obtain exponential bounds is by applying the Efron-Stein inequality to $\exp(\lambda X/2)$ with $\lambda > 0$. Then, by the mean-value theorem,

$$\mathbb{E}\left[\exp\left(\lambda X\right)\right] - \left(\mathbb{E}\left[\exp\left(\frac{\lambda X}{2}\right)\right]\right)^{2} \leq \mathbb{E}\left[\sum_{i=1}^{n} \left(\exp\left(\frac{\lambda X}{2}\right) - \exp\left(\frac{\lambda X'}{2}\right)\right)_{+}^{2}\right]$$
 (Efron-Stein inequality)
$$\leq \frac{\lambda^{2}}{4} \mathbb{E}\left[\exp\left(\lambda X\right) \sum_{i=1}^{n} \left(X - X'\right)_{+}^{2}\right]$$
 (mean-value theorem)

Now we may use our condition (29) to derive

$$\mathbb{E}\left[\exp\left(\lambda X\right)\right] - \left(\mathbb{E}\left[\exp\left(\frac{\lambda X}{2}\right)\right]\right)^{2} \leq \frac{\nu\lambda^{2}}{4}\mathbb{E}\left[\exp\left(\lambda X\right)\right]$$

or equivalently

$$\left(1 - \frac{\nu \lambda^2}{4}\right) \Phi(\lambda) \le \left(\Phi\left(\frac{\lambda}{2}\right)\right)^2,$$

where $\Phi(\lambda) := \mathbb{E}\left[\exp\left(\lambda(X - \mathbb{E}\left[X\right])\right)\right]$ is the moment generating function of $X - \mathbb{E}\left[X\right]$.

Lemma 2.9 Let $g:(0,1)\to (0,\infty)$ be a function such that $\lim_{x\to 0}(g(x)-1)/x=0$. If for every $x\in (0,1)$

$$(1-x^2)g(x) \le g(x/2)^2$$

then

$$g(x) \le (1 - x^2)^{-2}.$$

Since $\Phi(0) = 1$ and $\Phi'(0) = 0$, we may apply above Lemma to the function $x \to \Phi(2x\nu^{-1/2})$ and get, for every $\lambda \in (0, 2\nu^{-1/2})$,

$$\Phi(\lambda) \le \left(1 - \frac{\nu\lambda^2}{4}\right)^{-2}.\tag{31}$$

Thus, the Efron-Stein inequality may be used to prove exponential integrability of X.

Moreover, since by (31) $\Phi(\nu^{-1/2}) \leq 2$, by Markov's inequality, for every t > 0,

$$\mathbb{P}\left\{f(Z) - \mathbb{E}\left[f(Z)\right] \ge t\right\} \le 2\exp\left(-\frac{t}{\sqrt{\nu}}\right). \tag{32}$$

This inequality has the same form as the one derived using the first method of this section but now we *bound deviations* from the *mean* instead of the *median* and the constants are somewhat better.

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