Lecture 8.

3.3. **Stein's method of exchangeable pairs.** The exchangeable pairs approach within Stein's method was first used in the paper [Dia77] which, however, attributed the method to Charles Stein. Later, this technique was presented in a systematic way in Stein's monograph [St86]. We recall that a pair (X, X') of random elements on a common probability space is said to be *exchangeable*, if (X, X') has the same distribution as (X', X). In the book [St86, Lecture III], it is highlighted that a given real random variable W is close in distribution to a standard normal variable N, whenever one can construct an exchangeable pair (W, W') such that W' is close to W in *some* sense and such that the *linear regression property*

$$\mathbb{E}\big[W' - W \,\big|\, \mathcal{G}\big] = -\lambda W \tag{3.6}$$

is satisfied for some small $\lambda > 0$ and $\mathrm{Var}\big(\frac{1}{2\lambda}\mathbb{E}[(W'-W)^2|\mathcal{G}]\big)$ is small, where $\mathcal{G}$ is a σ-algebra that contains $\sigma\{W\}$. Note the relation (3.6) forces W to be centered.

Theorem 3.4 (C. Stein, 1986)**.** *Let (W, W') be an exchangeable pair of random variables defined on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ such that $\mathrm{Var}(W) = 1$, (3.6) holds for some $\lambda > 0$ and $W \in L^3(\mathbb{P})$, then we have*

$$d_{\mathrm{W}}(W, N) \le \sqrt{2/\pi}\sqrt{\mathrm{Var}\left(\frac{1}{2\lambda}\mathbb{E}\big[(W-W')^2|\mathcal{G}\big]\right)} + \frac{1}{2\lambda}\mathbb{E}\big[|W-W'|^3\big]\,,$$

where $N \sim \mathcal{N}(0,1)$.

Proof. Let $f : \mathbb{R} \to \mathbb{R}$ belong to $C^2(\mathbb{R})$ with $\|f\|_\infty \le 2$, $\|f'\|_\infty \le \sqrt{2/\pi}$ and $\|f''\|_\infty \le 2$, then it is clear that $f(W')W$ and $f(W)W$ are integrable. It follows from the exchangeability that $\mathbb{E}\big[(W-W')f(W)\big] = \mathbb{E}\big[(W'-W)f(W')\big]$, from which we get $\mathbb{E}\big[(W-W')[f(W)+f(W')]\big] = 0$. So

$$\begin{aligned}
0 &= \mathbb{E}\big[(W-W')[-f(W)+f(W')]\big] + 2\mathbb{E}\big[(W-W')f(W)\big] \\
&= \mathbb{E}\big[(W-W')[-f(W)+f(W')]\big] + 2\mathbb{E}\big[f(W)\mathbb{E}(W-W'|\mathcal{G})\big] \\
&= \mathbb{E}\big[(W-W')[-f(W)+f(W')]\big] + 2\lambda\mathbb{E}\big[f(W)W\big] \quad \text{by (3.6)}
\end{aligned}$$

that is, $\mathbb{E}\big[(W'-W)[f(W')-f(W)]\big] = 2\lambda\mathbb{E}\big[f(W)W\big]$; and particularly, $\mathbb{E}[(W'-W)^2] = 2\lambda$. Therefore,

$$\begin{aligned}
&2\lambda\mathbb{E}\big[f(W)W - f'(W)\big] = \mathbb{E}\Big((W'-W)[f(W')-f(W)] - 2\lambda f'(W)\Big) \\
&= \mathbb{E}\Big(f'(W)\big[(W'-W)^2 - 2\lambda\big]\Big) + \mathbb{E}\left[(W'-W)^3\int_0^1 (1-t)f''(W+t(W'-W))\,dt\right] \\
&= \mathbb{E}\Big[f'(W)\Big(\mathbb{E}\big[(W'-W)^2|\mathcal{G}\big] - 2\lambda\Big)\Big] + \mathbb{E}\left[(W'-W)^3\int_0^1 (1-t)f''(W+t(W'-W))\,dt\right],
\end{aligned}$$

which together with Proposition 3.3 gives us the desired bound. □

In the following, we will apply Stein's bound of exchangeable pairs to obtain a rate of convergence for the CLT under the assumption of finite fourth moment.

Proposition 3.5 (Quantitative CLT via exchangeable pairs)**.** *Let $\{X_i\}_i$ be i.i.d. with mean zero and variance one such that $\mathbb{E}[|X_1|^4] < \infty$ Then with $V_n = \frac{1}{\sqrt{n}}(X_1 + \dots + X_n)$,*

$$d_{\mathrm{W}}(V_n, \mathcal{N}(0,1)) \le \frac{C}{\sqrt{n}},$$

where $C = \left(\frac{\mathbb{E}[X_1^4]-1}{2\pi}\right)^{\frac{1}{2}} + 4\mathbb{E}[|X_1|^3]$.

Proof. Let us first construct the exchangeable pair:

$$V_n' = V_n + \frac{X_I' - X_I}{\sqrt{n}},$$

where $\{X_i'\}_i$ is an independent copy of $\{X_i\}_i$, and I is a uniform random variable with values in $\{1, ..., n\}$ such that I is independent from $\{X_i\}_i$ and $\{X_i'\}_i$. We claim that V_n and V_n' are exchangeable. Indeed, for any $t, s \in \mathbb{R}$, we have

$$\begin{aligned}
\mathbb{P}(V_n \le t, V_n' \le s) &= \sum_{k=1}^n \mathbb{P}(V_n \le t, V_n' \le s, I = k) \\
&= \sum_{k=1}^n \mathbb{P}\Big(U_k + \frac{X_k}{\sqrt{n}} \le t, U_k + \frac{X_k'}{\sqrt{n}} \le s, I = k\Big) \quad \text{with } U_k = V_n - \frac{X_k}{\sqrt{n}} \\
&= \sum_{k=1}^n \frac{1}{n}\mathbb{P}\Big(U_k + \frac{X_k}{\sqrt{n}} \le t, U_k + \frac{X_k'}{\sqrt{n}} \le s\Big) \\
&= \sum_{k=1}^n \frac{1}{n}\mathbb{P}\Big(U_k + \frac{X_k'}{\sqrt{n}} \le t, U_k + \frac{X_k}{\sqrt{n}} \le s\Big)
\end{aligned}$$

by the independence among U_k, X_k, X_k'. Then, we have

$$\begin{aligned}
\mathbb{P}(V_n \le t, V_n' \le s) &= \sum_{k=1}^n \mathbb{P}\Big(U_k + \frac{X_k'}{\sqrt{n}} \le t, U_k + \frac{X_k}{\sqrt{n}} \le s, I = k\Big) \\
&= \mathbb{P}(V_n' \le t, V_n \le s).
\end{aligned}$$

That is, $(V_n, V_n') \overset{\text{(law)}}{=} (V_n', V_n)$. Next, we write, with $\mathcal{G} = \sigma\{X_1, ..., X_n\}$,

$$\begin{aligned}
\mathbb{E}[V_n' - V_n|\mathcal{G}] &= \frac{1}{\sqrt{n}}\mathbb{E}[X_I' - X_I|\mathcal{G}] = \frac{1}{\sqrt{n}}\sum_{k=1}^n \mathbb{E}[(X_k' - X_k)\mathbf{1}_{\{I=k\}}|\mathcal{G}] \\
&= \frac{1}{\sqrt{n}}\frac{1}{n}\sum_{k=1}^n \mathbb{E}[X_k' - X_k|\mathcal{G}] \quad \text{as } I \text{ is independent from } \mathcal{G} \\
&= -\frac{1}{n}\frac{1}{\sqrt{n}}\sum_{k=1}^n X_k \quad \text{since } \mathbb{E}[X_k'|\mathcal{G}] = 0 \\
&= -\frac{1}{n}V_n.
\end{aligned}$$

That is, (3.6) holds true with $(W, W', \lambda) = (V_n, V_n', \frac{1}{n})$.

Next, by similar arguments, we can have

$$\begin{aligned}
\mathbb{E}\big[(V_n - V_n')^2|\mathcal{G}\big] &= \frac{1}{n}\mathbb{E}\big[(X_I - X_I')^2|\mathcal{G}\big] = \frac{1}{n^2}\sum_{k=1}^n \mathbb{E}\big[(X_k - X_k')^2|\mathcal{G}\big] \\
&= \frac{1}{n^2}\sum_{k=1}^n \mathbb{E}\big[|X_k|^2 - 2X_kX_k' + |X_k'|^2|\mathcal{G}\big] \\
&= \frac{1}{n^2}\sum_{k=1}^n (X_k^2 + 1).
\end{aligned}$$

Thus,

$$\mathrm{Var}\left(\frac{1}{2\lambda}\mathbb{E}\big[(V_n - V_n')^2|\mathcal{G}\big]\right) = \mathrm{Var}\left(\frac{1}{2n}\sum_{k=1}^{n}(1+X_k^2)\right) = \frac{1}{4n}\big(\mathbb{E}[X_1^4]-1\big).$$

Finally, let us look at the third moment of the difference $V_n' - V_n$:

$$\begin{aligned}\frac{1}{2\lambda}\mathbb{E}[|V_n' - V_n|^3] &= \frac{1}{2\sqrt{n}}\mathbb{E}[|X_I - X_I'|^3] = \frac{1}{2\sqrt{n}}\sum_{k=1}^{n}\frac{1}{n}\mathbb{E}[|X_k - X_k'|^3] \\ &= \frac{1}{2\sqrt{n}}\mathbb{E}[|X_1 - X_1'|^3] \leq \frac{1}{2\sqrt{n}}\mathbb{E}\big[4|X_1|^3 + 4|X_1'|^3\big] \\ &= \frac{4}{\sqrt{n}}\mathbb{E}[|X_1|^3].\end{aligned}$$

Combining the above bounds, we can get

$$d_{\mathrm{W}}(V_n, \mathcal{N}(0,1)) \leq \Big\{\big(\frac{\mathbb{E}[X_1^4]-1}{2\pi}\big)^{\frac{1}{2}} + 4\mathbb{E}[|X_1|^3]\Big\}n^{-\frac{1}{2}}.$$

Hence, the proof is completed. □

3.4. **2nd-order Gaussian Poincaré inequality.** The Gaussian Poincaré inequality (Proposition 2.5) indicates that the variance of $F = f(\mathbf{G})$, with $f \in \mathbb{D}^{1,2}(\mathbb{R}^d)$ and $\mathbf{G} \sim \mathcal{N}_d(0, \mathbf{I})$, is controlled by the average magnitude of DF (i.e., $\mathbb{E}[\|DF\|^2_{\mathbb{R}^d}]$). That is, when the latter is small, the random variable F has small variance, i.e., small fluctuation from its mean. The bound in Proposition 2.5) becomes an exact equality only when $F = f(\mathbf{G})$ is a linear combination of the components $G_1, ..., G_d$, that is, when F is a Gaussian random variable. Naively, if f is close to an affine function, then F would be expected to be close to a Gaussian distribution (with matched mean and variance). Then, if we have a good control over the "second-order" derivatives of f (i.e., $\mathrm{Hessf}(\mathbf{G})$), we should have a proximity of F to a Gaussian. It is S. Chatterjee who first came up with this idea and made it rigorous via Stein's method; see [Cha09]. Let us illustrate this idea more with the quadratic form. Let

$$F = \langle \mathbf{G}, A\mathbf{G}\rangle_{\mathbb{R}^d} = \sum_{i,j=1}^{d} A_{ij}G_iG_j,$$

where $A = (A_{ij})$ is a symmetric $d \times d$ matrix. By the orthogonal decomposition of a real symmetric matrix, we can write

$$A = Q^T\Lambda Q,$$

where $\Lambda = \mathrm{diag}(\lambda_1, ..., \lambda_d)$ is the diagonal matrix with entries being the eigenvalues of A, Q is an orthogonal matrix (i.e., $QQ^T = \mathbf{I}$). Then, we can rewrite $F = \sum_{i=1}^d \lambda_i Y_i^2$, with $(Y_1, ..., Y_d) = Q\mathbf{G}$ again a standard Gaussian vector. By the CLT heuristic, F is approximately Gaussian if no eigenvalue dominates in the sum, or $\max \lambda_i^2$ is much smaller than $\sum_i \lambda_i^2$. Note that for $f(x) = \langle x, Ax\rangle_{\mathbb{R}^d}$, we have the Hessian matrix

$$\mathrm{Hess}f(x) = 2A \quad \text{so that the operator norm } \|\mathrm{Hess}f(x)\|_{\mathrm{op}} = 2\max_i |\lambda_i|,$$

while $\mathrm{Var}(F) = 2\sum_{i=1}^d \lambda_i^2$. This leads to the heuristic that F is approximately Gaussian if the typical value of $\|\mathrm{Hess}f(x)\|^2_{\mathrm{op}}$ is much smaller than the variance of F.

Theorem 3.6 (2nd-order GPI, [Cha09]). *Suppose $f \in C^2(\mathbb{R}^d)$ and $F = f(\mathbf{G})$ with $\mathbf{G} \sim \mathcal{N}_d(0, \mathbf{I})$. Suppose F has zero mean and variance $\sigma^2 \in (0, \infty)$. Then, we have*

$$d_{\mathrm{TV}}\big(F, \mathcal{N}(0, \sigma^2)\big) \le \frac{3}{\sigma^2}\mathbb{E}\Big[\|\mathrm{Hess} f(\mathbf{G})\|_{\mathrm{op}}^4\Big]^{\frac14}\mathbb{E}\Big[\|\nabla f(\mathbf{G})\|_{\mathbb{R}^d}^4\Big]^{\frac14}. \tag{3.7}$$

Proof. By the definition of total-variation distance, we have $d_{\mathrm{TV}}(F, \mathcal{N}(0, \sigma^2)) = d_{\mathrm{TV}}(\frac{F}{\sigma}, \mathcal{N}(0, 1))$. Then, it is enough to consider the case where $\mathrm{Var}(F) = \sigma^2 = 1$. According to Stein's method, it suffices to prove a uniform bound for the expectation

$$\mathbb{E}[F\varphi(F)] - \mathbb{E}[\varphi'(F)] \ \text{ with } \|\varphi'\|_\infty \le 2.$$

In the rest of the proof, we assume that the RHS of (3.7) is finite, otherwise the proof is trivial. With F centered, we can write $F = \mathcal{L}\mathcal{L}^{-1}F$, and therefore with $\mathcal{L} = -\delta\nabla$ ($\nabla = D$),

$$\begin{aligned}\mathbb{E}[F\varphi(F)] &= \mathbb{E}[-\delta\nabla\mathcal{L}^{-1}F\varphi(F)] = \mathbb{E}[\langle -\nabla\mathcal{L}^{-1}F, \nabla\varphi(F)\rangle_{\mathbb{R}^d}] \quad \text{by duality relation}\\ &= \mathbb{E}[\langle -\nabla\mathcal{L}^{-1}F, \nabla F\rangle_{\mathbb{R}^d}\varphi'(F)] \quad \text{by chain rule,}\end{aligned}$$

and in particular, we have $1 = \mathbb{E}[F^2] = \mathbb{E}[\langle -\nabla\mathcal{L}^{-1}F, \nabla F\rangle_{\mathbb{R}^d}]$. Thus, the expression $\mathbb{E}[F\varphi(F)] - \mathbb{E}[\varphi'(F)]$ is uniformly bounded by $2\sqrt{\mathrm{Var}(\langle -\nabla\mathcal{L}^{-1}F, \nabla F\rangle_{\mathbb{R}^d})}$. From previous sections, we know that

$$-\nabla\mathcal{L}^{-1}F = \int_0^\infty e^{-t}P_t\nabla F dt \quad \text{and} \quad A\cdot(-\nabla\mathcal{L}^{-1}F) = \int_0^\infty e^{-t}A\cdot(P_t\nabla F)dt; \tag{3.8}$$

by the same arguments, we can get (with $\nabla^2 f = \mathrm{Hess} f \in \mathbb{R}^{d\times d}$)

$$-\nabla^2\mathcal{L}^{-1}F = \int_0^\infty e^{-2t}P_t\nabla^2 F dt \quad \text{and} \quad (-\nabla^2\mathcal{L}^{-1}F)\cdot y = \int_0^\infty e^{-2t}(P_t\nabla^2 F)\cdot y\, dt, \tag{3.9}$$

where $A\cdot y$ means that the matrix $A \in \mathbb{R}^{d\times d}$ acts on the vector $y \in \mathbb{R}^d$,

Applying the Gaussian Poincaré inequality, we have

$$\begin{aligned}\sqrt{\mathrm{Var}(\langle -\nabla\mathcal{L}^{-1}F, \nabla F\rangle_{\mathbb{R}^d})} &\le \sqrt{\mathbb{E}\big[\|\nabla\langle -\nabla\mathcal{L}^{-1}F, \nabla F\rangle_{\mathbb{R}^d}\|_{\mathbb{R}^d}^2\big]}\\ \le \sqrt{\mathbb{E}\big[\|(-\nabla^2\mathcal{L}^{-1}F)\cdot(\nabla F)\|_{\mathbb{R}^d}^2\big]} &+ \sqrt{\mathbb{E}\big[\|(\nabla^2 F)\cdot(-\nabla\mathcal{L}^{-1}F)\|_{\mathbb{R}^d}^2\big]},\end{aligned} \tag{3.10}$$

where in the last step, we applied Minkowski's inequality. Now let us deal with the first term in (3.10): using (3.9) with Minkowski's inequality, we write

$$\begin{aligned}\Big\|\|(-\nabla^2\mathcal{L}^{-1}F)\cdot(\nabla F)\|_{\mathbb{R}^d}\Big\|_{L^2(\mathbb{P})} &\le \Big\|\int_0^\infty e^{-2t}\|P_t\nabla^2 F\|_{\mathrm{op}}\|\nabla F\|_{\mathbb{R}^d}dt\Big\|_{L^2(\mathbb{P})}\\ &\le \int_0^\infty e^{-2t}\Big\|\|P_t\nabla^2 F\|_{\mathrm{op}}\|\nabla F\|_{\mathbb{R}^d}\Big\|_{L^2(\mathbb{P})}dt\\ &\le \int_0^\infty e^{-2t}\big\|\|P_t\nabla^2 F\|_{\mathrm{op}}\big\|_{L^4(\mathbb{P})}\big\|\|\nabla F\|_{\mathbb{R}^d}\big\|_{L^4(\mathbb{P})}dt\\ &\le \int_0^\infty e^{-2t}\big\|\|\nabla^2 F\|_{\mathrm{op}}\big\|_{L^4(\mathbb{P})}\big\|\|\nabla F\|_{\mathbb{R}^d}\big\|_{L^4(\mathbb{P})}dt \quad (*)\\ &= \frac12\big\|\|\nabla^2 F\|_{\mathrm{op}}\big\|_{L^4(\mathbb{P})}\big\|\|\nabla F\|_{\mathbb{R}^d}\big\|_{L^4(\mathbb{P})},\end{aligned}$$

where we used the contraction property of the O-U semigroup in the step $(*)$. The second term in (3.10) can be dealt with in the same way, so that the proof is concluded. □

Exercise 3.7. *Work out the details for the step $(*)$ and the details for the second term in (3.10).*

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