STEIN'S METHOD AND CENTRAL LIMIT THEOREMS FOR HAAR DISTRIBUTED ORTHOGONAL MATRICES: SOME RECENT DEVELOPMENTS

MICHAEL STOLZ

Abstract. In recent years, Stein's method of normal approximation has been applied to Haar distributed orthogonal matrices by several authors. We give an introduction to the relevant aspects of the method, highlight a few results thus obtained, and finally argue that the quantitative multivariate central limit theorem for traces of powers that was recently obtained by Döbler and the author for the special orthogonal group remains true for the full orthogonal group.

1. Introduction

The observation that random matrices, picked according to Haar measure from orthogonal groups of growing dimension, give rise to central limit theorems, dates back at least to Émile Borel, whose 1905 result on random elements of spheres can be read as saying that if the upper left entry of a Haar orthogonal $n \times n$ matrix is scaled by $\sqrt{n}$, it converges to a standard normal distribution as n tends to infinity. See [DDN03] for more historical background. Borel's observation may be seen as an early result in random matrix theory, but it must be emphasized that from this point of view it is rather atypical. In the best known random matrix models, such as the Gaussian Unitary Ensemble (GUE) or Wigner matrices, the distributions of the individual matrix entries are either known or subject to certain assumptions, and one is interested in various global and local features of the eigenvalues of the random matrix. On the other hand, for Haar orthogonal matrices or, more generally, for Haar distributed elements of a compact matrix group, properties of the distributions of the individual entries have to be inferred from the distribution of the matrix as a whole.

Nevertheless, GUE matrices and Wigner matrices give rise to central limit theorems in a different way: If M_n is an $n \times n$ GUE matrix, say, with (necessarily real) eigenvalues $\lambda_1, \ldots, \lambda_n$, then the empirical eigenvalue distribution

$$L_n := \mathbb{L}_n(M_n) := \frac{1}{n} \sum_{j=1}^{n} \delta_{\lambda_j}$$

Ruhr-Universität Bochum, Fakultät für Mathematik, D-44780 Bochum, Germany.
email: michael.stolz@ruhr-uni-bochum.de.
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is known to converge to Wigner's semicircular distribution σ in various senses. Then for suitable real valued test functions f the fluctuation

$$n\left(\int f dL_n - \mathbb{E}\left(\int f dL_n\right)\right)$$

tends to a Gaussian limit as $n \to \infty$, see, e.g., [LP09].

This type of question also makes sense for Haar distributed matrices from a compact group, such as the orthogonal group, the uniform distribution on the unit circle $\mathbb{T}$ of the complex plane replacing the semicircular distribution. If $f : \mathbb{T} \to \mathbb{R}$ is continuous and of bounded variation, then the fluctuation on the orthogonal group has a pointwise expression

$$\begin{aligned} n(L_n(f) - \mathbb{E}(L_n(f))) &= f(\lambda_{n1}) + \ldots + f(\lambda_{nn}) - n\hat{f}(0) \\ &= \sum_{j=1}^{\infty} \hat{f}(j) \operatorname{Tr}(M_n^j) + \sum_{j=1}^{\infty} \overline{\hat{f}(j) \operatorname{Tr}(M_n^j)} \\ &= 2\sum_{j=1}^{\infty} \operatorname{Re}(\hat{f}(j)) \operatorname{Tr}(M_n^j). \end{aligned} \tag{1}$$

This expansion shows that if f is a trigonometric polynomial, a CLT for fluctuations will be equivalent to a CLT for random vectors of the form

$$(\operatorname{Tr}(M_n), \operatorname{Tr}(M_n^2), \ldots, \operatorname{Tr}(M_n^d)).$$

This CLT was established in the famous paper of Diaconis and Shahshahani [DS94] from 1994 that turned traces of powers into a popular subject in the theory of Haar distributed matrices. It was used as a stepping stone for the treatment of more general test functions by Diaconis and Evans [DE01] in 2001.

Diaconis and Shahshahani proved their theorem using the method of moments. It turned out that the moment

$$\mathbb{E}\left((\operatorname{Tr}(M_n))^{a_1} (\operatorname{Tr}(M_n^2))^{a_2} \ldots (\operatorname{Tr}(M_n^d))^{a_d}\right)$$

actually coincided with the corresponding moment of the Gaussian limit distribution (to be described in Lemma 6.4 below) as soon as

$$2n \geq k_a := \sum_{j=1}^{d} j a_j \tag{2}$$

(see [Sto05] for the threshold given here). This led Diaconis to conjecture that the speed of convergence should be rather fast. Subsequently, only a few years later, Stein [Ste95] proved superpolynomial, and Johansson [Joh97] finally exponential convergence.

During the last decade several authors, certainly inspired by Stein's paper, have turned to the broader approach to normal approximation that bears the name "Stein's method" to investigate the speed of convergence in various CLTs for Haar orthogonals (and Haar distributed elements of other compact matrix groups), obtaining worse rates of convergence, but a wider range of results. It is the aim of this survey paper to introduce the relevant techniques, present some results on the linear combinations and traces of powers problems, and extend the multivariate traces of powers result from the special orthogonal to the full orthogonal group.

2. Univariate normal approximation via Stein's method

Consider random variables W and Z, with distributions P and Q, respectively. A useful recipe to quantify the distance between P and Q is to choose a family $\mathcal{H}$ of test functions and define

$$d_{\mathcal{H}}(P,Q) := \sup_{h\in\mathcal{H}} |\mathbb{E}(h(W)) - \mathbb{E}(h(Z))|.$$

Well-known examples are $\mathcal{H} = \{1_{]-\infty,z]} \mid z \in \mathbb{R}\}$, giving rise to the Kolmogorov distance

$$d_{\mathcal{H}}(P,Q) = \sup_{z\in\mathbb{R}} |\mathbb{P}(W \leq z) - \mathbb{P}(Z \leq z)|,$$

and $\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R}, \text{Lipschitz with constant } \leq 1\}$, which defines the Wasserstein distance.

Stein's method, developed by Charles Stein since the early 1970s (see [Ste72]), serves to bound distances of this type. Stein himself developed his method for normally distributed Z, his student L.H.Y. Chen developed a parallel theory for the Poisson distribution, see [BHJ92] for a monographic treatment. Nowadays, the methods for normal and Poisson limits are still the best developed instances of Stein's approach, but progress has been made on other distributions as well (see, e.g., [CFR11] and [Döb12]). In accordance with the nature of the limit theorems to be discussed in this survey, we will focus on the normal case and start with a sketch of the case of a univariate normal distribution. A much more detailed picture of the fundamentals (and a lot more) of Stein's method of normal approximation can be found in the recent textbook [CGS11].

Write φ for the density of the univariate standard normal distribution. Since φ is strictly positive, for h measurable and $\mathbb{E}|h(Z)| < \infty$ we may define

$$f_h(x) := \frac{1}{\varphi(x)} \int_{-\infty}^{x} (h(y) - \mathbb{E}(h(Z)))\ \varphi(y)\ dy.$$

Then it can be verified by partial integration that f_h solves the *Stein equation*

$$f'(x) = xf(x) + h(x) - \mathbb{E}(h(Z)).$$

For Z a standard normal random variable and W such that $h(W)$ is integrable for all $h \in \mathcal{H}$, this implies that

$$|\mathbb{E}(h(W)) - \mathbb{E}(h(Z))| = |\mathbb{E}(f_h'(W)) - \mathbb{E}(Wf_h(W))|. \tag{3}$$

So to bound the distance, defined by the class $\mathcal{H}$ of test functions, between the law of W and the standard normal distribution, which is the law of Z, it suffices to bound the right hand side of the last equation for all Stein solutions f_h, where h runs over $\mathcal{H}$. Note that this right-hand side involves only W, not Z. A crucial fact to be used in what follows is that estimates on f_h and its first and second derivatives are available that require only little information about h. To be specific, one has that if h is absolutely continuous, then

(i) $\|f_h\|_\infty \leq 2\|h'\|_\infty$.

(ii) $\|f_h'\|_\infty \leq \sqrt{2/\pi}\ \|h'\|_\infty$.
(iii) $\|f_h''\|_\infty \leq 2\|h'\|_\infty$.

Actually there are several approaches to bound the right-hand side of (3), see, e.g., [Rei05]. The orthogonal group examples will use "exchangeable pairs", a device that was introduced by Stein in his monograph [Ste86] of 1986. To illustrate the main ideas of this variant of the method, we will extract a few steps from an argument that Stein provided in his book.

An exchangeable pair is a pair (W, W') of random variables, defined on the same probability space and taking values in the same state space, such that (W, W') and (W', W) have the same distribution. An elementary, but crucial, consequence is that

$$\mathbb{E}\ g(W, W') = 0$$

for any antisymmetric function g defined on pairs of elements of the state space. For concreteness, we assume for now that W and W' are real-valued. In later applications they will be elements of a finite dimensional real vector space.

One further condition that has to be imposed on (W, W') is that there exist $0 < \lambda < 1$ such that

$$\mathbb{E}(W'|W) = (1-\lambda)W.$$

This "regression condition" is quite natural in the context of normal approximation, since it is known to hold if (W, W') has a bivariate normal distribution. Actually, it is desirable to weaken the condition to the effect that the regression property needs to hold only approximately, and indeed this may be done, as shown by Rinott and Rotar in [RR97]. But for our purely illustrative purposes, we assume the condition as it stands.
Since λ is assumed to lie strictly between 0 and 1, W, W' must be centered, as

$$\mathbb{E}(W) = \mathbb{E}(W') = \mathbb{E}(\mathbb{E}(W'|W)) = \mathbb{E}((1-\lambda)W) = (1-\lambda)\mathbb{E}(W).$$

Making the specific choice

$$g(x, y) := (x-y)(f(x) + f(y))$$

of an antisymmetric function, where f is a function that will be specialized to a Stein solution later on, one obtains that

$$\begin{aligned}
0 &= \mathbb{E}((W-W')(f(W) + f(W'))) \\
&= \mathbb{E}((W-W')(f(W') - f(W)) + 2\mathbb{E}((W-W')f(W)) \\
&= \mathbb{E}((W-W')(f(W') - f(W)) + 2\mathbb{E}(f(W)\mathbb{E}((W-W')|W)) \\
&= \mathbb{E}((W-W')(f(W') - f(W)) + 2\lambda\mathbb{E}(Wf(W)).
\end{aligned}$$

From this one concludes that

$$\begin{aligned}
\mathbb{E}(Wf(W)) &= \frac{1}{2\lambda}\mathbb{E}((W-W')(f(W)-f(W')) \\
&= \frac{1}{2\lambda}\mathbb{E}\left[\int_{W'}^{W}(W-W')f'(t)dt\right] \\
&= \frac{1}{2\lambda}\mathbb{E}\left[\int_{-(W-W')}^{0}f'(W+t)(W-W')dt\right] \\
&= \frac{1}{2\lambda}\mathbb{E}\left[\int_{\mathbb{R}}f'(W+t)K(t)dt\right],
\end{aligned}$$

where

$$K(t) = (W-W')\left(1_{\{-(W-W')\leq t\leq 0\}} - 1_{\{0<t\leq -(W-W')\}}\right).$$

On the other hand, a similar argument yields

$$\mathbb{E}(f'(W)) = \mathbb{E}\left[f'(W)(1-\frac{1}{2\lambda}\mathbb{E}((W-W')^2|W)\right] + \frac{1}{2\lambda}\mathbb{E}\left[\int_{\mathbb{R}}f'(W)K(t)dt\right].$$

Assume h Lipschitz with minimal constant $\|h'\|_\infty$, and choose the Stein solution f_h in the place of f. Then it follows from the above that

$$\begin{aligned}
|\mathbb{E}(h(W)) - \mathbb{E}(h(Z))| =& \ |\mathbb{E}(f_h'(W)) - \mathbb{E}(Wf_h(W))| \\
\leq& \ \mathbb{E}\left|f_h'(W)\left(1-\frac{1}{2\lambda}\mathbb{E}((W-W')^2|W)\right)\right| \\
&+ \frac{1}{2\lambda}\mathbb{E}\left[\int_{\mathbb{R}}|f_h'(W)-f_h'(W+t)|K(t)dt\right].
\end{aligned}$$

Observing that

$$|f'(W) - f_h'(W+t)| \leq \|f_h''\|_\infty|t| \leq 2\|h'\|_\infty|t|$$

and recalling the bound

$$\|f_h'\|_\infty \leq (2/\pi)\|h'\|_\infty$$

on the solutions of Stein's equation, one finally arrives at a bound

$$\begin{aligned}
|\mathbb{E}(h(W))-&\mathbb{E}(h(Z))| \\
&\leq \frac{2}{\pi}\|h'\|_\infty \ \mathbb{E}\left[\left|1-\frac{1}{2\lambda}\mathbb{E}((W-W')^2|W)\right|\right] + \frac{\|h'\|_\infty}{2\lambda}\ \mathbb{E}(|W-W'|^3).
\end{aligned}$$

Since this bound in particular holds for all 1-Lipschitz functions h, this means that the Wasserstein distance between the distribution of W and the standard normal law has been bounded from above by the expression

$$\frac{2}{\pi}\ \mathbb{E}\left[\left|1-\frac{1}{2\lambda}\mathbb{E}((W-W')^2|W)\right|\right] + \frac{1}{2\lambda}\ \mathbb{E}(|W-W'|^3). \tag{4}$$

This is a crude version of a bound. In the proofs of the orthogonal group results to be presented in what follows, more elaborate results will be required. In particular, in a situation which exhibits continuous rather than discrete symmetries, such as in a Lie group context, it may be an advantage to consider a continuous family of exchangeable pairs simultaneously, yealding theorems of the type given in Prop. 3.1 below. Nonetheless, the proof of the present crude version illustrates how the exchangeability condition and the regression condition fit together.

It should be noted that there is no guarantee at all that (4) will yield a reasonable bound. The true challenge is to find an exchangeable pair such that the moments of $W - W'$ which appear in (4) get small in the relevant limit, satisfying a regression condition for which λ does not become too small in this limit.

3. Stein's method in the multivariate case

Against the backdrop of the sketch of univariate normal approximation that has been provided above, it does not seem straightforward to extend Stein's approach to the multivariate case. For instance, it is not obvious which differential operator should be used to construct a Stein equation. The most popular choice is the Ornstein-Uhlenbeck (OU) generator $L = \Delta - x \cdot \nabla$. To see that it serves this purpose, denote by (T_t) the operator semigroup corresponding to the OU process in $\mathbb{R}^d$, and by ν_d the d-dimensional standard normal distribution. It is known that the OU process is stationary w.r.t. ν_d. Hence, for f from a suitable class of test functions, one has that

$$\frac{d}{dt} \int T_t f \; d\nu_d = 0,$$

hence

$$\int Lf \; d\nu_d = 0.$$

This observation was exploited by Götze [Göt91] in 1991 in his treatment of the multivariate CLT in euclidean space. On the other hand, a multivariate version of the exchangeable pairs method is only a recent achivement. The handy version that will be presented below, due to E. Meckes [Mec09], builds upon her previous joint work with Chatterjee [CM08] from 2008 as well as on a paper of Reinert and Röllin [RR09] that appeared in 2009.

For a vector $x \in \mathbb{R}^d$ let $\|x\|_2$ denote its euclidean norm induced by the standard scalar product on $\mathbb{R}^d$ that will be denoted by $\langle \cdot, \cdot \rangle$. For $A, B \in \mathbb{R}^{d\times k}$ let $\langle A, B\rangle_{\mathrm{HS}} := \mathrm{Tr}(A^T B) = \mathrm{Tr}(B^T A) = \mathrm{Tr}(AB^T) = \sum_{i=1}^d \sum_{j=1}^k a_{ij} b_{ij}$ be the usual Hilbert-Schmidt scalar product on $\mathbb{R}^{d\times k}$ and denote by $\|\cdot\|_{\mathrm{HS}}$ the corresponding norm. For random matrices $M_n, M \in \mathbb{R}^{k\times d}$, defined on a common probability space $(\Omega, \mathcal{A}, \mathbb{P})$, we will say that M_n converges to M in $\mathrm{L}^1(\|\cdot\|_{\mathrm{HS}})$ if $\|M_n - M\|_{\mathrm{HS}}$ converges to 0 in $\mathrm{L}^1(\mathbb{P})$.
For $A \in \mathbb{R}^{d\times d}$ let $\|A\|_{\mathrm{op}}$ denote the operator norm induced by the euclidean norm, i.e., $\|A\|_{\mathrm{op}} = \sup\{\|Ax\|_2 : \; \|x\|_2 = 1\}$. We now state a multivariate normal approximation theorem, due to E. Meckes ([Mec09, Thm. 4]) that has been used in [DS11] to treat the multivariate CLT for traces of powers of Haar orthogonals. $Z = (Z_1, \ldots, Z_d)^T$ denotes a standard d-dimensional normal random vector, $\Sigma \in \mathbb{R}^{d\times d}$ a positive definite matrix and $Z_\Sigma := \Sigma^{1/2} Z$ with distribution $\mathrm{N}(0, \Sigma)$.

Proposition 3.1. *Let W, W_t $(t > 0)$ be $\mathbb{R}^d$-valued $\mathrm{L}^2(\mathbb{P})$ random vectors on the same probability space $(\Omega, \mathcal{A}, \mathbb{P})$ such that for any $t > 0$ the pair (W, W_t) is exchangeable. Suppose there exist an invertible non-random matrix Λ, a positive definite matrix Σ, a random vector $R = (R_1, \ldots, R_d)^T$, a random $d\times d$-matrix S, a sub-σ-field $\mathcal{F}$ of $\mathcal{A}$ such that W is measurable* *w.r.t.* $\mathcal{F}$ *and a non-vanishing deterministic function* $s :]0,\infty[\to \mathbb{R}$ *such that the following three conditions are satisfied:*

$$\text{(i)} \qquad \frac{1}{s(t)}\mathbb{E}[W_t - W|\mathcal{F}] \xrightarrow{t\to 0} -\Lambda W + R \text{ in } \mathrm{L}^1(\mathbb{P}).$$

$$\text{(ii)} \qquad \frac{1}{s(t)}\mathbb{E}[(W_t - W)(W_t - W)^T|\mathcal{F}] \xrightarrow{t\to 0} 2\Lambda\Sigma + S \text{ in } \mathrm{L}^1(\|\cdot\|_{\mathrm{HS}}).$$

$$\text{(iii)} \qquad \lim_{t\to 0}\frac{1}{s(t)}\mathbb{E}\left[\|W_t - W\|_2^2\, 1_{\{\|W_t-W\|_2^2>\epsilon\}}\right] = 0 \text{ for each } \epsilon > 0.$$

Then

$$d_{\mathcal{W}}(W, Z_\Sigma) \le \|\Lambda^{-1}\|_{\mathrm{op}}\left(\mathbb{E}[\|R\|_2] + \frac{1}{\sqrt{2\pi}}\|\Sigma^{-1/2}\|_{\mathrm{op}}\ \mathbb{E}[\|S\|_{\mathrm{HS}}]\right). \tag{5}$$

It should be remarked that the more complete statement of this theorem given in [Mec09, Thm. 4] also treats the case that Σ is only positive semidefinite.

4. Exchangeable pairs and quantitative Borel type theorems

As mentioned in the introduction, the historical precursor of CLTs for Haar distributed orthogonal matrices is Borel's result about the first coordinate of a random unit vector in euclidean space. This result is a special case (for $A^{(n)}$ specialized to a matrix with 1 in the $(1,1)$ coordinate and 0 elsewhere) of the following result, due to D'Aristotile, Diaconis, and Newman [DDN03]:

Theorem 4.1. *For* $n \in \mathbb{N}$ *choose (deterministic)* $A^{(n)} \in \mathbb{R}^{n\times n}$ *such that* $\mathrm{Tr}(A^{(n)}(A^{(n)})') = n$ *and let* $M_n \in \mathrm{O}_n$ *be distributed according to Haar measure. Then* $\mathrm{Tr}(A^{(n)}M_n)$ *converges in distribution to* $\mathrm{N}(0,1)$ *as* n *tends to infinity.*

Quantitative versions of this result, both with a rate of order $\frac{1}{n-1}$ in total variation distance and with only slightly different constants, have been proven by E. Meckes in [Mec08] and by Fulman and Röllin in [FR11]. In both papers the method of exchangeable pairs is applied, but the specific exchangeable pairs are quite different. Meckes uses a family (W, W_ϵ), where $W = \mathrm{Tr}(AM)$ and $W_\epsilon = \mathrm{Tr}(AM_\epsilon.)$ Here, for any $\epsilon > 0$, the matrix M_ϵ is defined by $M_\epsilon = HB_\epsilon H^T M$, where H is a Haar orthogonal independent of M, and

$$B_\epsilon = \begin{pmatrix} \sqrt{1-\epsilon^2} & \epsilon & & & \\ -\epsilon & \sqrt{1-\epsilon^2} & & 0 & \\ & & 1 & & \\ & 0 & & \ddots & \\ & & & & 1 \end{pmatrix}.$$

Fulman and Röllin, on the other hand, obtain a family $(\mathrm{Tr}(AM_0), \mathrm{Tr}(AM_t))$ $(t > 0)$ of exchangeable pairs from a Brownian motion on O_n that is started in Haar measure, which is the stationary distribution of this process. This construction will be explained more carefully below in the context of the multivariate CLT for traces of powers.

5. Exchangeable pairs and vectors of traces of powers

Let $M = M_n$ be distributed according to Haar measure on $K_n = \mathrm{SO}_n$ or $K_n = \mathrm{O}_n$. For $d \in \mathbb{N},\ r = 1, \ldots, d$, consider the r-dimensional real random vector

$$W := W(d, r, n) := (f_{d-r+1}(M), f_{d-r+2}(M), \ldots, f_d(M)),$$

where

$$f_j(M) = \begin{cases} \mathrm{Tr}(M^j), & j \text{ odd}, \\ \mathrm{Tr}(M^j) - 1, & j \text{ even} \end{cases}$$

Theorem **5.1.** *If $K_n = \mathrm{SO}_n$ and $n \geq 4d + 1$ or $K_n = \mathrm{O}_n$ and $n \geq 2d$, the Wasserstein distance between W and Z_Σ is*

$$d_{\mathcal{W}}(W, Z_\Sigma) = \mathrm{O}\left(\frac{\max\left\{ \frac{r^{7/2}}{(d-r+1)^{3/2}},\ (d-r)^{3/2}\sqrt{r} \right\}}{n} \right). \tag{6}$$

In particular, for $r = d$ we have

$$d_{\mathcal{W}}(W, Z_\Sigma) = \mathrm{O}\left(\frac{d^{7/2}}{n} \right),$$

and for $r \equiv 1$

$$d_{\mathcal{W}}(W, Z_\Sigma) = \mathrm{O}\left(\frac{d^{3/2}}{n} \right).$$

If $1 \leq r = \lfloor cd \rfloor$ for $0 < c < 1$, then

$$d_{\mathcal{W}}(W, Z_\Sigma) = \mathrm{O}\left(\frac{d^2}{n} \right).$$

For the special orthogonal group this result is proven in [DS11] (where the conditions on n in the special orthogonal and symplectic cases have been interchanged in the statement of the main result). The main steps of this proof will be indicated in Section 6 below, where it will also be shown how to adapt this strategy of proof to O_n in the place of SO_n. The univariate version of this theorem, including the construction of the exchangeable pair that will be explained below, is due to Fulman [Ful10].

Remark 5.2. In the case of a single fixed power, the rate of convergence in Theorem 5.1 is clearly significantly worse than the exponential rate that was obtained by Johansson [Joh97] in the context of limit theorems for Toeplitz determinants. The merit of Theorem 5.1 may be seen in the fact that it is multivariate and that the powers under consideration may grow with n. That the latter property yields practical benefits is demonstrated by Döbler and the author in [DS12]. There this property is used to prove, actually in the case of the unitary group, that the fluctuation of the linear eigenvalue statistic in (1) will converge to a normal limit with a rate of $\mathrm{O}(n^{-(1-\epsilon)})$ for any $\epsilon > 0$ if the test function f is of class C^∞. This result extends to the orthogonal group in a straightforward way.

6. On the proof of the multivariate traces of powers result

The aim of this section is to summarize the main steps of the proof of Theorem 5.1, as provided in [DS11], for the special orthogonal group, and indicate how this argument can be supplemented to yield a proof of the full orthogonal case.

The overall strategy is to apply Proposition 3.1 to the traces of powers problem. To do so, one has to find a suitable family of exchangeable pairs. The following construction has been proposed by Fulman in [Ful10] to treat the univariate case. See [IW89, Section V.4] for the relevant facts about diffusions on manifolds.

Let $(M_t)_{t\geq 0}$ be Brownian motion on the compact connected Lie group $K = \mathrm{SO}_n$, started in the Haar measure λ_K on K, which is known to be its stationary distribution. What is more, (M_t) is reversible w.r.t. λ_K. In particular, for any $t > 0$ and measurable f, $(f(M_0), f(M_t))$ is an exchangeable pair. Let $(T_t)_{t\geq 0}$ be the associated semigroup of transition operators on $\mathrm{C}^2(K)$ corresponding to (M_t). Its infinitesimal generator is the Laplace-Beltrami operator Δ, and the map $(t, g) \mapsto (T_t f)(g)$ satisfies the heat equation on K. Hence

$$\begin{aligned} T_t f(g) &= T_0 f(g) + t\, \frac{d}{dt}\bigg|_{t=0} T_t f(g) + \mathrm{O}(t^2) \\ &= f(g) + t(\Delta f)(g) + \mathrm{O}(t^2), \end{aligned} \tag{7}$$

and basic Markov process theory yields an expansion that will be useful to establish the regression property that is fundamental for applying the method of exchangeable pairs:

$$\mathbb{E}[f(M_t)|M_0] = (T_t f)(M_0) = f(M_0) + t(\Delta f)(M_0) + \mathrm{O}(t^2). \tag{8}$$

To study traces of powers within this framework, it is useful to express them via power sum symmetric polynomials. To this end, consider $g \in \mathbb{C}^{n\times n}$ with eigenvalues $c_1, \ldots, c_n$ (with multiplicities). Then

$$\mathrm{Tr}(g^k) = c_1^k + \ldots + c_n^k,$$

i.e., the power sum symmetric polynomial $p_k = X_1^k + \ldots + X_n^k$ evaluated at $(c_1, \ldots, c_n) \in \mathbb{C}^n$. As p_k is symmetric in its arguments, we may unambiguously consider p_k as a function on $\mathbb{C}^{n\times n}$, in accordance with the usual functional calculus for operators. For $k, l \in \mathbb{N}$ we write

$$p_{k,l}(g) := p_k(g)p_l(g) = \mathrm{Tr}(g^k)\,\mathrm{Tr}(g^l),$$

which is but a special instance of the general definition of power sum symmetric polynomials, as in [Mac95]. Recalling the notation introduced in Section 5, we have that

$$f_j(M) = \begin{cases} p_j(M), & j \text{ odd}, \\ p_j(M) - 1, & j \text{ even}. \end{cases}$$

Setting

$$W := (f_{d-r+1}(M), f_{d-r+2}(M), \ldots, f_d(M))$$

and

$$W_t := (f_{d-r+1}(M_t), f_{d-r+2}(M_t), \ldots, f_d(M_t)),$$

we see from the discussion above that for any $t > 0$ the pair (W, W_t) is exchangeable.

We will have to verify that this family of exchangeable pairs satisfies the regression property in the refined form of (i), (ii) from Proposition 3.1. Obviously, the expansion (8) may be used to this end, as soon as one is able to describe the action of the Laplacian on the polynomials p_j in an explicit way. Fortunately, such formulae are available from work of Rains [Rai97] and Lévy [Lév08]. The latter reference provides a conceptual account of how they follow from an extension of Schur-Weyl duality to the universal enveloping algebra of the Lie algebra of K, hence to invariant differential operators on K. In concrete terms, we have the following lemma:

LEMMA **6.1.** *For the Laplacian* Δ_{SO_n} *on* SO_n*,*

(i)
$$\Delta_{\mathrm{SO}_n} p_j = -\frac{(n-1)}{2} j p_j - \frac{j}{2}\sum_{l=1}^{j-1} p_{l,j-l} + \frac{j}{2}\sum_{l=1}^{j-1} p_{2l-j}.$$

(ii)
$$\begin{aligned}\Delta_{\mathrm{SO}_n} p_{j,k} = &-\frac{(n-1)(j+k)}{2}\ p_{j,k} - \frac{j}{2}\ p_k \sum_{l=1}^{j-1} p_{l,j-l} - \frac{k}{2}\ p_j\ \sum_{l=1}^{k-1} p_{l,k-l}\\ &- jk\ p_{j+k} + \frac{j}{2}\ p_k\ \sum_{l=1}^{j-1} p_{j-2l}\ + \frac{k}{2}\ p_j\ \sum_{l=1}^{k-1} p_{k-2l}\ + jk\ p_{j-k}.\end{aligned}$$

The expansion (8) and Lemma 6.1 make it possible to identify the vector R and the matrices Λ and S in Proposition 3.1. By way of illustration, one may argue as follows:

LEMMA **6.2.** *For all* $j = d-r+1, \ldots, d$

$$\mathbb{E}[W_{t,j} - W_j | M] = \mathbb{E}[f_j(M_t) - f_j(M)|M] = t \cdot \left(-\frac{(n-1)j}{2} f_j(M) + R_j + \mathrm{O}(t) \right),$$

where

$$\begin{aligned} R_j &= -\frac{j}{2}\sum_{l=1}^{j-1} p_{l,j-l}(M) + \frac{j}{2}\sum_{l=1}^{j-1} p_{2l-j}(M) \quad \text{if } j \text{ is odd,}\\ R_j &= -\frac{(n-1)j}{2} - \frac{j}{2}\sum_{l=1}^{j-1} p_{l,j-l}(M) + \frac{j}{2}\sum_{l=1}^{j-1} p_{2l-j}(M) \quad \text{if } j \text{ is even.}\end{aligned}$$

Proof. First observe that always $f_j(M_t) - f_j(M) = p_j(M_t) - p_j(M)$, no matter what the parity of j is. By (8) and Lemma 6.1

$$\begin{aligned}\mathbb{E}[p_j(M_t) - p_j(M)|M] &= t(\Delta p_j)(M) + \mathrm{O}(t^2)\\ &= t\left(-\frac{(n-1)j}{2} p_j(M) - \frac{j}{2}\sum_{l=1}^{j-1} p_{l,j-l}(M) + \frac{j}{2}\sum_{l=1}^{j-1} p_{2l-j}(M) \right) + \mathrm{O}(t^2),\end{aligned}$$

and the claim follows from the definition of f_j in the even and odd cases. $\square$

From Lemma 6.2 and the compactness of the group K we conclude

$$\frac{1}{t}\mathbb{E}[W_t - W|M] \overset{t\to 0}{\longrightarrow} -\Lambda W + R \text{ almost surely and in } \mathrm{L}^1(\mathbb{P}),$$

where $\Lambda = \operatorname{diag}\left(\frac{(n-1)j}{2}\,,\, j = d-r+1,\ldots,d\right)$ and $R = (R_{d-r+1},\ldots,R_d)^T$. Thus, Condition (i) of Proposition 3.1 is satisfied, and we have identified Λ and R. The verification of (ii), and identification of Σ and S, is based on the following lemma, which is proven along the same lines as Lemma 6.2.

Lemma **6.3.** *For all $j,k = d-r+1,\ldots,d$*

$$\mathbb{E}[(p_j(M_t) - p_j(M))(p_k(M_t) - p_k(M))|M] = t\,(jkp_{j-k}(M) - jkp_{j+k}(M)) + \mathrm{O}(t^2).$$

With Lemma 6.3 in hand, we obtain that

$$\begin{aligned}\frac{1}{t}\mathbb{E}[(W_{t,j} - W_j)(W_{t,k} - W_k)|M] &= \frac{1}{t}\mathbb{E}[(f_j(M_t) - f_j(M))(f_k(M_t) - f_k(M))|M] \\ &= \frac{1}{t}\mathbb{E}[(p_j(M_t) - p_j(M))(p_k(M_t) - p_k(M))|M] = jkp_{j-k}(M) - jkp_{j+k}(M) + \mathrm{O}(t^2) \\ &\overset{t\to 0}{\to} jkp_{j-k}(M) - jkp_{j+k}(M) \text{ a.s. and in } \mathrm{L}^1(\mathbb{P}),\end{aligned}$$

for all $j,k = 1,\ldots,d$. Noting that for $j = k$ the last expression is $j^2 n - j^2 p_{2j}(M)$ and that $2\Lambda\Sigma = \operatorname{diag}((n-1)j^2\,,\, j = d-r+1,\ldots,d)$ we see that Condition (ii) of Proposition 3.1 is satisfied with the matrices $\Sigma = \operatorname{diag}(d-r+1,\ldots,d)$ and $S = (S_{j,k})_{j,k=d-r+1,\ldots,d}$ given by

$$S_{j,k} = \begin{cases} j^2(1 - p_{2j}(M)), & j = k \\ jkp_{j-k}(M) - jkp_{j+k}(M), & j \neq k\,. \end{cases}$$

To proceed further, i.e., to verify Condition (iii) of Proposition 3.1 and bound the right hand side of (5), one has to be able to integrate products of traces of powers with respect to Haar measure. Such formulae are available from the moment-based proof of the CLT for vectors of traces of powers given by Diaconis and Shahshahani in [DS94], and subsequent work. A version for the special orthogonal group, due to Pastur and Vasilchuk [PV04], is as follows:

Lemma **6.4.** *If $M = M_n$ is a Haar-distributed element of SO_n, $n-1 \geq k_a$, $Z_1,\ldots,Z_r$ iid real standard normals, then*

$$\mathbb{E}\left(\prod_{j=1}^{r}(\mathrm{Tr}(M^j))^{a_j}\right) = \mathbb{E}\left(\prod_{j=1}^{r}(\sqrt{j}Z_j + \eta_j)^{a_j}\right) = \prod_{j=1}^{r} f_a(j), \tag{9}$$

where

$$f_a(j) := \begin{cases} 1 & \text{if } a_j = 0, \\ 0 & \text{if } ja_j \text{ is odd}, a_j \geq 1, \\ j^{a_j/2}(a_j - 1)!! & \text{if } j \text{ is odd and } a_j \text{ is even}, a_j \geq 2, \\ 1 + \sum_{d=1}^{\lfloor a_j/2\rfloor} j^d \binom{a_j}{2d}(2d-1)!! & \text{if } j \text{ is even}, a_j \geq 1. \end{cases}$$

Here we have used the notations $(2m-1)!! = (2m-1)(2m-3)\cdot\ldots\cdot 3\cdot 1$,

$$k_a := \sum_{j=1}^{r} ja_j, \quad \text{and} \quad \eta_j := \begin{cases} 1, & \text{if } j \text{ is even}, \\ 0, & \text{if } j \text{ is odd}. \end{cases}$$

Using Lemma 6.4, it is tedious, but straightforward, to complete the proof of Theorem 5.1 in the special orthogonal case.

It should be evident from this sketch that an extension of Theorem 5.1 to the full orthogonal group will be proven once one has extended the construction of the exchangeable pair in a way that preserves the expansion (8), and verified the validity of Lemma 6.1 for the full orthogonal group. Lemma 6.4 for the full orthogonal group is due to Diaconis and Shahshahani [DS94], and the condition on n can be even weakened to $2n \geq k_a$ as a consequence of the invariant-theoretic proof given in [Sto05] (which does not directly carry over to the special orthogonal group).

In a nutshell, the arguments involving the Laplacian extend to the full orthogonal group because the special orthogonal group is the connected component of the full orthogonal group that contains the identity. Consequently, both groups share the same Lie algebra, and the action of one-parameter semigroups, hence of differential operators, can be extended from SO_n to O_n in a canonical way. Although this has already been briefly discussed by Fulman and Röllin [FR11] in the context of linear functions of matrix entries, it is perhaps useful to close this survey by expanding a bit on this argument in the present situation.

The full orthogonal group has two connected components, consisting of orthogonal matrices of determinant 1 and -1, respectively. Writing J for the diagonal matrix $\mathrm{diag}(-1, 1, 1, \ldots, 1)$, the connected components of the group $K := \mathrm{O}_n$ are the cosets $K_+ := \mathrm{SO}_n$ and $K_- := J\,\mathrm{SO}_n$. For any $f \in \mathrm{C}(K)$ denote by $f_+ \in \mathrm{C}(K_+)$ and $f_- \in \mathrm{C}(K_-)$ its restrictions to K_+ and K_-, respectively. Then we may extend the family (T_t) of transition operators from $\mathrm{C}(K_+)$ to $\mathrm{C}(K)$ by requiring that for $f \in \mathrm{C}(K)$ there hold $(T_t f)_+ = T_t(f_+)$ and $(T_t f)_- = T_t(f_- \circ \tau_J) \circ \tau_J$, where τ_J is the left translation $(x \mapsto Jx)$. To verify that the process that corresponds to the extended semigroup is reversible w.r.t. Haar measure, one deduces from the invariance of Haar measure under translations and from reversibiliy of the process on the special orthogonal group that for $f, g \in \mathrm{C}(K)$ one has

$$
\begin{aligned}
\int_{K_-} (T_t f)_-(x)\ g_-(x)\ \lambda_K(dx) &= \int_{K_-} ((T_t(f_- \circ \tau_J)) \circ \tau_J)(x)\ g_-(x)\ \lambda_K(dx) \\
&= \int 1_{K_+}(Jx)\ ((T_t(f_- \circ \tau_J))(Jx)\ g_-(x)\ \lambda_K(dx) \\
&= \int_{K_+} (T_t(f_- \circ \tau_J))(x)\ g_-(Jx)\ \lambda_K(dx) \\
&= \int_{K_+} (f_- \circ \tau_J)(x)\ T_t(g_- \circ \tau_J)(x)\ \lambda_K(dx) \\
&= \int_{K_-} f_-(x)\ (T_t(g_- \circ \tau_J)) \circ \tau_J)(x)\ \lambda_K(dx) \\
&= \int_{K_-} f_-(x)\ (T_t g)_-(x)\ \lambda_K(dx).
\end{aligned}
$$

Since a Laplacian is invariant under translations, the action of $\Delta = \Delta_{K_+}$ on $\mathrm{C}^2(K)$ in particular satisfies

$$\Delta(f \circ \tau_J) = (\Delta f) \circ \tau_J. \tag{10}$$

So we have that for any $x \in K_-$

$$\frac{d}{dt}(T_t f)_-(x) = \frac{d}{dt} T_t(f_- \circ \tau_J)(Jx) = \Delta(f_- \circ \tau_J)(Jx) = \Delta(f_-)(x).$$

That Lemma 6.1 extends to the full orthogonal group is a direct consequence of (10).

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