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Exponential approximation and Stein's method of exchangeable pairs

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Abstract. We derive a new result for exponential approximation using Stein's method of exchangeable pairs. As an application, an exponential limit theorem with error term is derived for $|Tr(U)|^2$, where $Tr(U)$ denotes the trace of a matrix chosen from the Haar measure of the unitary group $U(n, \mathbb{C})$.

1. Introduction

The purpose of this paper is to further develop exponential approximation, using Stein's method of exchangeable pairs. The first use of exchangeable pairs in exponential approximation was in the paper Chatterjee et al. (2011), which studied the spectrum of the Bernoulli-Laplace Markov chain. Unfortunately the results in Chatterjee et al. (2011), which use the Kolmogorov metric, are very complicated and seem quite hard to apply in other examples. We provide approximation results similar to those in Chatterjee et al. (2011), but which are significantly easier to compute. In particular, we do not see how to apply the results of Chatterjee et al. (2011) to the example in this paper.

We work in a "smooth" test function metric, but also provide bounds in the Kolmogorov metric, which is defined for random variables W and Z to be

$$d_K(W, Z) = \sup_{t \in \mathbb{R}} |\mathbb{P}(W \le t) - \mathbb{P}(Z \le t)|.$$

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Our main theoretical result is the following theorem (see also Theorem 2.1 below).

Theorem 1.1. *Let Z be a mean one exponential random variable. If $W \geq 0$ is a random variable with finite second moment and (W, W') is an exchangeable pair such that for some $a > 0$ and sigma-field $\mathcal{F} \supseteq \sigma(W)$,*

$$\mathbb{E}[W' - W|\mathcal{F}] = -a(W - 1) + R, \tag{1.1}$$

then for all $\delta > 0$,

$$d_K(W, Z) \leq \frac{8}{\delta}\mathbb{E}\left|W - \frac{\mathbb{E}[(W' - W)^2|\mathcal{F}]}{2a}\right| + \frac{2}{\delta}|\mathbb{E}W - 1|$$
$$+ \left(\frac{(5 - 6/e)}{\delta} + \frac{3}{\delta^2}\right)\frac{\mathbb{E}|W' - W|^3}{a} + \frac{8}{\delta}\frac{\mathbb{E}|R|}{a} + \delta/2.$$

Remark: The theorem is stated with a choice of δ in order to simplify the error bound, but it is obvious that in applications δ should be chosen to minimize the bound.

One of the attractive points about this result is that the terms are very similar to those which one encounters in normal approximation. To see the parallels, here is a normal approximation theorem of Rinott and Rotar (2000) (in the Kolmogorov metric).

Theorem 1.2. *Let (W, W') be an exchangeable pair of real random variables such that $\mathbb{E}(W) = 0, \mathbb{E}(W^2) = 1$ and $\mathbb{E}(W'|W) = (1 - a)W + R(W)$ with $0 < a < 1$. Then for all real x_0,*

$$\left|\mathbb{P}(W \leq x_0) - \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{x_0} e^{-\frac{x^2}{2}}dx\right|$$
$$\leq \frac{6}{a}\sqrt{Var(\mathbb{E}[(W' - W)^2|W])} + 19\frac{\sqrt{\mathbb{E}(R^2)}}{a} + 6\sqrt{\frac{1}{a}\mathbb{E}|W' - W|^3}.$$

For normal approximation, there are natural examples related to Markov chain spectra and random matrices (see Fulman 2008, 2009, 2012; Fulman and Röllin 2011), which are perfectly suited for the bounding of terms such as $Var(\mathbb{E}[(W' - W)^2|W])$ and $\mathbb{E}|W' - W|^3$. This is why we believe the bound in Theorem 1.1 will be useful for exponential approximation.

Indeed, in Section 3, we consider the random variable $W = |Tr(U)|^2$, where Tr denotes trace and U is from the Haar measure of the unitary group $U(n, \mathbb{C})$. Since $Tr(U)$ converges to a complex normal Diaconis and Shahshahani (1994), it follows that $|Tr(U)|^2$ converges to an exponential with mean 1. In studying the correspondence between unitary eigenvalues and zeros of the Riemann zeta function, it is conjectured in Coram and Diaconis (2003) that the convergence of $|Tr(U)|^2$ to an exponential limit is extremely rapid, more precisely that there are positive c, δ such that for all $n \geq 1, t \geq 0$,

$$|\mathbb{P}(|Tr(U)|^2 \geq t) - e^{-t}| \leq cn^{-\delta n}.$$

The authors suggest that this should follow from methods in the remarkable paper Johansson (1997). This seems challenging to make rigorous, particularly if one wants to make c, δ explicit. In Section 3, we give the first rigorous and explicit error term for this problem, proving that the Kolmogorov distance between $|Tr(U)|^2$ and a standard mean 1 exponential is at most $2^{9/4}/\sqrt{n}$. Another approach to this result might be to use the multivariate central limit theorems in Döbler and Stolz (2011); we do not pursue this here.

To close the introduction, we mention some related results using Stein's method for exponential approximation. Aside from Chatterjee et al. (2011) which we already mentioned, the recent paper Chatterjee and Shao (2011) (and similar results in Section 13.4 of the text Chen et al. (2011)), use Stein's method of exchangeable pairs for exponential approximation. However our approach is quite different than theirs since they assume the exchangeable pair (W, W') satisfies

$$\mathbb{E}(W' - W|W) = 1/c_0 + R(W),$$

with c_0 a positive constant, rather than the linearity condition (1.1) assumed here. Another approach to Stein's method for exponential approximation is the "equilibrium distribution" coupling for which we refer the reader to the papers Peköz and Röllin (2011a,b), and to the references therein. For the generator method (in the more general context of chi-squared approximation), one can consult Luk (1994) or Reinert (2005). We note that the examples in Luk (1994) and Reinert (2005) are about independent random variables, whereas the example in the current paper involves dependence. Finally, the introductory survey Ross (2011) has some discussion of these approaches in the wider context of Stein's method.

2. General theorem

The purpose of this section is to prove Theorem 1.1 from the introduction. We first prove an intermediate result which can be thought of as an approximation result for "smooth" test functions. In what follows $\|\cdot\|$ denotes the supremum norm.

Theorem 2.1. *Let Z be a mean one exponential random variable. If $W \geq 0$ is a random variable with finite second moment and (W, W') is an exchangeable pair such that for some $a > 0$ and sigma-field $\mathcal{F} \supseteq \sigma(W)$,*

$$\mathbb{E}[W' - W|\mathcal{F}] = -a(W - 1) + R, \tag{2.1}$$

then for all twice differentiable functions h with $\|h'\|, \|h''\| < \infty$,

$$|\mathbb{E}h(W) - \mathbb{E}h(Z)| \leq 4\|h'\|\mathbb{E}\left|W - \frac{\mathbb{E}[(W' - W)^2|\mathcal{F}]}{2a}\right| + \|h'\||\mathbb{E}W - 1| \tag{2.2}$$

$$+ (2(5 - 6/e)\|h'\| + 3\|h''\|)\frac{\mathbb{E}|W' - W|^3}{4a} + 4\|h'\|\frac{\mathbb{E}|R|}{a}. \tag{2.3}$$

The proof of Theorem 2.1 roughly follows the usual development of Stein's method of exchangeable pairs for distributional approximation. Specifically, for W the random variable of interest and Z having the exponential distribution, we want to bound $|\mathbb{E}h(W) - \mathbb{E}h(Z)|$ for functions h in some predetermined family of test functions (here, twice differentiable functions h with $\|h'\|, \|h''\| < \infty$). Typically, this program has three components.

1. Define a *characterizing operator* $\mathcal{A}$ for the exponential distribution which has the property that

$$\mathbb{E}\mathcal{A}f(Z) = 0$$

for all f in a large enough class of functions if and only if $Z \sim Exp(1)$.

2. For functions h in the class of interest, define f_h to solve
$$\mathcal{A}f_h(x) = h(x) - \mathbb{E}h(Z). \tag{2.4}$$
3. Using (2.4), note that
$$|\mathbb{E}h(W) - \mathbb{E}h(Z)| = |\mathbb{E}\mathcal{A}f_h(W)|.$$
Now use properties of the solutions f_h and the auxiliary randomization of exchangeable pairs to bound this last term.

The next lemma takes care of Items 1 and 2 and also provides the bounds on the solutions f_h needed for Item 3 in the program above. The proof of Theorem 2.1 is immediately after the proof of the lemma.

Lemma 2.2. *Let Z be a mean one exponential random variable. If h is a function such that the following integrals are well defined, then*
$$f(w) = f_h(w) = -\frac{e^w}{w}\int_w^\infty (h(x) - \mathbb{E}h(Z))e^{-x}dx \tag{2.5}$$
defined for $w > 0$, solves the differential equation
$$wf'(w) - (w-1)f(w) = h(w) - \mathbb{E}h(Z). \tag{2.6}$$
If h is absolutely continuous with $\|h'\| < \infty$, then
$$\|f\| \le \left(1 + \frac{2}{e}\right)\|h'\|, \qquad \|f'\| \le 2\|h'\|. \tag{2.7}$$
If in addition, $h'(0) = 0$ and h' is absolutely continuous with $\|h''\| < \infty$, then
$$\|f''\| \le (5 - 6/e)\|h'\| + 3\|h''\|.$$

Proof: The fact that (2.5) solves (2.6) is straightforward to verify. Now, using that $\mathbb{E}h(Z) = \int_0^\infty h(x)e^{-x}dx$, we can rewrite (2.5) as
$$\begin{aligned} f(w) &= -\frac{e^w}{w}\int_w^\infty h(x)e^{-x}dx + \frac{1}{w}\int_0^\infty e^{-x}h(x)dx \\ &= -\frac{e^w(1-e^{-w})}{w}\int_w^\infty h(x)e^{-x}dx + \frac{1}{w}\int_0^w h(x)e^{-x}dx. \end{aligned} \tag{2.8}$$
To prove (2.7), first note that since translating h by a constant leaves f unchanged, we may (and do) assume without loss of generality that $h(0) = 0$, so that $h(x) \le \|h'\||x|$. Using this fact and also that $\int xe^{-x}dx = -e^{-x}(x+1)$ in the equality below, we find
$$\begin{aligned} |f(w)| &\le \|h'\|\left[\frac{e^w(1-e^{-w})}{w}\int_w^\infty xe^{-x}dx + \frac{1}{w}\int_0^w xe^{-x}dx\right] \\ &= \|h'\|\left[\frac{(1-e^{-w})(w+2)}{w} - e^{-w}\right]. \end{aligned}$$
To bound this last expression, we compare derivatives to find
$$(1-e^{-w})(w+2) - we^{-w} \le (1+2/e)w, \qquad w \ge 0,$$
which yields the first assertion of (2.7).

For the second assertion note that (2.6) implies that
$$f'(w) = \frac{h(w)}{w} - \left(\frac{(1-w)f(w) + \mathbb{E}h(Z)}{w}\right). \tag{2.9}$$

Since $|h(x)| \leq \|h'\||x|$, the first term of (2.9) is bounded in absolute value by $\|h'\|$, so we only need to find an appropriate bound on the term of (2.9) that is in parentheses. We have by (2.8) that

$$\begin{aligned}\frac{(1-w)f(w)+\mathbb{E}h(Z)}{w} &= \left(\frac{e^w-1}{w}-\frac{e^w-1-w}{w^2}\right)\int_w^\infty h(x)e^{-x}dx \\ &\quad + \frac{1}{w^2}\int_0^w h(x)e^{-x}dx.\end{aligned} \tag{2.10}$$

One easily checks that

$$\frac{e^w-1}{w}-\frac{e^w-1-w}{w^2}\geq 0.$$

Indeed, this is equivalent to $we^w \geq e^w-1$, which is proved by comparing derivatives. Now taking the absolute value of (2.10), using the triangle inequality, bounding $|h(x)| \leq \|h'\||x|$, and using $\int xe^{-x}dx = -e^{-x}(x+1)$, we find

$$\begin{aligned}&\left|\frac{(1-w)f(w)+\mathbb{E}h(Z)}{w}\right| \\ &\quad\leq \|h'\|\left(\frac{(w+1)(w+e^{-w}-1)}{w^2}+\frac{1-(w+1)e^{-w}}{w^2}\right) = \|h'\|,\end{aligned}$$

which now yields the second assertion of (2.7).

To prove the final statement of the lemma, take the derivative of (2.9) using the expression (2.10) to find

$$f''(w) = \frac{h'(w)}{w}+\frac{(w-2)h(w)}{w^2} \tag{2.11}$$

$$\quad + \frac{2-(w^2-2w+2)e^w}{w^3}\int_w^\infty h(x)e^{-x}dx + \frac{2}{w^3}\int_0^w h(x)e^{-x}dx. \tag{2.12}$$

To bound these expressions we first note that since $h'(0)=h(0)=0$,

$$|h(x)| \leq \min\{\|h'\||x|, \|h''\|x^2/2\}, \text{ and } |h'(x)| \leq \|h''\||x|$$

and in particular, $|h(x)|$ is bounded above by both terms appearing in the minimum. Thus, the absolute value of the right hand side of (2.11) is bounded above by

$$\begin{aligned}\|h''\| + \min\{|w/2-1|\|h''\|, |1-2/w|\|h'\|\} &\leq \|h''\| + \max\{\|h'\|, \|h''\|\}, \\ &\leq 2\|h''\| + \|h'\|\end{aligned}$$

where we have used that $\min\{|w/2-1|, |1-2/w|\} \leq 1$.

We bound the second term (2.12) differently according to $w \geq 1$ or $w < 1$. Suppose that $w \geq 1$. Then note that $(w^2-2w+2)e^w \geq e^w \geq 2$. Using that $|h(x)| \leq \|h'\||x|$ and $\int xe^{-x}dx = -e^{-x}(x+1)$, we find the absolute value of (2.12) is bounded above by

$$\begin{aligned}&\|h'\|\left[\frac{((w^2-2w+2)e^w-2)(w+1)e^{-w}}{w^3}+\frac{2(1-(w+1)e^{-w})}{w^3}\right] \\ &\quad = \|h'\|\frac{w^3-w^2+4-4(w+1)e^{-w}}{w^3} \\ &\quad \leq \|h'\|\frac{w^3+3(1-(w+1)e^{-w})}{w^3},\end{aligned} \tag{2.13}$$

where we have used that $1-w^2 \le 0$. By comparing derivatives we find

$$1-(w+1)e^{-w} \le (1-2/e)w^3, \qquad w \ge 1,$$

so that (2.13) (and hence (2.12)) is bounded above by $(4-6/e)\|h'\|$ for $w \ge 1$.

If $0 \le w < 1$, then

$$(w^2-2w+2)e^w \ge (w^2-2w+2)\left(1+w+\frac{w^2}{2}\right) = \frac{w^4+4}{2} \ge 2.$$

Using that $|h(x)| \le \|h''\|x^2/2$ and $\int x^2 e^{-x}dx = -e^{-x}(2+2x+x^2)$, we find the absolute value of (2.12) is bounded above by

$$\begin{aligned}\|h''\| &\left[\frac{((w^2-2w+2)e^w-2)(2+2w+w^2)e^{-w}}{2w^3} + \frac{2-(2+2w+w^2)e^{-w}}{w^3}\right] \\ &= \|h''\|\frac{w^4+8-4e^{-w}(2+2w+w^2)}{2w^3}. \end{aligned} \tag{2.14}$$

Again by comparing derivatives we find

$$w^4+8-4e^{-w}(2+2w+w^2) \le 2w^3, \qquad 0 \le w < 1,$$

so that (2.14) (and hence (2.12)) is bounded above by $\|h''\|$ for $0 < w \le 1$. □

Proof of Theorem 2.1: We show that for h as in the theorem, $|\mathbb{E}h(W)-\mathbb{E}h(Z)|$ is appropriately bounded. We would like to follow the program outlined at the beginning of the section, but in order to apply the bounds of Lemma 2.2, we must have $h'(0)=0$, which is not assumed in Theorem 2.1. We circumvent this problem by replacing h with $\tilde{h}(x) = h(x) - xh'(0)$, and we have

$$\begin{aligned}|\mathbb{E}h(W)-\mathbb{E}h(Z)| &\le |\mathbb{E}\tilde{h}(W)-\mathbb{E}\tilde{h}(Z)| + |h'(0)||\mathbb{E}W-\mathbb{E}Z| \\ &\le |\mathbb{E}\tilde{h}(W)-\mathbb{E}\tilde{h}(Z)| + \|h'\||\mathbb{E}W-1|. \end{aligned} \tag{2.15}$$

In order to bound $|\mathbb{E}\tilde{h}(W)-\mathbb{E}\tilde{h}(Z)|$, we use Lemma 2.2 in conjunction with Item 3 of the program outlined at the beginning of this section to show that the absolute value of

$$\mathbb{E}[Wf'(W)-(W-1)f(W)] \tag{2.16}$$

is appropriately bounded, where f satisfies (2.6) with h replaced by $\tilde{h}$.

Using exchangeability and the linearity condition (2.1), we observe that

$$\begin{aligned}\mathbb{E}[(W'-W)(f(W)-f(W'))] &= 2\mathbb{E}[f(W)(W'-W)] \\ &= -2a\mathbb{E}[(W-1)f(W)] + 2\mathbb{E}[Rf(W)], \end{aligned}$$

so that (2.16) is equal to

$$\mathbb{E}[Wf'(W)] - (2a)^{-1}\mathbb{E}[(W'-W)(f(W')-f(W))] - a^{-1}\mathbb{E}[Rf(W)].$$

We rewrite this expression as

$$\begin{aligned}\mathbb{E}&\left[f'(W)\left(W - \frac{\mathbb{E}[(W'-W)^2|\mathcal{F}]}{2a}\right)\right] \\ &- \mathbb{E}\left[\frac{(W'-W)}{2a}\int_0^{W'-W}[f'(W+t)-f'(W)]dt\right] - a^{-1}\mathbb{E}[Rf(W)]. \end{aligned}$$

Now taking the absolute value of this last expression, we find that (2.16) in absolute value is bounded above by

$$\|f'\|\mathbb{E}\left|W - \frac{\mathbb{E}[(W'-W)^2|\mathcal{F}]}{2a}\right| \\ + \|f''\|\mathbb{E}\left[\frac{|W'-W|}{2a}\int_0^{W'-W}|t|dt\right] + \|f\|\frac{\mathbb{E}|R|}{a}.$$

The result now easily follows after applying the bounds of Lemma 2.2, with h replaced by $\tilde{h}$, noting that $\|\tilde{h}''\| = \|h''\|$ and $\|\tilde{h}'\| = \|h' - h'(0)\| \leq 2\|h'\|$, and recalling (2.15). □

We are now in a position to prove Theorem 1.1. First define the function for $t, x \geq 0$, and $\delta > 0$,

$$h_{t,\delta}(x) = \begin{cases} 1, & x \leq t-\delta, \\ 1 - \frac{2(x-t+\delta)^2}{\delta^2}, & t-\delta < x \leq t-\delta/2, \\ \frac{2(x-t)^2}{\delta^2}, & t-\delta/2 < x \leq t, \\ 0, & x > t. \end{cases} \tag{2.17}$$

The next lemma states some important facts regarding the use of $h_{t,\delta}$ in our framework.

Lemma 2.3. *If $t \geq 0$, $\delta > 0$, and $h_{t,\delta}$ is defined by (2.17), then*

$$\|h_{t,\delta}\| \leq 1, \qquad \|h'_{t,\delta}\| \leq 2/\delta, \qquad \|h''_{t,\delta}\| = 4/\delta^2.$$

If $W \geq 0$ is a random variable and Z has the exponential distribution with mean one, then

$$d_K(W,Z) \leq \sup_{t\geq 0}|\mathbb{E}h_{t,\delta}(W) - \mathbb{E}h_{t,\delta}(Z)| + \delta/2. \tag{2.18}$$

Proof: The first assertion follows from direct computation; to be precise, the first inequality is an equality if $t \geq \delta$, the second is an equality if $t \geq \delta/2$, and these are strict inequalities otherwise. For the second, note that

$$\begin{aligned} \mathbb{P}(W \leq t) - \mathbb{P}(Z \leq t) &\leq \mathbb{E}h_{t+\delta,\delta}(W) - \mathbb{P}(Z \leq t) \\ &= \mathbb{E}h_{t+\delta,\delta}(W) - \mathbb{E}h_{t+\delta,\delta}(Z) + \mathbb{E}h_{t+\delta,\delta}(Z) - \mathbb{P}(Z \leq t) \\ &\leq |\mathbb{E}h_{t+\delta,\delta}(W) - \mathbb{E}h_{t+\delta,\delta}(Z)| + \int_t^{t+\delta} h_{t+\delta,\delta}(x)e^{-x}dx. \end{aligned}$$

Since $e^{-x} \leq 1$ for $x > 0$, we find by direct computation that

$$\int_t^{t+\delta} h_{t+\delta,\delta}(x)e^{-x}dx \leq \int_t^{t+\delta} h_{t+\delta,\delta}(x)dx = \delta/2.$$

Taking supremums, we have shown

$$\sup_{t\geq 0}[\mathbb{P}(W \leq t) - \mathbb{P}(Z \leq t)] \leq \sup_{t\geq 0}|\mathbb{E}h_{t,\delta}(W) - \mathbb{E}h_{t,\delta}(Z)| + \delta/2. \tag{2.19}$$

A similar argument starting from

$$\mathbb{P}(Z \leq t) - \mathbb{P}(W \leq t) \leq \mathbb{P}(Z \leq t) - \mathbb{E}h_{t,\delta}(W)$$

establishes (2.19) with the left hand side replaced by

$$\sup_{t\geq 0}[\mathbb{P}(Z \leq t) - \mathbb{P}(W \leq t)],$$

which proves the lemma. □

Proof of Theorem 1.1: First apply Theorem 2.1 with h replaced by $h_{t,\delta}$ to obtain a bound on $\sup_{t\geq 0} |\mathbb{E}h_{t,\delta}(W) - \mathbb{E}h_{t,\delta}(Z)|$. From this point, the result follows from the bounds of Lemma 2.3 and (2.18). □

3. Exponential approximation of $|Tr(U)|^2$

The main purpose of this section is to prove the following result.

Theorem 3.1. *Let $W = |Tr(U)|^2$, where U is from the Haar measure of $U(n, \mathbb{C})$. Then for $n \geq 8$, the Kolmogorov distance between W and an exponential with mean one is at most $2^{9/4}/\sqrt{n}$.*

To construct an exchangeable pair to be used in our application, we use the heat kernel of $U(n, \mathbb{C})$. This has proved useful in other Stein's method problems about random matrices Fulman (2012); Fulman and Röllin (2011); Döbler and Stolz (2011). See Grigor'yan (2009); Rosenberg (1997) for a detailed discussion of heat kernels on compact Lie groups. The papers Lévy (2008); Liu (1999); Rains (1997) illustrate combinatorial uses of heat kernels on compact Lie groups, and Liu (1999) also discusses the use of the heat kernel for finite groups.

The heat kernel on a compact Lie group G is defined by setting for $x, y \in G$ and $t \geq 0$,

$$K(t, x, y) = \sum_{n\geq 0} e^{-\lambda_n t}\phi_n(x)\overline{\phi_n(y)}, \tag{3.1}$$

where the λ_n are the eigenvalues of the Laplacian repeated according to multiplicity, and the ϕ_n are an orthonormal basis of eigenfunctions of $L^2(G)$; these can be taken to be the irreducible characters of G.

We use the following properties of the heat kernel, where Δ denotes the Laplacian of G. Part 1 of Lemma 3.2 is from Section 3.4 of Rosenberg (1997). Part 2 of Lemma 3.2 is immediate from the expansion (3.1). Part 3 of Lemma 3.2 is Lemma 2.5 of Döbler and Stolz (2011).

Lemma 3.2. *Let G be a compact Lie group, $x, y \in G$, and $t \geq 0$.*

1. *$K(t, x, y)$ converges and is non-negative for all x, y, t.*
2. *$\int_{y\in G} K(t, x, y)dy = 1$, where the integration is with respect to Haar measure of G.*
3. *For smooth ϕ, as $t \to 0$, one has that*

$$\int_{y\in G} K(t, x, y)\phi(y)dy = \phi(x) + t(\Delta\phi)(x) + O(t^2).$$

The symmetry in x and y of $K(t, x, y)$ shows that the heat kernel is a reversible Markov process with respect to the Haar measure of G. It is a standard fact Rinott and Rotar (1997); Stein (1986) that reversible Markov processes lead to exchangeable pairs (W, W'). Namely suppose one has a Markov chain with transition probabilities $K(x, y)$ on a state space X, and that the Markov chain is reversible with respect to a probability distribution π on X. Then given a function f on X, if one lets $W = f(x)$ where x is chosen from π and $W' = f(x')$ where x' is obtained by moving from x according to $K(x, y)$, then (W, W') is an exchangeable pair. In the special case of the heat kernel on a compact Lie group G, given a function f on G, one can construct an exchangeable pair (W, W') by letting $W = f(U)$ where

U is chosen from Haar measure, and $W' = f(U')$, where U' is obtained by moving time t from U via the heat kernel. To define the exchangeable pair (W, W') used in this paper, we further specialize by setting $f(U) = |Tr(U)|^2$.

If λ is an integer partition, and m_j denotes the multiplicity of part j in λ, we define $p_\lambda(U) = \prod_j Tr(U^j)^{m_j}$. For example, $p_{5,3,3}(U) = Tr(U^5)Tr(U^3)^2$. Typically we suppress the U and use the notation p_λ.

The next three lemmas are from Rains (1997); here $\nabla f \cdot \nabla g$ is defined by

$$\nabla f \cdot \nabla g = \frac{1}{2}[\Delta(fg) - g\Delta f - f\Delta g].$$

Lemma 3.3. $\Delta_{U(n)} p_1 = -np_1$.

Lemma 3.4. *For all integers k and l (not necessarily positive), and unitary U,*

$$(\nabla p_k(U)) \cdot (\nabla p_l(U)) = -kl \cdot p_{k+l}(U).$$

Lemma 3.5. *For all unitary matrices U and class functions $f_1, \cdots, f_k$*

$$\begin{aligned} &\Delta\left(\prod_{1\le i\le k} f_i(U)\right) \\ = &\left(\prod_{1\le i\le k} f_i(U)\right)\left(\sum_{1\le i\le k} \frac{\Delta f_i(U)}{f_i(U)} + 2\sum_{1\le i<j\le k} \frac{(\nabla f_i(U)) \cdot (\nabla f_j(U))}{f_i(U) f_j(U)}\right). \end{aligned}$$

The next lemma is a moment computation from Diaconis and Evans (2001).

Lemma 3.6. *If U is Haar distributed on $U(n, \mathbb{C})$, $(a_1, \cdots, a_k)$ and $(b_1, \cdots, b_k)$ are vectors of non-negative integers, then for all $n \geq max(\sum_{j=1}^k ja_j, \sum_{j=1}^k jb_j)$,*

$$\mathbb{E}\left[\prod_{j=1}^k Tr(U^j)^{a_j} \overline{Tr(U^j)^{b_j}}\right] = \delta_{\vec{a}\vec{b}} \prod_{j=1}^k j^{a_j} a_j!.$$

Throughout we let $W(U) = |Tr(U)|^2 = p_1(U)\overline{p_1(U)}$.

Lemma 3.7 computes the conditional expectation $\mathbb{E}[W' - W|U]$.

Lemma 3.7.

$$\mathbb{E}[W' - W|U] = 2nt(1 - W) + O(t^2).$$

Proof: Applying part 3 of Lemma 3.2,

$$\begin{aligned} \mathbb{E}[W'|U] &= W + t\Delta(p_1\overline{p_1}) + O(t^2) \\ &= W + t[\overline{p_1}\Delta(p_1) + p_1\Delta(\overline{p_1}) + 2(\nabla p_1) \cdot (\nabla \overline{p_1})] + O(t^2) \\ &= W + t[-2np_1\overline{p_1} + 2n] + O(t^2). \end{aligned}$$

The second equality was Lemma 3.5. The final equality used Lemmas 3.3 and 3.4, and the fact that $\overline{p_1} = p_{-1}$. □

Lemma 3.8 computes $\mathbb{E}[(W' - W)^2|U]$.

Lemma 3.8.

$$\mathbb{E}[(W' - W)^2|U] = t[-2p_2\overline{p_{1,1}} - 2\overline{p_2}p_{1,1} + 4nW] + O(t^2).$$

Proof: Clearly

$$\mathbb{E}[(W'-W)^2|U] = \mathbb{E}[(W')^2|U] - 2W\mathbb{E}[W'|U] + W^2.$$

By part 3 of Lemma 3.2,

$$\mathbb{E}[(W')^2|U] = W^2 + t\Delta[p_{1,1}\overline{p_{1,1}}] + O(t^2).$$

Using Lemma 3.5, and then Lemmas 3.3 and 3.4, one computes that

$$\begin{aligned}
& \Delta[p_{1,1}\overline{p_{1,1}}] \\
= \quad & p_{1,1}\overline{p_{1,1}}\left[\frac{2\Delta p_1}{p_1} + \frac{2\Delta\overline{p_1}}{\overline{p_1}} + \frac{2\nabla p_1\cdot\nabla p_1}{p_{1,1}} + \frac{2\nabla\overline{p_1}\cdot\nabla\overline{p_1}}{\overline{p_{1,1}}} + \frac{8\nabla p_1\cdot\nabla\overline{p_1}}{p_1\overline{p_1}}\right] \\
= \quad & -4np_{1,1}\overline{p_{1,1}} - 2p_2\overline{p_{1,1}} - 2\overline{p_2}p_{1,1} + 8np_1\overline{p_1}.
\end{aligned}$$

Thus

$$\mathbb{E}[(W')^2|U] = W^2 + t\left[-4np_{1,1}\overline{p_{1,1}} - 2p_2\overline{p_{1,1}} - 2\overline{p_2}p_{1,1} + 8np_1\overline{p_1}\right] + O(t^2).$$

By Lemma 3.7,

$$-2W\mathbb{E}[W'|U] = -2W^2 + t[-4nW + 4nW^2] + O(t^2).$$

Thus

$$\mathbb{E}[(W')^2|U] - 2W\mathbb{E}[W'|U] + W^2 = t[-2p_2\overline{p_{1,1}} - 2\overline{p_2}p_{1,1} + 4nW] + O(t^2).$$

□

Next we compute low order moments of $W'-W$.

Lemma 3.9. *Suppose that $n \geq 8$. Then*
(1) $\mathbb{E}(W'-W)^2 = 4nt + O(t^2)$.
(2) $\mathbb{E}(W'-W)^4 = O(t^2)$.
(3) $\mathbb{E}|W'-W|^3 = O(t^{3/2})$.

Proof: Lemma 3.8 implies that

$$\mathbb{E}(W'-W)^2 = t\mathbb{E}\left[-2p_2\overline{p_{1,1}} - 2\overline{p_2}p_{1,1} + 4nW\right] + O(t^2).$$

By Lemma 3.6, $\mathbb{E}[p_2\overline{p_{1,1}}] = 0$, $\mathbb{E}[\overline{p_2}p_{1,1}] = 0$, and $\mathbb{E}[W] = 1$; the first part of the lemma follows.

For part 2, first note that since

$$\mathbb{E}[(W'-W)^4] = \mathbb{E}(W^4) - 4\mathbb{E}(W^3W') + 6\mathbb{E}[W^2(W')^2] - 4\mathbb{E}[W(W')^3] + \mathbb{E}[(W')^4],$$

exchangeability of (W, W') gives that

$$\begin{aligned}
\mathbb{E}(W'-W)^4 &= 2\mathbb{E}(W^4) - 8\mathbb{E}(W^3W') + 6\mathbb{E}[W^2(W')^2] \\
&= 2\mathbb{E}(W^4) - 8\mathbb{E}[W^3\mathbb{E}[W'|U]] + 6\mathbb{E}[W^2\mathbb{E}[(W')^2|U]].
\end{aligned}$$

By Lemma 3.7,

$$\begin{aligned}
-8\mathbb{E}[W^3\mathbb{E}[W'|U]] &= -8\mathbb{E}[W^3(W + t(2n - 2nW) + O(t^2))] \\
&= -8\mathbb{E}(W^4) + t\mathbb{E}[-16nW^3 + 16nW^4] + O(t^2) \\
&= -8\mathbb{E}(W^4) + tn[-16(6) + 16(24)] + O(t^2) \\
&= -8\mathbb{E}(W^4) + 288tn + O(t^2),
\end{aligned}$$

where the penultimate equality used Lemma 3.6.

By the proof of Lemma 3.8, and then Lemma 3.6,

$$\begin{aligned}
& 6\mathbb{E}[W^2\mathbb{E}[(W')^2|U]] \\
= \ & 6\mathbb{E}\left[W^2\left(W^2+t[-4nW^2-2p_2\overline{p_{1,1}}-2\overline{p_2}p_{1,1}+8nW]+O(t^2)\right)\right] \\
= \ & 6\mathbb{E}[W^4]+tn\mathbb{E}[-24W^4+48W^3]+O(t^2) \\
= \ & 6\mathbb{E}[W^4]+tn[-24(24)+48(6)]+O(t^2) \\
= \ & 6\mathbb{E}[W^4]-288tn+O(t^2).
\end{aligned}$$

Summarizing, it follows that

$$\begin{aligned}
\mathbb{E}(W'-W)^4 &= 2\mathbb{E}(W^4)-8\mathbb{E}[W^3\mathbb{E}[W'|U]]+6\mathbb{E}[W^2\mathbb{E}[(W')^2|U]] \\
&= O(t^2),
\end{aligned}$$

proving part 2 of the lemma.

For part 3 of the lemma, one uses the Cauchy-Schwarz inequality to obtain that

$$\mathbb{E}|W'-W|^3 \leq \sqrt{\mathbb{E}(W'-W)^2\mathbb{E}(W'-W)^4}.$$

Part 3 then follows from parts 1 and 2 of the lemma. □

Now we proceed to the proof of Theorem 3.1.

Proof of Theorem 3.1: By Lemma 3.7, one can apply Theorem 1.1 with $a=2nt$. By Lemma 3.8, and the triangle inequality,

$$\begin{aligned}
& \mathbb{E}\left|W-\frac{\mathbb{E}[(W'-W)^2|W]}{2a}\right| \\
= \ & \mathbb{E}\left|W-\frac{t[-2p_2\overline{p_{1,1}}-2\overline{p_2}p_{1,1}+4nW]}{4nt}+\frac{O(t^2)}{4nt}\right| \\
= \ & \frac{1}{2n}\mathbb{E}|p_2\overline{p_{1,1}}+\overline{p_2}p_{1,1}|+O(t) \\
\leq \ & \frac{1}{2n}\sqrt{\mathbb{E}(p_{2,2}\overline{p_{1,1,1,1}}+2p_{2,1,1}\overline{p_{2,1,1}}+\overline{p_{2,2}}p_{1,1,1,1})}+O(t).
\end{aligned}$$

By Lemma 3.6, this is $\frac{\sqrt{2}}{n}+O(t)$; letting $t\to 0$ gives an upper bound

$$\mathbb{E}\left|W-\frac{\mathbb{E}[(W'-W)^2|W]}{2a}\right| \leq \frac{\sqrt{2}}{n}.$$

The second term in Theorem 1.1 is 0 since by Lemma 3.6, $\mathbb{E}(W)=1$.

To bound $\frac{\mathbb{E}|W'-W|^3}{a}$, note by Lemma 3.9 that $\mathbb{E}|W'-W|^3=O(t^{3/2})$. Since $a=2nt$, the term $\frac{\mathbb{E}|W'-W|^3}{a}$ tends to 0 as $t\to 0$.

Finally, note from Lemma 3.7 that $R=O(t^2)$. Since $a=2nt$, it follows that

$$\frac{\mathbb{E}|R|}{a} \leq \frac{\sqrt{\mathbb{E}(R(W)^2)}}{a}=O(t)$$

tends to 0 as $t\to 0$.

Summarizing, by letting $t\to 0$, Theorem 1.1 implies that for $\delta>0$,

$$d_K(W,Z) \leq \frac{8\sqrt{2}}{\delta n}+\delta/2.$$

Choosing $\delta=4\cdot 2^{1/4}/\sqrt{n}$, yields the claimed result. □

Remarks:

(1) The moments of the random variable $|Tr(U)|^2$ have a combinatorial interpretation. Indeed, from Rains (1998) one has for all positive integers l, n that

$$\mathbb{P}(L_n \leq l) = \frac{1}{n!} \int_{U(l,\mathbb{C})} |Tr(U)|^{2n}.$$

Here L_n is the length of the longest increasing subsequence of a random permutation on n symbols.

(2) The technique used in this section can be used to prove that for positive integers k, $|Tr(U^k)|^2/k$ tends to an exponential with mean 1, for U a Haar distributed unitary matrix from $U(n,\mathbb{C})$, as $n \to \infty$. The bookkeeping is quite tedious, so we do not carry this out.

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