

STEIN'S METHOD, HEAT KERNEL, AND LINEAR FUNCTIONS ON THE ORTHOGONAL GROUPS

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ABSTRACT. Combining Stein's method with heat kernel techniques, we study the function $Tr(AO)$, where A is a fixed $n \times n$ matrix over \mathbb{R} such that $Tr(AA^t) = n$, and O is from the Haar measure of the orthogonal group $O(n, \mathbb{R})$. It is shown that the total variation distance of the random variable $Tr(AO)$ to a standard normal random variable is bounded by $\frac{2\sqrt{2}}{n-1}$, slightly improving the constant in a bound of Meckes, which was obtained by completely different methods.

1. INTRODUCTION

Let $O(n, \mathbb{R})$ denote the group of $n \times n$ real orthogonal matrices, and let O be from the Haar measure on $O(n, \mathbb{R})$. Let A be a fixed $n \times n$ real matrix, satisfying the constraint $Tr(AA^t) = n$, and let $W = Tr(AO)$. Letting $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x e^{-t^2/2} dt$ denote the cumulative distribution function of a standard normal random variable, a result of D'Aristotile, Diaconis and Newman [6] is that

$$\sup_{-\infty < x < \infty} \sup_{Tr(AA^t)=n} |\mathbb{P}(W \leq x) - \Phi(x)| \rightarrow 0$$

as $n \rightarrow \infty$. A recent paper of Meckes [23] shows that for all $n \geq 2$, the total variation distance between the law of W and a standard normal is at most $\frac{2\sqrt{3}}{n-1}$. In this paper we use a very different construction than that of Meckes and obtain a slightly better total variation bound of $\frac{2\sqrt{2}}{n-1}$.

As Meckes observes, this problem has quite a bit of history. Borel in [2] showed that if X is a random vector on the $n - 1$ dimensional unit sphere, with first coordinate X_1 , then $\mathbb{P}(\sqrt{n}X_1 \leq t) \rightarrow \Phi(t)$ as $n \rightarrow \infty$. Since the first column of a Haar distributed orthogonal matrix is uniformly distributed on the sphere, Borel's theorem follows from the central limit theorem for W , taking $A = \sqrt{n} \oplus \mathbf{0}$. Various generalizations of Borel's theorem, focusing on blocks of entries of a Haar distributed orthogonal matrix, can be found in the papers [8], [9], [16].

In the special case that $A = I$, W becomes the trace of a Haar distributed orthogonal matrix. Diaconis and Mallows (see [7]) proved that $Tr(O)$ is approximately normal. Stein [27] proved there exists a constant C_r so that the total variation distance between $Tr(O)$ and a standard normal is at most $C_r(n-1)^{-r}$, and Johansson [17] proved a central limit in the Kolmogorov metric with error term $O(e^{-cn})$ for some $c > 0$. Diaconis and Shahshahani

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[10] proved multivariate central limit theorems (without error terms) for the joint limiting distribution of $Tr(O), Tr(O^2), \dots, Tr(O^k)$, with k fixed. Fulman [12] used heat kernel methods to prove central limit theorems with error terms for $Tr(O^k)$ with k growing; this was extended to the multivariate setting by Döbler and Stolz [11].

Another reason for studying $Tr(AO)$ is the similarity with Hoeffding's combinatorial central limit theorem [15], which proves a central limit theorem for $Tr(AP)$ where P is a random permutation matrix. Stein's method has been used to give explicit bounds for Hoeffding's theorem; see [1] or [4].

It should be possible to extend the results in the current paper to a multivariate setting. Indeed, Chatterjee and Meckes [3] prove bounds in the Wasserstein metric between the distribution of $Tr(A_1O), \dots, Tr(A_kO)$ and a multivariate normal, where A_1, \dots, A_k are fixed and O is from Haar measure of the orthogonal group; see also Collins and Stolz [5] for an extension of [3] (without error terms) to compact symmetric spaces.

Extensions of our results to the unitary and symplectic groups appear in the companion paper [13], which slightly improves Meckes' constant in the unitary case [23]. For the unitary groups there is also an interesting recent paper [19] which uses characteristic functions and a heavy dose of analysis to prove a central limit theorem for $Tr(AU)$ with error term $O(n^{-2+b})$ where $0 \leq b < 1$ depends on the leading order asymptotics of the greatest singular value of A .

Although our results are only a slight improvement of those of Meckes [23], the heat kernel is a remarkable tool appearing in many parts of mathematics (see [18] for a spirited defense of this statement with many references), and we suspect that the blending of heat kernel techniques with Stein's method will be useful for other problems.

The organization of this paper is as follows. Section 2 gives background on symmetric functions and the orthogonal group. Section 3 gives background on the heat kernel and Laplacian of the orthogonal group. Section 4 uses tools from Section 2 and Section 3 to prove our main results.

2. SYMMETRIC FUNCTIONS AND THE ORTHOGONAL GROUP

In this paper we use the zonal polynomial Z_λ (with parameter 2) defined in Section 7.2 of Macdonald [22]. To show the usefulness of symmetric functions, we give a quick proof that $W = Tr(AO)$ is asymptotically normal, if O is from Haar measure of the orthogonal group and A satisfies $AA^t = n$. As noted in Meckes [23] one can assume without loss of generality that A is diagonal: let $A = UDV$ be the singular value decomposition of A . Then $W = Tr(UDVO) = Tr(DVOU)$, and the distribution of VOU is the same as the distribution of O by the translation invariance of Haar measure.

The key to proving a central limit theorem for W is the following lemma from page 423 of [22] (which should also prove useful for carrying the results of [19] over to the orthogonal case). For its statement, recall that the hooklength of a box x is $1 +$ number of boxes in same row as x to right of $x +$ number of boxes in same column of x beneath x . In the diagram below

representing a partition of 7, each box is filled with its hook length:

$$\begin{array}{cccc} \boxed{6} & \boxed{4} & \boxed{2} & \boxed{1} \\ \boxed{3} & \boxed{1} & & \\ \boxed{1} & & & \end{array} .$$

Lemma 2.1. *Let Z_λ be the zonal polynomial (with parameter 2) and let $h(2\lambda)$ be the product of the hooklengths of the partition 2λ , whose rows have length twice those of λ . Let A have singular values a_1, \dots, a_n . Then*

$$\int_{O(n, \mathbb{R})} \exp(t \cdot \text{Tr}[AO]) dO = \sum_{\lambda} \frac{t^{|\lambda|}}{h(2\lambda)} \frac{Z_\lambda(a_1^2, \dots, a_n^2)}{Z_\lambda(1, \dots, 1)}.$$

Lemma 2.1 immediately implies that $\mathbb{E}(W) = 0$. Since by page 410 of [22] one has that $Z_1(a_1^2, \dots, a_n^2) = a_1^2 + \dots + a_n^2 = n$, it follows that $\text{Var}(W) = 1$. Lemma 2.1 also implies the following central limit theorem for W .

Corollary 2.2. *Let A satisfy $\text{Tr}(AA^t) = n$, and let O be from the Haar measure of the orthogonal group $O(n, \mathbb{R})$. Then as $n \rightarrow \infty$, $W = \text{Tr}(AO)$ tends to the standard normal distribution with mean 0 and variance 1.*

Proof. Lemma 2.1 implies that $\mathbb{E}(W^r) = 0$ for r odd, so suppose that r is even. From page 409 of [22],

$$Z_\lambda(1, \dots, 1) = \prod_{(i,j) \in \lambda} (n - i + 2j - 1).$$

With λ fixed this is asymptotic to $n^{|\lambda|}(1 + O(1/n))$.

Recall we can assume that A is diagonal with entries (a_1, \dots, a_n) . Hence by Lemma 2.1, $\mathbb{E}[\text{Tr}(AO)^r]$, with A fixed, r fixed and even, is asymptotic to

$$\begin{aligned} & \frac{r!}{n^{r/2}} \sum_{|\lambda|=r/2} \frac{Z_\lambda(a_1^2, \dots, a_n^2)}{h(2\lambda)} \\ &= \frac{r!}{n^{r/2} 2^{r/2} (r/2)!} \sum_{|\lambda|=r/2} \frac{2^{r/2} (r/2)! Z_\lambda(a_1^2, \dots, a_n^2)}{h(2\lambda)} \\ &= \frac{r!}{n^{r/2} 2^{r/2} (r/2)!} (a_1^2 + \dots + a_n^2)^{r/2} \\ &= \frac{r!}{2^{r/2} (r/2)!}. \end{aligned}$$

The penultimate equality was from page 406 of [22].

It follows that for fixed r , $E(W^r)$ is 0 for r odd, and is asymptotic to $(r-1) \dots (3)(1)$ for r even. The method of moments ([7]) implies that W is asymptotically normal with mean 0 and variance 1. \square

It will also be useful to work with Schur functions $s_\lambda(AO)$ evaluated on the eigenvalues of AO . An in-depth treatment of Schur functions is in Chapter 1 of [22]. From pages 421-422 of [22], one can express the integral of a Schur function over the orthogonal group in terms of zonal polynomials as follows:

Lemma 2.3. *Let s_λ be the Schur function and Z_λ be the zonal polynomial with parameter 2. Then for any partition λ of length $\leq n$,*

$$\int_{O(n, \mathbb{R})} s_\lambda(AO) dO = \begin{cases} \frac{Z_\kappa(a_1^2, \dots, a_n^2)}{Z_\kappa(1, \dots, 1)} & \text{if } \lambda = 2\kappa \\ 0 & \text{otherwise} \end{cases}$$

The power sum symmetric functions p_λ will also be useful. To define these, given a matrix M , if λ is an integer partition and m_j denotes the multiplicity of part j in λ , we set $p_\lambda(M) = \prod_j \text{Tr}(M^j)^{m_j}$. For example, $p_{5,3,3}(M) = \text{Tr}(M^5)\text{Tr}(M^3)^2$. Sometimes we suppress the M and use the notation p_λ . Lemma 2.4, from page 114 of [22], expresses power sum symmetric functions in terms of Schur functions s_λ , and will be used later in the paper.

Lemma 2.4. *Let χ_ρ^λ denote the value of the irreducible character of the symmetric group parameterized by λ on the conjugacy class of elements of type ρ . Then*

$$p_\rho = \sum_\lambda \chi_\rho^\lambda s_\lambda.$$

3. HEAT KERNEL AND LAPLACIAN OF THE ORTHOGONAL GROUP

Recall that a pair (W, W') of random variables is called exchangeable if (W, W') has the same distribution as (W', W) . To construct an exchangeable pair to be used in our applications, we use the heat kernel of G . See [14], [26] for a detailed discussion of heat kernels on compact Lie groups. The papers [20],[21], [24] illustrate combinatorial uses of heat kernels on compact Lie groups, and [21] also discusses the use of the heat kernel for finite groups.

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

$$(1) \quad K(t, x, y) = \sum_{n \geq 0} e^{-\lambda_n t} \phi_n(x) \overline{\phi_n(y)},$$

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. Here Δ denotes the Laplacian of G , and $e^{t\Delta}$ is defined as $I + t\Delta + t^2 \frac{\Delta^2}{2!} + \dots$. Part 2 of Lemma 3.1 is immediate from the expansion (1), and parts 1 and 3 of Lemma 3.1 are on page 198 of [14].

Lemma 3.1. *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) $e^{t\Delta} \phi(x) = \int_{y \in G} K(t, x, y) \phi(y) dy$ for smooth ϕ .

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 [25], [28] 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 $W = f(O)$ where O is chosen from Haar measure, and $W' = f(O')$, where O' is obtained by moving time t from O via the heat kernel. To define the exchangeable pair (W, W') used in this paper, we further specialize by setting $f(O) = \text{Tr}(AO)$.

To analyze the heat kernel on the orthogonal groups, we need to understand the corresponding Laplacian. Proposition 2.7 of the paper [20] gave an explicit description of the Laplacian for $SO(n, \mathbb{R})$. The same calculations work for $O(n, \mathbb{R})$ (which shares the same Lie algebra with $SO(n, \mathbb{R})$), and yield the following result.

Lemma 3.2. *Let A satisfy $\text{Tr}(AA^t) = n$. Then*

(1)

$$\Delta_{O(n)} p_1(AO) = -\frac{(n-1)}{2} p_1(AO).$$

(2)

$$\Delta_{O(n)} p_{1,1}(AO) = -(n-1)p_{1,1}(AO) - p_2(AO) + n.$$

4. MAIN RESULTS

To begin we describe the exchangeable pair (W, W') . Namely $W = \text{Tr}(AO) = p_1(AO)$, where as explained earlier one can assume A is diagonal. We fix $t > 0$, and motivated by Section 3, define

$$W' = e^{t\Delta}(W) = W + \sum_{k \geq 1} \frac{t^k}{k!} \Delta^k(W).$$

Lemma 4.1 computes the conditional expectation $\mathbb{E}[W'|O]$.

Lemma 4.1.

$$\mathbb{E}[W'|O] = \left(1 - \frac{t(n-1)}{2}\right) W + O(t^2).$$

Proof. Applying part 3 of Lemma 3.1 and part 1 of Lemma 3.2,

$$\begin{aligned} \mathbb{E}[W'|O] &= e^{t\Delta}(W) \\ &= W + t\Delta W + O(t^2) \\ &= W + t\frac{-(n-1)}{2}W + O(t^2), \end{aligned}$$

as desired. □

Lemma 4.2 computes $\mathbb{E}[(W' - W)^2|O]$.

Lemma 4.2.

$$\mathbb{E}[(W' - W)^2|O] = t[n - p_2(AO)] + O(t^2).$$

Proof. Clearly

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

By part 3 of Lemma 3.1 and part 2 of Lemma 3.2,

$$\begin{aligned} \mathbb{E}[(W')^2|O] &= W^2 + t\Delta p_{1,1}(AO) + O(t^2) \\ &= W^2 + t[-(n-1)p_{1,1}(AO) - p_2(AO) + n] + O(t^2). \end{aligned}$$

By Lemma 4.1, $-2W\mathbb{E}[W'|O]$ is equal to

$$-2W^2 + t(n-1)p_{1,1}(AO) + O(t^2).$$

Thus

$$\mathbb{E}[(W')^2|O] - 2W\mathbb{E}[W'|O] + W^2 = t[n - p_2(AO)] + O(t^2).$$

□

Lemma 4.3 bounds the variance of $p_2(AO)$.

Lemma 4.3. *Suppose that $n \geq 4$. Then $\text{Var}[p_2(AO)] \leq 2$.*

Proof. By definition, $\text{Var}[p_2(AO)] = \mathbb{E}[p_{2,2}(AO)] - (\mathbb{E}[p_2(AO)])^2$.

From Lemma 2.4,

$$p_2(AO) = -s_{(1,1)}(AO) + s_2(AO).$$

Then Lemma 2.3 gives that $\int_{O(n, \mathbb{R})} -s_{(1,1)}(AO)dO = 0$ and (combined with page 410 of [22]) that

$$\int_{O(n, \mathbb{R})} s_2(AO)dO = \frac{Z_1(a_1^2, \dots, a_n^2)}{Z_1(1, \dots, 1)} = \frac{a_1^2 + \dots + a_n^2}{n} = 1.$$

Thus $\mathbb{E}[p_2(AO)] = 1$.

To compute $\mathbb{E}[p_{2,2}(AO)]$, Lemma 2.4 gives that

$$p_{2,2}(AO) = \chi_{(2,2)}^4 s_4 + \chi_{(2,2)}^{(3,1)} s_{(3,1)} + \chi_{(2,2)}^{(2,2)} s_{(2,2)} + \chi_{(2,2)}^{(2,1,1)} s_{(2,1,1)} + \chi_{(2,2)}^{(1,1,1,1)} s_{(1,1,1,1)}.$$

Lemma 2.3 and the character table of S_4 then give that

$$\begin{aligned} \mathbb{E}[p_{(2,2)}(AO)] &= \mathbb{E}[\chi_{(2,2)}^4 s_4(AO) + \chi_{(2,2)}^{(2,2)} s_{(2,2)}(AO)] \\ &= \mathbb{E}[s_4(AO) + 2s_{(2,2)}(AO)] \\ &= \frac{Z_2(a_1^2, \dots, a_n^2)}{Z_2(1, \dots, 1)} + 2 \frac{Z_{(1,1)}(a_1^2, \dots, a_n^2)}{Z_{(1,1)}(1, \dots, 1)}. \end{aligned}$$

From pages 382 and 383 of [22], it follows that

$$\frac{Z_2(a_1^2, \dots, a_n^2)}{Z_2(1, \dots, 1)} = \frac{n^2 + 2(a_1^4 + \dots + a_n^4)}{n^2 + 2n}$$

and that

$$\frac{Z_{(1,1)}(a_1^2, \dots, a_n^2)}{Z_{(1,1)}(1, \dots, 1)} = \frac{n^2 - (a_1^4 + \dots + a_n^4)}{n^2 - n}.$$

Thus

$$\text{Var}[p_2(AO)] = \left[\frac{n^2}{n^2 + 2n} + \frac{2n^2}{n^2 - n} - 1 \right] - (a_1^4 + \cdots + a_n^4) \left[\frac{2}{n^2 - n} - \frac{2}{n^2 + 2n} \right]$$

By the method of Lagrange multipliers, $a_1^4 + \cdots + a_n^4$ is minimized subject to the constraint $a_1^2 + \cdots + a_n^2 = n$ when $a_1 = \cdots = a_n = 1$. But

$$\left[\frac{n^2}{n^2 + 2n} + \frac{2n^2}{n^2 - n} - 1 \right] - n \left[\frac{2}{n^2 - n} - \frac{2}{n^2 + 2n} \right] = 2,$$

implying that $\text{Var}[p_2(AO)] \leq 2$, as claimed. \square

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

Lemma 4.4. *Suppose that $n \geq 4$. Then*

- (1) $\mathbb{E}(W' - W)^2 = t(n - 1) + O(t^2)$.
- (2) $\mathbb{E}(W' - W)^4 = O(t^2)$.
- (3) $\mathbb{E}|W' - W|^3 = O(t^{3/2})$.

Proof. Lemma 4.2 implies that $\mathbb{E}(W' - W)^2 = t\mathbb{E}[n - p_2(AO)] + O(t^2)$. By the proof of Lemma 4.3, $\mathbb{E}[p_2(AO)] = 1$. Thus

$$\mathbb{E}(W' - W)^2 = t(n - 1) + O(t^2),$$

as claimed.

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

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

By Lemma 4.1,

$$\mathbb{E}[W'|O] = \left(1 - \frac{t(n-1)}{2} \right) W + O(t^2),$$

and by the proof of Lemma 4.2,

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

Thus

$$\begin{aligned} &\mathbb{E}(W' - W)^4 \\ &= 2\mathbb{E}(W^4) - 8\mathbb{E}(W^4) + 6\mathbb{E}(W^4) \\ &\quad + t[4(n-1)\mathbb{E}(W^4) + 6\mathbb{E}[W^2[-(n-1)p_{1,1}(AO) - p_2(AO) + n]]] \\ &\quad + O(t^2) \\ &= t[-2(n-1)\mathbb{E}[p_{1,1,1,1}(AO)] - 6\mathbb{E}[p_{2,1,1}(AO)] + 6n] + O(t^2), \end{aligned}$$

where we used that $\mathbb{E}(W^2) = 1$.

From Lemma 2.4, $p_{1,1,1,1}(AO)$ is equal to

$$\chi_{(1,1,1,1)}^4 s_4 + \chi_{(1,1,1,1)}^{(3,1)} s_{(3,1)} + \chi_{(1,1,1,1)}^{(2,2)} s_{(2,2)} + \chi_{(1,1,1,1)}^{(2,1,1)} s_{(2,1,1)} + \chi_{(1,1,1,1)}^{(1,1,1,1)} s_{(1,1,1,1)}.$$

From Lemma 2.3 and the fact that $\chi_{(1,1,1,1)}^4 = 1$ and $\chi_{(1,1,1,1)}^{(2,2)} = 2$, it follows that

$$\begin{aligned}\mathbb{E}[p_{1,1,1,1}(AO)] &= \mathbb{E}[s_4(AO) + 2s_{2,2}(AO)] \\ &= \frac{Z_2(a_1^2, \dots, a_n^2)}{Z_2(1, \dots, 1)} + 2 \frac{Z_{1,1}(a_1^2, \dots, a_n^2)}{Z_{1,1}(1, \dots, 1)},\end{aligned}$$

where Z_λ denotes the zonal polynomial with parameter two.

Similarly, $p_{2,1,1}(AO)$ is equal to

$$\chi_{(2,1,1)}^4 s_4 + \chi_{(2,1,1)}^{(3,1)} s_{(3,1)} + \chi_{(2,1,1)}^{(2,2)} s_{(2,2)} + \chi_{(2,1,1)}^{(2,1,1)} s_{(2,1,1)} + \chi_{(2,1,1)}^{(1,1,1,1)} s_{(1,1,1,1)}.$$

From Lemma 2.3 and the fact that $\chi_{(2,1,1)}^4 = 1$ and $\chi_{(2,1,1)}^{(2,2)} = 0$, it follows that

$$\mathbb{E}[p_{2,1,1}(AO)] = \mathbb{E}[s_4(AO)] = \frac{Z_2(a_1^2, \dots, a_n^2)}{Z_2(1, \dots, 1)},$$

with Z_λ the zonal polynomial with parameter 2.

As in the proof of Lemma 4.3, one has that

$$\frac{Z_2(a_1^2, \dots, a_n^2)}{Z_2(1, \dots, 1)} = \frac{n^2 + 2(a_1^4 + \dots + a_n^4)}{n^2 + 2n}$$

and that

$$\frac{Z_{(1,1)}(a_1^2, \dots, a_n^2)}{Z_{(1,1)}(1, \dots, 1)} = \frac{n^2 - (a_1^4 + \dots + a_n^4)}{n^2 - n}.$$

Plugging in these values, one obtains that

$$\begin{aligned}& \mathbb{E}(W' - W)^4 \\ &= -2(n-1)t \left[\frac{n^2 + 2(a_1^4 + \dots + a_n^4)}{n^2 + 2n} + \frac{2(n^2 - (a_1^4 + \dots + a_n^4))}{n^2 - n} \right] \\ & \quad - 6t \left[\frac{n^2 + 2(a_1^4 + \dots + a_n^4)}{n^2 + 2n} \right] + 6nt + O(t^2) \\ &= O(t^2),\end{aligned}$$

proving part 2 of the theorem.

For part 3 of the theorem, 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 theorem. \square

Lemma 4.5. *Let f be a twice differentiable function with bounded second derivative. Then*

$$\mathbb{E}[f'(W) - Wf(W)] = \mathbb{E} \left[\frac{p_2(AO) - 1}{n-1} f'(W) \right].$$

Proof. Since (W, W') is an exchangeable pair,

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

Now by Lemma 4.1,

$$\begin{aligned} 2\mathbb{E}[(W' - W)f(W)] &= 2\mathbb{E}[f(W)\mathbb{E}[(W' - W)|O]] \\ &= -t(n-1)\mathbb{E}[f(W)W] + O(t^2). \end{aligned}$$

By Taylor's theorem and Lemma 4.2, it follows that

$$\begin{aligned} \mathbb{E}[(W' - W)(f(W') - f(W))] &= \mathbb{E}[(W' - W)[f'(W)(W' - W)] + R] \\ &= \mathbb{E}[f'(W)\mathbb{E}[(W' - W)^2|O]] + R \\ &= \mathbb{E}[tf'(W)[n - p_2(AO)] + R] + O(t^2), \end{aligned}$$

with $|R| \leq \frac{\|f''\|}{2}|W' - W|^3$, where $\|\cdot\|$ denotes the supremum norm. From part 3 of Lemma 4.4, it follows that $R = O(t^{3/2})$.

Summarizing, we have that

$$\begin{aligned} 0 &= 2\mathbb{E}[(W' - W)f(W)] + \mathbb{E}[(W' - W)(f(W') - f(W))] \\ &= -t(n-1)\mathbb{E}[f(W)W] + t\mathbb{E}[f'(W)[n - p_2(AO)]] + O(t^{3/2}). \end{aligned}$$

Dividing both sides of this equation by t and then letting $t \rightarrow 0$ completes the proof. \square

Now we prove our main result.

Theorem 4.6. *The total variation distance between W and a standard normal is at most $\frac{2\sqrt{2}}{n-1}$.*

Proof. Note that the total variation distance between two random variables W and Z can be described as

$$d_{TV}(W, Z) = \sup_h |\mathbb{E}h(W) - \mathbb{E}h(Z)|,$$

where the supremum ranges over all h that are continuous and bounded from below by 0 and from above by 1 and have compact support.

Any such function h can be approximated by C^∞ functions in the supremum norm. For fixed h let h_m be a sequence of C^∞ functions such that $\|h - h_m\| \rightarrow 0$ as $m \rightarrow \infty$ where $\|\cdot\|$ denotes the supremum norm.

Let f_m be the solution to the Stein equation

$$f'_m(x) - xf_m(x) = h_m(x) - \mathbb{E}h_m(Z),$$

where Z has the standard normal distribution. Since we approximate h by a compactly supported C^∞ function, Formula (47) on page 25 of [28] allows us to assume that $\|f''_m\|$ is bounded. Applying Lemma 4.5 (so taking $T(AO) = \frac{p_2(AO)-1}{n-1}$ in the formulas below), we have

$$\begin{aligned}
& |\mathbb{E}h(W) - \mathbb{E}h(Z)| \\
& \leq 2\|h - h_m\| + |\mathbb{E}h_m(W) - \mathbb{E}h_m(Z)| \\
& \leq 2\|h - h_m\| + |\mathbb{E}[f'_m(W) - Wf_m(W)]| \\
& \leq 2\|h - h_m\| + \sqrt{\text{Var}(T)}\|f'_m\| \\
& \leq 2\|h - h_m\| + 2\sqrt{\text{Var}(T)}\|h_m - \mathbb{E}h_m(Z)\| \\
& \leq (2 + 4\sqrt{\text{Var}(T)})\|h - h_m\| + 2\sqrt{\text{Var}(T)}\|h - \mathbb{E}h(Z)\|.
\end{aligned}$$

(The inequality $\|f'_m\| \leq 2\|h_m - \mathbb{E}h_m(Z)\|$ is Formula (46) on page 25 of Stein [28]).

Letting $m \rightarrow \infty$ we therefore have

$$|\mathbb{E}h(W) - \mathbb{E}h(Z)| \leq 2\sqrt{\text{Var}(T)}\|h - \mathbb{E}h(Z)\|$$

for any continuous function h . As $\|h - \mathbb{E}h(Z)\| \leq 1$ and $\text{Var}(T) \leq \frac{2}{(n-1)^2}$ by Lemma 4.3, the total variation bound now follows. \square

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