

On the Maximal Halfspace Depth of Permutation-invariant Distributions on the Simplex

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Abstract

We compute the maximal halfspace depth for a class of permutation-invariant distributions on the probability simplex. The derivations are based on stochastic ordering results that so far were only showed to be relevant for the Behrens-Fisher problem.

Keywords: α -unimodality, Dirichlet distribution, Halfspace depth, Majorization, Stochastic ordering

1. Introduction

Denoting as $\mathcal{S}^{k-1} := \{x \in \mathbb{R}^k : \|x\|^2 = x'x = 1\}$ the unit sphere in \mathbb{R}^k , the Tukey (1975) halfspace depth $HD(\theta, P) = \inf_{u \in \mathcal{S}^{k-1}} P[u'(X - \theta) \geq 0]$ measures the centrality of the k -vector θ with respect to a probability measure $P = P^X$ over \mathbb{R}^k . Any probability measure P admits a deepest point, that generalizes to the multivariate setup the univariate median; see, e.g., Proposition 7 in Rousseeuw and Ruts (1999). Parallel to the univariate

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median, this deepest point is not unique in general. Whenever a unique representative of the collection C_P of P 's deepest points is needed, the *Tukey median* θ_P , that is defined as the barycentre of C_P , is often considered. The convexity of C_P (see, e.g., the corollary of Proposition 1 in Rousseeuw and Ruts, 1999) implies that θ_P has maximal depth. The depth of θ_P is larger than or equal to $1/(k+1)$; see Lemma 6.3 in Donoho and Gasko (1992).

In this paper, we determine the Tukey median and the corresponding maximal depth for a class of permutation-invariant distributions on the probability simplex $\mathcal{D}_k := \{x \in \mathbb{R}^k : x_1, \dots, x_k \geq 0, \sum_{\ell=1}^k x_\ell = 1\}$. The results identify the most central location for some of the most successful models used for compositional data. They have also recently proved useful in the context of depth for shape matrices; see Paindaveine and Van Bever (2017).

The outline of the paper is as follows. In Section 2, we define the class of distributions we will consider and state a stochastic ordering result on which our derivations will be based. In Section 3, we state and prove the main results of the paper. Finally, in Section 4, we illustrate the results through numerical exercises and we shortly comment on open research questions.

2. Preliminaries

Let \mathcal{F} be the collection of cumulative distribution functions F such that (i) $F(0) = 0$ and (ii) F is concave on $(0, +\infty)$. In other words, \mathcal{F} collects the cumulative distribution functions of random variables that are (i) almost surely positive and (ii) unimodal at 0. Any F in \mathcal{F} admits a probability

density function f that is non-increasing on $(0, +\infty)$.

For an integer $k \geq 2$ and F in \mathcal{F} , consider the random k -vector

$$X_k = (X_{k1}, \dots, X_{kk})' = (V_{k1}, \dots, V_{kk})' / \sum_{\ell=1}^k V_{k\ell}, \quad (1)$$

where V_{k1}, \dots, V_{kk} are mutually independent and have cumulative distribution function F . The corresponding probability measure over \mathbb{R}^k will be denoted as $P_{k,F}$. Obviously, the random vector X_k takes its values in the probability simplex \mathcal{D}_k . This includes, for example, the Dirichlet distribution with parameter $(\alpha, \dots, \alpha)' \in \mathbb{R}^k$, obtained for the cumulative distribution function $F = F_\alpha$ of the Gamma($\alpha, \frac{1}{2}$) distribution (that corresponds to the probability density function $x \mapsto x^{\alpha-1} \exp(-x/2) / (2^\alpha \Gamma(\alpha))$ on $(0, +\infty)$, where Γ is the Euler Gamma function). The unimodality constraint in (ii) above imposes to restrict to $\alpha \leq 1$. Note that, irrespective of F , the mean vector of X_k is $\mu_k = k^{-1} \mathbf{1}_k = k^{-1}(1, \dots, 1)'$.

To state the stochastic ordering result used in the sequel, we need to introduce the following notation. For n -vectors a, b with $\sum_{\ell=1}^n a_\ell = \sum_{\ell=1}^n b_\ell$, we will say that a is *majorized by* b if and only if, after permuting the components of these vectors in such a way that $a_1 \geq a_2 \geq \dots \geq a_n$ and $b_1 \geq b_2 \geq \dots \geq b_n$ (possible ties are unimportant below), $\sum_{\ell=1}^r a_\ell \leq \sum_{\ell=1}^r b_\ell$, for any $r = 1, \dots, n-1$; see, e.g., Marshall et al. (2011). For random variables Y_1 and Y_2 , we will say that Y_1 is stochastically smaller than Y_2 ($Y_1 \leq_{\text{st}} Y_2$) if and only if $P[Y_1 > t] \leq P[Y_2 > t]$ for any $t \in \mathbb{R}$. To the best of our knowledge,

the following stochastic ordering result so far was only used in the framework of the Behrens-Fisher problem; see Hájek (1962), Lawton (1968), and Eaton and Olshen (1972).

Lemma 1 (Eaton and Olshen, 1972). *Let W be a random variable with a cumulative distribution function in \mathcal{F} . Let Q_1, \dots, Q_n be exchangeable positive random variables that are independent of W . Then, $W/(\sum_{\ell=1}^n a_\ell Q_\ell) \leq_{\text{st}} W/(\sum_{\ell=1}^n b_\ell Q_\ell)$ for any $a, b \in \mathbb{R}^n$ such that a is majorized by b .*

In Eaton and Olshen (1972), the result is stated in a vectorial context that requires the α -unimodality concept from Olshen and Savage (1970). In the present scalar case, the minimal unimodality assumption in Eaton and Olshen (1972) is that \sqrt{W} is 2-unimodal about zero, which, in view of Lemma 2 in Olshen and Savage (1970), is strictly equivalent to requiring that W is unimodal about zero.

3. Main results

Our main goal is to determine the Tukey median of the probability measure $P_{k,F}$ and the corresponding maximal depth. Permutation invariance of $P_{k,F}$ and affine invariance of halfspace depth allows to obtain

Theorem 1. *The Tukey median of $P_{k,F}$ is $\mu_k = k^{-1}1_k$.*

PROOF OF THEOREM 1. Let $\theta_* = (\theta_{*1}, \dots, \theta_{*k})'$ be a point maximizing $HD(\theta, P_{k,F})$ and let $\alpha_* = HD(\theta_*, P_{k,F})$ be the corresponding maximal depth. Of course, $\theta_* \in \mathcal{D}_k$ (if $\theta \notin \mathcal{D}_k$, then $HD(\theta, P_{k,F}) = 0$). Denote by π_i ,

$i = 1, \dots, k!$, the $k!$ permutation matrices on k -vectors. By affine invariance of halfspace depth and permutation invariance of $P_{k,F}$, all $\pi_i \theta_*$'s have maximal depth α_* with respect to $P_{k,F}$. Now, for any $\ell = 1, \dots, k$,

$$\frac{1}{k!} \sum_{i=1}^{k!} (\pi_i \theta_*)_\ell = \frac{1}{k!} \sum_{\ell=1}^k (k-1)! \theta_{*\ell} = \frac{1}{k} \sum_{\ell=1}^k \theta_{*\ell} = \frac{1}{k} = (\mu_k)_\ell.$$

Since this holds for any θ_* maximizing $HD(\theta, P_{k,F})$, the result is proved. \square

Note that the unimodality of F about zero is not used in the proof of Theorem 1, so that the result also holds at F_α with $\alpha \geq 1$. In contrast, the proof of the following result, that derives the halfspace depth of the Tukey median of $P_{k,F}$, requires unimodality.

Theorem 2. *Let $X_k = (X_{k1}, \dots, X_{kk})'$ have distribution $P_{k,F}$ with $F \in \mathcal{F}$. Then, $HD(\mu_k, P_{k,F}) = P[X_{k1} \geq 1/k]$.*

The proof requires the following preliminary result.

Lemma 2. *For any positive integer k , let $h_{k,F} = P[X_{k1} \geq 1/k]$, where $X_k = (X_{k1}, \dots, X_{kk})'$ has distribution $P_{k,F}$ with $F \in \mathcal{F}$. Then, the sequence $(h_{k,F})$ is monotone non-increasing.*

PROOF OF LEMMA 2. Since $k^{-1}1_k$ is majorized by the k -vector $(k-1)^{-1}(1, \dots, 1, 0)'$, Lemma 1 readily provides

$$\begin{aligned} h_{k+1,F} &= P \left[V_{k+1,1} \geq \frac{1}{k+1} \sum_{\ell=1}^{k+1} V_{k+1,\ell} \right] = P \left[\frac{k}{k+1} V_{k+1,1} \geq \frac{1}{k+1} \sum_{\ell=2}^{k+1} V_{k+1,\ell} \right] \\ &= P \left[\frac{V_{k+1,1}}{\frac{1}{k} \sum_{\ell=2}^{k+1} V_{k+1,\ell}} \geq 1 \right] \leq P \left[\frac{V_{k+1,1}}{\frac{1}{k-1} \sum_{\ell=2}^k V_{k+1,\ell}} \geq 1 \right] \end{aligned}$$

$$= P \left[V_{k1} \geq \frac{1}{k-1} \sum_{\ell=2}^k V_{k\ell} \right] = P \left[V_{k1} \geq \frac{1}{k} \sum_{\ell=1}^k V_{k\ell} \right] = h_{k,F},$$

which establishes the result. \square

Note that this result shows that, for any F in \mathcal{F} , the maximal depth, $h_{k,F}$, in Theorem 2 is monotone non-increasing in k , hence converges as k goes to infinity. Clearly, the law of large numbers and Slutsky's theorem imply that $V_{k1}/(\frac{1}{k} \sum_{\ell=1}^k V_{k\ell}) \rightarrow V_{11}/\mathbb{E}[V_{11}]$ in distribution, so that $h_{k,F}$ converges to $h_{\infty,F} = P[V_{11} \geq \mathbb{E}[V_{11}]]$ as k goes to infinity. In particular, for $F = F_\alpha$, the limiting value is $h_{\infty,F_\alpha} = P[Z_\alpha > \alpha]$, where Z_α is Gamma($\alpha, 1$) distributed.

We can now prove the main result of this paper.

PROOF OF THEOREM 2. We are looking for the infimum with respect to $u = (u_1, \dots, u_k)'$ in \mathcal{S}^{k-1} , or equivalently in $\mathbb{R}^k \setminus \{0\}$, of

$$\begin{aligned} p(u) &:= P \left[\sum_{\ell=1}^k u_\ell \left(X_{k\ell} - \frac{1}{k} \right) \geq 0 \right] = P \left[\sum_{\ell=1}^k u_\ell X_{k\ell} \geq \bar{u} \right] \\ &= P \left[\sum_{\ell=1}^k u_\ell V_{k\ell} \geq \bar{u} \sum_{\ell=1}^k V_{k\ell} \right] = P \left[\sum_{\ell=1}^k (u_\ell - \bar{u}) V_{k\ell} \geq 0 \right], \end{aligned}$$

where we wrote $\bar{u} := \frac{1}{k} \sum_{\ell=1}^k u_\ell$. Without loss of generality, we may assume that $u_1 \geq u_2 \geq \dots \geq u_k$, which implies that $u_1 \geq \bar{u}$. Actually, if $u_1 = \bar{u}$, then all u_ℓ 's must be equal to \bar{u} , which makes the probability $p(u)$ equal to one. Since this cannot be the infimum, we may assume that $u_1 > \bar{u}$, which implies that $u_k < \bar{u}$. Therefore, denoting as m the largest integer for which $u_m \geq \bar{u}$,

we have $1 \leq m \leq k - 1$. Then, letting $s_m(u) = \sum_{\ell=1}^m (u_\ell - \bar{u})$, we may then write

$$p(u) = P \left[\sum_{\ell=1}^m (u_\ell - \bar{u}) V_{k\ell} \geq \sum_{\ell=m+1}^k (\bar{u} - u_\ell) V_{k\ell} \right] = P \left[\frac{\sum_{\ell=m+1}^k d_\ell(u) V_{k\ell}}{\sum_{\ell=1}^m c_\ell(u) V_{k\ell}} \leq 1 \right],$$

where $c_\ell(u) = (u_\ell - \bar{u})/s_m(u)$, $\ell = 1, \dots, m$ and $d_\ell(u) = (\bar{u} - u_\ell)/s_m(u)$, $\ell = m + 1, \dots, k$ are nonnegative and satisfy $\sum_{\ell=1}^m c_\ell(u) = 1$ and

$$\sum_{\ell=m+1}^k d_\ell(u) = \frac{\sum_{\ell=m+1}^k (\bar{u} - u_\ell)}{\sum_{\ell=1}^m (u_\ell - \bar{u})} = \frac{(k - m)\bar{u} - \sum_{\ell=m+1}^k u_\ell}{\sum_{\ell=1}^m u_\ell - m\bar{u}} = 1.$$

Since $\sum_{\ell=1}^m d_\ell(u) V_{k\ell}$ is unimodal at zero and since $(c_1(u), c_2(u), \dots, c_m(u))'$ is majorized by $(1, 0, \dots, 0)' \in \mathbb{R}^m$, Lemma 2 yields

$$p(u) \geq P \left[\frac{\sum_{\ell=m+1}^k d_\ell(u) V_{k\ell}}{V_{k1}} \leq 1 \right] = P \left[\frac{V_{km}}{\sum_{\ell=m+1}^k d_\ell(u) V_{k\ell}} \geq 1 \right],$$

where the lower bound is obtained for $c_1(u) = 1$ and $c_2(u) = \dots = c_m(u) = 0$, that is, for $u_1 (> \bar{u})$ arbitrary and $u_2 = \dots = u_m = \bar{u}$. Now, since $(k - m)^{-1} \mathbf{1}_{k-m}$ is majorized by $(d_{m+1}(u), \dots, d_k(u))'$ for any u , the same result provides

$$\begin{aligned} p(u) &\geq P \left[\frac{V_{km}}{\frac{1}{k-m} \sum_{\ell=m+1}^k V_{k\ell}} \geq 1 \right] = P \left[(k - m) V_{km} \geq \sum_{\ell=m+1}^k V_{k\ell} \right] \\ &= P \left[(k - m + 1) V_{km} \geq \sum_{\ell=m}^k V_{k\ell} \right] = P \left[X_{k-m+1,1} \geq \frac{1}{k - m + 1} \right] = h_{k-m+1, F}, \end{aligned}$$

with the lower bound obtained for $d_\ell(u) = 1/(k - m)$, $\ell = m + 1, \dots, k$, that is, for $u_\ell = \bar{u} - \frac{1}{k-m}(u_1 - \bar{u})$, $\ell = m + 1, \dots, k$. Therefore, the global minimum is the minimum of $h_{k-m+1, F}$, $m = 1, \dots, k - 1$, which, in view of Lemma 2, is $h_{k, F}$. This establishes the result. \square

Figure 1 plots the maximal depth h_{k, F_α} as a function of k for several α , where F_α still denotes the cumulative distribution function of the $\text{Gamma}(\alpha, \frac{1}{2})$ distribution. In accordance with Lemma 2, the maximal depth is decreasing in k and is seen to converge to the limiting value h_{∞, F_α} that was obtained below that lemma. For any α , the maximal depth is equal to $1/2$ if and only if $k = 2$, which is in line with the fact that the (non-atomic) probability measure P_{k, F_α} is (angularly) symmetric about μ_k if and only if $k = 2$; see Rousseeuw and Struyf (2004). Interestingly, thus, the asymmetry of $P_{k, F}$ for $k \geq 3$ would typically be missed by a test of symmetry that would reject the null when the sample (Tukey) median is too far from the sample mean.

4. Numerical illustration

We conducted two numerical exercises to illustrate Theorems 1 and 2, both in the trivariate case $k = 3$. In the first exercise, we generated $N = 1,000$ random locations $\theta_1, \dots, \theta_N$ from the uniform distribution over \mathcal{D}_k (that is the distribution P_{k, F_1} associated with the $\text{Gamma}(1, \frac{1}{2})$ distribution of the $V_{k\ell}$'s; see, e.g., Proposition 2 in Bélisle, 2011). Our goal is to compare, for various values of α , the depths $HD(\theta_i, P_{k, F_\alpha})$, $i = 1, \dots, N$ with the depth $HD(\mu_k, P_{k, F_\alpha})$. For each α , these $N + 1$ depth values were estimated

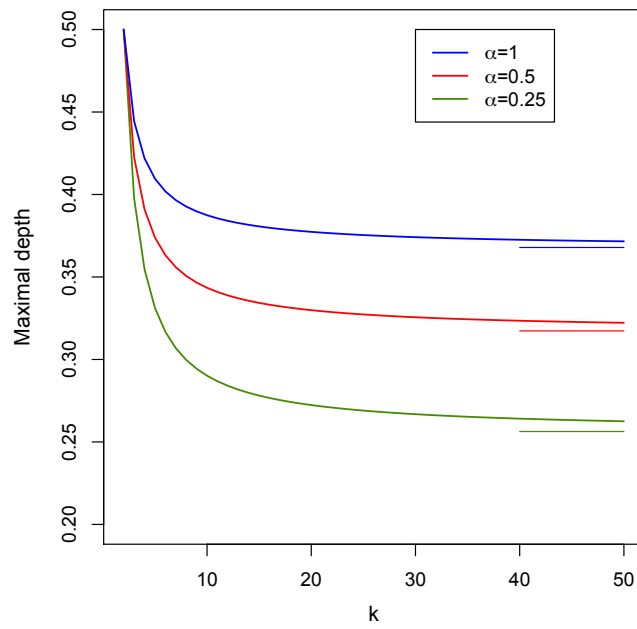


Figure 1: Plots of the maximal depth h_{k,F_α} as a function of k for several values of α , where F_α denotes the cumulative distribution function of the $\text{Gamma}(\alpha, \frac{1}{2})$ distribution. For each value of α considered, the limiting value as k goes to infinity is also showed.

by the depths $HD(\theta_i, P_n)$, $i = 1, \dots, N$, and $HD(\mu_k, P_n)$, computed with respect to the empirical measure P_n of a random sample of size $n = 100,000$ from P_{k, F_α} (these $N+1$ sample depth values were actually averaged over $M = 100$ mutually independent such samples). For each α , Figure 2 reports the boxplots of the resulting estimates of $HD(\theta_i, P_{k, F_\alpha})$, $i = 1, \dots, N$, and marks the estimated value of $HD(\mu_k, P_{k, F_\alpha})$. The results clearly support the claim in Theorem 1 that $\mu_k = \arg \max_{\theta} HD(\theta, P_{k, F_\alpha})$.

In the second numerical exercise, we generated, for various values of α and n , a collection of $M = 1,000$ mutually independent random samples of size n from the distribution P_{k, F_α} . For each sample, we evaluated the half-space depth of μ_k with respect to the corresponding empirical distribution P_n . Figure 3 provides, for each α and n , the boxplot of the resulting M depth values. Clearly, the results, through the consistency of sample depth, support the theoretical depth values provided in Theorem 2. Actually, while the theorem was only proved above for $\alpha \leq 1$ (due to the unimodality condition in Lemma 1), these empirical results suggest that the theorem might hold also for $\alpha > 1$. The extension of the proof of Theorem 2 to further distributions is an interesting research question, that requires another approach (simulations indeed reveal that Lemma 1 does not hold if the cumulative distribution function of W is F_α with $\alpha > 1$). Of course, another challenge is to derive a closed form expression for $HD(\theta, P_{k, F})$ for an arbitrary θ . After putting some effort into this question, it seemed to us that such a computation calls for a more general stochastic ordering result than the one in Lemma 1.

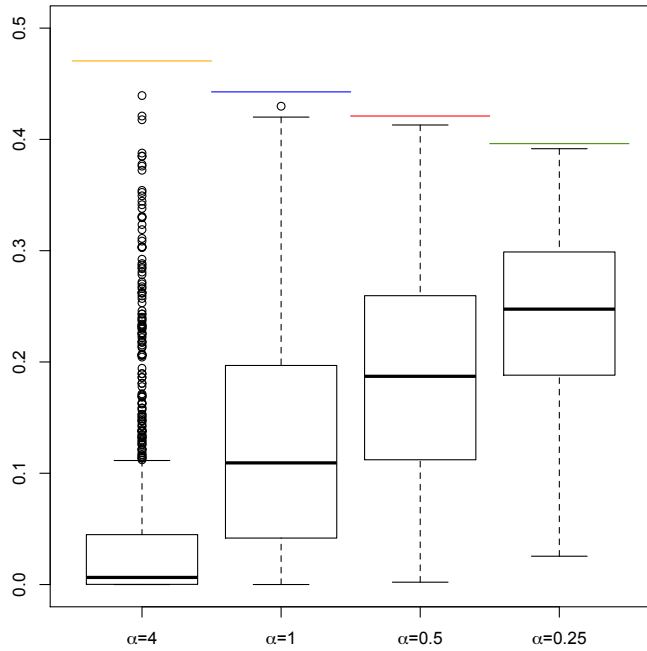


Figure 2: Boxplots, for $k = 3$ and for various values of α , of the sample depth values $HD(\theta_i, P_n)$, $i = 1, \dots, N$, of $N = 1,000$ locations randomly drawn from the uniform distribution over the probability simplex \mathcal{D}_k , where P_n denotes the empirical probability measure associated with a random sample of size $n = 100,000$ from the distributions P_{k, F_α} , with $\alpha = 4, 1, 0.5, 0.25$. For each value of α considered, the sample depth $HD(\mu_k, P_n)$ is also provided (as explained in Section 4, these sample depths were actually averaged over $M = 100$ mutually independent samples in each case).

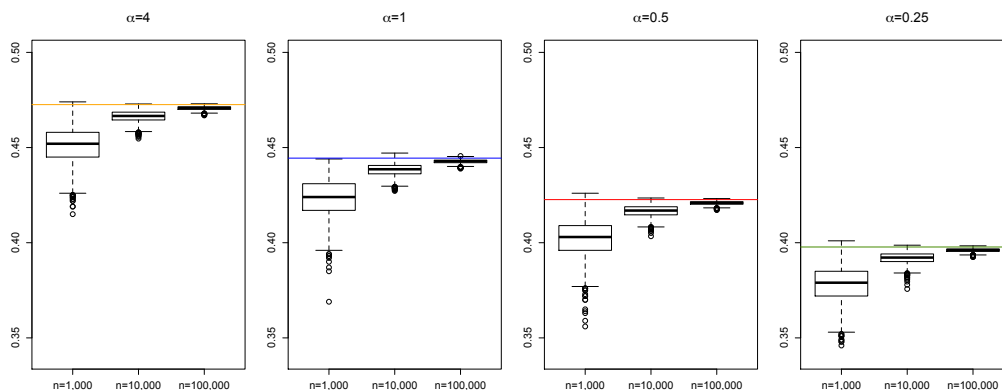


Figure 3: Boxplots, for $k = 3$ and for various values of α and n , of $M = 1,000$ mutually independent values of the depth $HD(\mu_k, P_n)$, where P_n denotes the empirical probability measure associated with a random sample of size n from the same distributions P_{k, F_α} as in Figure 2.

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