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Research Article

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The diameter of the Birkhoff polytope

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Abstract: The geometry of the compact convex set of all $n \times n$ doubly stochastic matrices, a structure frequently referred to as the Birkhoff polytope, has been an active subject of research as of late. Geometric characteristics such as the Chebyshev center and the Chebyshev radius with respect to the operator norms from ℓ_n^p to ℓ_n^p and the Schatten *p*-norms, both for the range $1 \le p \le \infty$, have only recently been studied in depth. In this article, we continue in this vein by determining the diameter of the Birkhoff polytope with respect to the metrics induced by the aforementioned matrix norms.

Keywords: Doubly stochastic matrices, Birkhoff polytope, diameter, operator norm, Schatten p-norms

MSC 2020: 15B51, 46B20, 52B12, 47B10

1 Introduction

A square matrix $A = [a_{ij}]$ with nonnegative real entries is said to be *row-stochastic* (or *right stochastic*) if

$$\sum_{j=1}^n a_{ij} = 1, \quad \forall i = 1, \dots, n.$$

Similarly, it is said to be column-stochastic (or left stochastic) if

$$\sum_{i=1}^{n} a_{ij} = 1, \quad \forall j = 1, \dots, n$$

A *doubly stochastic matrix* is one that is both row-stochastic and column-stochastic.

The theory of stochastic and doubly stochastic matrices was first developed alongside the Markov chain by the Russian mathematician Andrei Andreevich Markov (1856–1922) at the beginning of the twentieth century.

Markov first began developing his ideas about chains of linked events (where what happens next depends on the current state of the system) in 1906. The initial intended uses of the new branch of probability theory that he was elaborating were for linguistic analysis. Delving into the text of Alexander Pushkin's novel in verse *Eugene Onegin*, Markov treated the text as a mere stream of letters. He spent hours sifting through patterns of vowels and consonants with the aim of estimating to what extent there is an exaggerated tendency in Pushkin's text for vowels and consonants to alternate, thus violating the principle of independence. Although Markov's analysis remains on a superficial level from a linguistic point of view, it made a lasting impression because the technique involved presciently extended the theory of probability in a new direction [27].

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In the 100 years since Markov's early work, stochastic and doubly stochastic matrices have found use in almost every field of science, from econometrics [31,35] to geology [37,38], ecology [23], and population genetics [24,33].

The ubiquity of stochastic and doubly stochastic matrices in science as a tool for statistical analysis alone justifies the study of these sets of matrices. But they are not without intrinsic interest. For instance, it is well known that the set of doubly stochastic matrices of size $n \times n$, which we denote by Ω_n , forms a semigroup with respect to matrix multiplication. It is also a convex polytope (i.e., a compact convex set with a finite number of extreme points) of dimension $(n - 1)^2$ in the Euclidean space of dimension n^2 . Most interestingly, it was shown by Birkhoff [3] that the extreme points of Ω_n are precisely the $n \times n$ permutation matrices, denoted by \mathcal{P}_n , and that each $D \in \Omega_n$ admits a (not necessarily unique) *Birkhoff decomposition* $D = \sum_{i=1}^r \alpha_i P_i$, where $P_i \in \mathcal{P}_n$, $\alpha_i \ge 0$, and $\sum_{i=1}^r \alpha_i = 1$. Due to this fundamental characterization, Ω_n is sometimes referred to as the *Birkhoff polytope*.

In the last few decades, the geometric features of the Birkhoff polytope have been an active subject of research. For instance, in the 1970s, Brualdi and Gibson studied the Euclidean geometry structure of Ω_n . In a series of four articles [7–10], they characterized the faces, the edges, and the facets of Ω_n . At the turn of the millennium, several teams of researchers sought to characterize the volume of the Birkhoff polytope. In particular, formulas for the volume of Ω_n were given by Sturmfels [36] for $n \leq 7$, by Chan and Robbins [13] for n = 8, and by Beck and Pixton [2] for n = 9, 10. As for the case of $10 \leq n \leq 15$, estimates were obtained by Emiris and Fisikopoulos in 2014 [21], and by Cousins and Vempala in 2016 [16]. In 2009, De Loera et al. [19] presented a combinatorial formula for the volume of Ω_n , while Canfield and MacKay [11] discovered an asymptotic formula during the same year. In a different but related vein, an intensive investigation of combinatorial and geometric properties of the acyclic Birkhoff polytope has been done in [14,15,22,29], and interesting combinatorial peculiarities of the facial structure of the polytope consisting of the tridiagonal doubly stochastic matrices of order *n* have been extensively considered in [12,17,18].

Despite their frequent applications in some areas of mathematics, geometric notions such as the radius and the diameter of Ω_n have so far received little attention. The few articles dealing with these issues include papers from 1998 by Glunt et al. [25,26], by Khoury [30], and more recently by the authors of this manuscript [5,6]. While studying numerical simulation of large linear semiconductor circuit networks, Glunt et al. [25] naturally came across the following question: given a matrix *B* of order *n* subject to the constraints $e_1^{\top}D^ke_1 = e_1^{\top}B^ke_1$, $k \ge 1$, where $e_1 = (1, 0, ..., 0)^{\top}$, which generalized doubly stochastic matrix *D* is closest to *B* in the sense of Frobenius? They were able to give an algorithm to numerically find the solution. Khoury [30] independently studied the same question, bar the constraints mentioned above. He showed that $D = WBW + J_n$, where $W = I_n - J_n$ and J_n is the $n \times n$ matrix with every entry uniformly equal to 1/n. This line of investigation was later pursued by Glunt et al. in [26] and further developed in the more specific case of doubly stochastic matrices (as opposed to generalized doubly stochastic matrices) in [1] by Bai et al. in 2007. Finally, in [5,6], the authors carried out a detailed analysis of Chebyshev's center and radius of the Birkhoff polytope, when equipped with the operator norms from ℓ_n^p to ℓ_n^p ($1 \le p \le \infty$) and that of the Schatten p-norms ($1 \le p < \infty$). Along the way, they discussed classical problems such as finding the radius of a minimal bounding ball for the Birkhoff polytope and the smallest enclosing ball problem.

The present article is fully in line with the latter two above-mentioned papers in that the question addressed is centered around studying the geometry of the Birkhoff polytope when the ambient space is endowed with the metric induced by the operator norm from ℓ_n^p to ℓ_n^p ($1 \le p \le \infty$) and, in turn, with the Schatten *p*-norm ($p \ge 1$).

This article is structured as follows. In Section 2, we establish the preliminaries needed for later use. More precisely, we recall the definitions of the norms considered therein. We then state a few elementary results on the spectrum of doubly stochastic matrices as well as on a special matrix that plays a central role in the theory of doubly stochastic matrices. In Section 3, we briefly review the definition of the diameter of a nonempty set in a metric space. In Section 4, we determine by fairly elementary means that the diameter of the Birkhoff polytope in the case of the operator norms from ℓ_n^p to ℓ_n^p is 2 for $1 \le p \le \infty$. Finally, in Section 5, we first derive that the diameter of the Birkhoff polytope with respect to the metric induced by the Schatten *p*-norms $(1 \le p < \infty)$ is given by $\max_{p \in \mathcal{P}_n} ||I_n - P||_{S_p}$. A calculation then shows that

$$||I_n - P||_{\mathcal{S}_p} = 2\left(\sum_{k=1}^{n_1} \sin^p\left(\frac{\pi k}{n_1}\right) + \sum_{k=1}^{n_2} \sin^p\left(\frac{\pi k}{n_2}\right) + \dots + \sum_{k=1}^{n_r} \sin^p\left(\frac{\pi k}{n_r}\right)\right)^{\frac{1}{p}},$$

for some positive integer $n_1, ..., n_r$ such that $n_1 + ... + n_r = n$. From this point onward, the problem of calculating the diameter of the Birkhoff polytope becomes a trigonometric maximization problem. Using numerous identities, we establish in turn that

$$\operatorname{diam}_{\mathcal{S}_{p}}(\Omega_{n}) = \begin{cases} 2 \cot\left(\frac{\pi}{2n}\right), & \text{if } p = 1, \\ 2 \left[\sum_{k=1}^{n} \sin^{p}\left(\frac{\pi k}{n}\right)\right]^{\frac{1}{p}}, & \text{if } 1 2. \end{cases}$$

2 Definitions, properties, and preliminary results

In this section, we recall the definition of some standard matrix norms that will be considered in the rest of this article. We also explore some properties of doubly stochastic matrices that are used extensively in the rest of this article.

2.1 Operator norms induced by the vector *p*-norms

For $p \ge 1$, the *p*-norm of a given vector $x = (x_1, ..., x_n)$ is defined by:

$$||x||_p = \left(\sum_{k=1}^n |x_k|^p\right)^{1/p},$$

and the ∞ -norm is defined by:

$$||x||_{\infty} = \max\{|x_1|, ..., |x_n|\}.$$

We shall denote the space \mathbb{C}^n equipped with the vector *p*-norm by $\ell_n^p(\mathbb{C})$, or by ℓ_n^p for short.

Any $n \times n$ matrix A can be interpreted as an operator from ℓ_n^p to ℓ_n^p . The operator norm of A induced by the vector *p*-norm is given by:

$$||A||_{\ell_n^p \to \ell_n^p} \coloneqq \sup_{x \neq 0} \frac{||Ax||_p}{||x||_p}.$$

For all $1 \le p \le \infty$, we have $||B||_{\ell_n^p \to \ell_n^p} = ||B^*||_{\ell_n^q \to \ell_n^q}$, where B^* denotes the conjugate transpose of B and q is the Hölder conjugate exponent of p, i.e., $\frac{1}{p} + \frac{1}{q} = 1$ [28, p. 357].

It is also worth mentioning two properties of the operator norms induced by the vector *p*-norms, which will prove useful in the remainder of this article. Both easily derive from the definition. These are: 1. *Sub-multiplicativity*: For all $p \in [1, \infty]$ and all $n \times n$ matrices *A* and *B*,

$$||AB||_{\ell^p_n \to \ell^p_n} \leq ||A||_{\ell^p_n \to \ell^p_n} ||B||_{\ell^p_n \to \ell^p_n};$$

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2. *Permutation invariance*: For all $p \in [1, \infty]$, all $n \times n$ matrix A, and all $n \times n$ permutation matrices P and Q,

$$|PAQ||_{\ell_n^p \to \ell_n^p} = ||A||_{\ell_n^p \to \ell_n^p}.$$

Finally, since the sets of interest to us in what follows (i.e., Ω_n and \mathcal{P}_n) are invariant under the conjugate transpose action, many operators considered below have the same norm, whether we see them as $\ell_n^p \to \ell_n^p$ or as $\ell_n^q \to \ell_n^q$ mappings. For the sake of concision, when such situations arise, we shall only consider the case $1 \le p \le 2$.

2.2 Schatten *p*-norms

Given an $n \times n$ matrix A, let $\lambda_1, ..., \lambda_n$ denote the eigenvalues of A^*A , with repetitions counted. Note that for all i = 1, 2, ..., n we have

$$\lambda_i ||x||_2^2 = \langle \lambda_i x, x \rangle = \langle A^* A x, x \rangle = \langle A x, A x \rangle \ge 0.$$

Hence, λ_i s are non-negative real numbers. Order these so that $\lambda_1 \ge \cdots \ge \lambda_n \ge 0$. Let $\sigma_i = \sqrt{\lambda_i}$, so that $\sigma_1 \ge \cdots \ge \sigma_n \ge 0$. These latter numbers are called the *singular values* of *A*.

It follows from the Courant-Fischer min-max theorem [28, Thm 4.2.6] that the *i*th singular value of *A* is given by:

$$\sigma_i(A) = \inf_{\substack{V \subseteq \mathbb{C}^n \\ \dim(V) = n - i + 1 ||X||_p = 1}} \sup_{x \in V} ||Ax||_2, \quad (i = 1, 2, ..., n).$$

It is easy to see that the largest singular value of *A* is equal to the operator norm of *A* induced by the vector 2-norm. More explicitly,

$$\sigma_1(A) = \|A\|_{\ell_p^2 \to \ell_p^2}.$$
(2.1)

For a given $p \in [1, \infty]$, the Schatten *p*-norm of an $n \times n$ matrix *A*, which we denote by $||A||_{S_p}$, is defined as the *p*-norm of the sequence of its singular values, i.e.,

$$||A||_{\mathcal{S}_p} \coloneqq \left(\sum_{i=1}^n |\sigma_i(A)|^p\right)^{1/p}, \quad (1 \le p < \infty),$$

and

$$||A||_{\mathcal{S}_{\infty}} \coloneqq \max\{|\sigma_1(A)|, \dots, |\sigma_n(A)|\} = \sigma_1(A).$$

Remark that the definition of the Schatten ∞-norm coincides with that of the spectral norm 2.1.

Being closely related to vector *p*-norms, Schatten *p*-norms naturally inherit the following monotonic behavior of the latter:

$$||A||_{S_1} \ge ||A||_{S_p} \ge ||A||_{S_q} \ge ||A||_{S_{\infty}},$$

for all $n \times n$ matrix A and for $1 \le p \le q \le \infty$.

Finally, the following two properties of Schatten *p*-norms are immediate consequences of the singular value decomposition (SVD). These are as follows:

1. *Sub-multiplicativity*: For all $p \in [1, \infty]$ and all $n \times n$ matrices *A* and *B*,

$$|AB||_{\mathcal{S}_n} \leq ||A||_{\mathcal{S}_n} ||B||_{\mathcal{S}_n};$$

2. Unitarily invariance (and a fortiori permutation invariance): For all $p \in [1, \infty]$, all $n \times n$ matrix A, and all $n \times n$ unitary matrices U and V,

$$||UAV||_{\mathcal{S}_p} = ||A||_{\mathcal{S}_p}.$$

2.3 Elementary spectral properties of doubly stochastic matrices

Let us recall some basic yet useful facts concerning doubly stochastic matrices, which will be needed in our studies:

- (i) The spectrum of a doubly stochastic matrix always includes 1. This eigenvalue is associated with the "obvious" eigenvector $e = (1, 1, ..., 1)^T$. All other eigenvalues have magnitude at most 1 [34, Lemma 1].
- (ii) The spectrum of a doubly stochastic matrix *D* is a subset of the unit circle if and only if *D* is a permutation matrix [34, Theorem 5].
- (iii) A convex real-valued function on Ω_n attains its maximum at a permutation matrix [28, Corollary 8.7.4].

2.4 A special doubly stochastic matrix

The $n \times n$ matrix where every entry is equal to 1/n, which we denote by J_n , plays a central role in the theory of doubly stochastic matrices and is quite special in a number of regards. But for the purposes of the following discussion, it suffices to note that it acts as *the absorbing element* of Ω_n , i.e.,

$$DJ_n = J_n D = J_n$$
,

for every $n \times n$ doubly stochastic matrix *D*.

2.5 Minimum and maximum distance of an element of the Birkhoff polytope from the origin

For the purposes of our study of the diameter of the Birkhoff polytope with respect to various norms, it will be useful to have upper and lower bounds for the value of these norms when the operand runs through the Birkhoff polytope. The following lemma provides such elementary bounds.

Lemma 2.1. Let $\|\cdot\|$ be a permutation invariant sub-multiplicative matrix norm and let D be an $n \times n$ doubly stochastic matrix. Then, $1 \le \|D\| \le \|I_n\|$, where I_n is the $n \times n$ identity matrix.

Proof. On the one hand, it follows from the absorbing property of the special matrix J_n that

$$||J_n|| = ||DJ_n|| \le ||D|| ||J_n||.$$
(2.2)

Thus, $||D|| \ge 1$. On the other hand, if $\sum_{i=1}^{r} \alpha_i P_i$ is a Birkhoff decomposition of *D*, then

$$||D|| = \left\| \sum_{i=1}^{r} \alpha_{i} P_{i} \right\| \le \sum_{i=1}^{r} \alpha_{i} ||P_{i}|| = \sum_{i=1}^{r} \alpha_{i} ||I_{n}|| = ||I_{n}||.$$

3 Definition of the diameter of a set

In any given metric space (X, d), the diameter of a nonempty set of points $\mathcal{B} \subseteq X$ is defined as the supremum of the distances between pairs of points in \mathcal{B} , i.e.,

$$\operatorname{diam}_d(\mathcal{B}) \coloneqq \sup_{x,y \in \mathcal{B}} d(x,y).$$

If diam_d(\mathcal{B}) < ∞ , then *B* is called a bounded set (Figure 1).

In the following two sections, we determine the diameter of Ω_n with respect to the operator norms from ℓ_n^p to ℓ_n^p and also with respect to the Schatten *p*-norms ($1 \le p \le \infty$). While the former is fairly straightforward, the latter requires a few non-trivial results and identities and gives rise to quite a surprising answer.

4 Diameter of the Birkhoff polytope relative to the operator norms from ℓ_n^p to ℓ_n^p for $1 \le p \le \infty$

First, we turn our attention to the diameter of the Birkhoff polytope relative to the operator norms from ℓ_n^p to $\ell_n^p (1 \le p \le \infty)$. Here, we find that this diameter is constant and independent of the parameter p. This elegant and simple result mainly rests on Lemma 2.1.

Theorem 4.1. For every $1 \le p \le \infty$, diam $\ell_n^p(\Omega_n) = 2$.

Proof. One can easily check straight from the definition of the operator norm from ℓ_n^p to ℓ_n^p that $||I_n||_{\ell_n^p \to \ell_n^p} = 1$ for all $1 \le p \le \infty$. Lemma 2.1 therefore ensures that for any $D \in \Omega_n$, $||D||_{\ell_n^p \to \ell_n^p} = 1$. Thus,

$$||D - S||_{\ell_n^p \to \ell_n^p} \le ||D||_{\ell_n^p \to \ell_n^p} + ||S||_{\ell_n^p \to \ell_n^p} = 2$$

for every $D, S \in \Omega_n$. Hence, diam $_{\ell_n^p}(\Omega_n) \le 2$. Moreover, let $D = I_{n-2} \oplus \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ and $S = I_n$. Then, $D - S = I_n$.

 $0_{n-2} \oplus \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$. The singular values of this matrix are 2 with multiplicity 1, and 0 with multiplicity n - 1. Consequently, the diameter of Ω_n relative to the operator norm from ℓ_n^p to ℓ_n^p is equal to 2.

Remark 4.2. In the space of $n \times n$ matrices with real coefficients equipped with the metric induced by the $\|\cdot\|_{\ell_n^p \to \ell_n^p}$ norm, the Birkhoff polytope Ω_n has certain properties reminiscent of those of the unit circle. For example, $\|D\|_{\ell_n^p \to \ell_n^p} = 1$ for all $D \in \Omega_n$ and diam $_p(\Omega_n) = 2$.

Note, however, that the unit circle also verifies a property that is easily taken for granted: its diameter is equal to twice its radius (in Chebyshev's sense). A set in a metric space that verifies both of the aforementioned properties of the unit circle as well as this latter property is called a *centrable* set.

The authors of this article have shown in [5, Theorem 6.8] that the Chebyshev radius of the Birkhoff polytope with respect to the metric induced by the spectral norm is 1, which makes Ω_n a centrable set with respect to this metric space. However, for $p \neq 2$, Ω_n is not a centrable set with respect to $\|\cdot\|_{\ell_n^p \to \ell_n^p}$ since its radius is strictly greater than 1.

5 Diameter of the Birkhoff polytope relative to the Schatten *p*-norms for $p \ge 1$

We begin by using the fact that $||D - S||_{S_p}$ is convex relative to both operand $D, S \in \Omega_n$ to deduce from property (iii) of doubly stochastic matrices in Section 2.3 that $\operatorname{diam}_{S_p}(\Omega_n) = \operatorname{diam}_{S_p}(\mathcal{P}_n)$. But, since Schatten *p*-norms are unitarily-invariant (and thus permutation-invariant), we have

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = \max_{P,Q\in\mathcal{P}_n} ||P-Q||_{\mathcal{S}_p} = \max_{P,Q\in\mathcal{P}_n} ||I_n-QP^*||_{\mathcal{S}_p} = \max_{P\in\mathcal{P}_n} ||I_n-P||_{\mathcal{S}_p}.$$



Figure 1: Diameter of the nonempty closed bounded set \mathcal{B} with respect to the metric d.

Now observe that $(I_n - P)^*(I_n - P) = 2I_n - P - P^*$ and that, if (λ, x) is an eigenpair of the permutation matrix P, then

$$(2I_n - P - P^*)x = (2 - \lambda - \lambda^{-1})x.$$

Thus, if $\lambda_k (1 \le k \le n)$ are the eigenvalues of P, then the singular values of $I_n - P$ are equal to $\sqrt{2 - \lambda_k - \lambda_k^{-1}}$. But, the eigenvalues of the permutation matrices are unimodular. So if $\lambda_k \coloneqq e^{i\theta_k}$, we find

$$\sqrt{2 - \lambda_k - \lambda_k^{-1}} = \sqrt{2(1 - \cos(\theta_k))} = 2\sin\left(\frac{\theta_k}{2}\right), \quad (0 \le \theta_k \le 2\pi)$$

It follows that

$$||I_n - P||_{S_p} = 2 \left(\sum_{k=1}^n \sin^p \left(\frac{\theta_k}{2} \right) \right)^{\frac{1}{p}},$$

where θ_k are the arguments of the eigenvalues of *P*. Recall that the eigenvalues of a permutation matrix are of the following particular form: there exist natural numbers $n_1, n_2, ..., n_r$ satisfying $n_1 + n_2 + \cdots + n_r = n$ for which the eigenvalues of *P* are $e^{2\pi i k/n_1}(1 \le k \le n_1)$, $e^{2\pi i k/n_2}(1 \le k \le n_2)$,..., $e^{2\pi i k/n_r}$ $(1 \le k \le n_r)$ [20]. Therefore,

$$||I_n - P||_{S_p} = 2\left(\sum_{k=1}^{n_1} \sin^p\left(\frac{\pi k}{n_1}\right) + \sum_{k=1}^{n_2} \sin^p\left(\frac{\pi k}{n_2}\right) + \dots + \sum_{k=1}^{n_r} \sin^p\left(\frac{\pi k}{n_r}\right)\right)^{\frac{1}{p}},$$

and thus,

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2 \max_{\sum n_j = n} \left(\sum_{k=1}^{n_1} \sin^p \left(\frac{\pi k}{n_1} \right) + \dots + \sum_{k=1}^{n_r} \sin^p \left(\frac{\pi k}{n_r} \right) \right)^{\frac{1}{p}}.$$

Finding this maximum is a difficult problem. Indeed, a partition maximizing the aforementioned quantity not only depends on the parameter p, but also, as we shall see, on the parity of n when p > 2. We therefore divide the problem into three subcases. In the first case, where $1 \le p < 2$, we will use some non-trivial identities to achieve our goal. In the second case, certain peculiarities of the Schatten 2-norm will be exploited to find precisely for which doubly stochastic matrices the diameter is realized. Finally, we will characterize the case p > 2 using estimates.

5.1 Case $1 \le p < 2$

In [4], it is shown that for every $p \in [0, 2)$, the function

$$S(n) \coloneqq \frac{1}{n} \sum_{k=1}^{n} \sin^p \left(\frac{\pi k}{n} \right)$$

is monotonically increasing relative to the natural numbers n. It thus follows that

$$diam_{S_p}(\Omega_n) = 2 \max_{\sum n_j = n} \left(\sum_{k=1}^{n_1} \sin^p \left(\frac{\pi k}{n_1} \right) + \dots + \sum_{k=1}^{n_r} \sin^p \left(\frac{\pi k}{n_r} \right) \right)^{\frac{1}{p}}$$

= $2 \max_{\sum n_j = n} (n_1 S(n_1) + \dots + n_r S(n_r))^{\frac{1}{p}}$
 $\leq 2 \max_{\sum n_j = n} (n_1 S(n) + \dots + n_r S(n))^{\frac{1}{p}}$
= $2(nS(n))^{\frac{1}{p}} = 2 \left(\sum_{k=1}^n \sin^p \left(\frac{\pi k}{n} \right) \right)^{\frac{1}{p}}.$

The reverse inequality being realized by the trivial partition (n), it follows that

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2\left(\sum_{k=1}^n \sin^p\left(\frac{\pi k}{n}\right)\right)^{\frac{1}{p}}, \quad (1 \le p < 2).$$

Hence, the following holds true:

Theorem 5.1. For $1 \le p < 2$, the diameter of Ω_n relative to the Schatten *p*-norm is

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2\left(\sum_{k=1}^n \sin^p\left(\frac{\pi k}{n}\right)\right)^{\frac{1}{p}}.$$

Remark 5.2. It can be shown (see [4]) that

$$\lim_{n\to\infty}\frac{1}{n}\sum_{j=1}^n\sin^p\left(\frac{\pi k}{n}\right)\sim\int_0^1\sin^p(\pi x)\,\mathrm{d}x=\binom{(p-1)/2}{p/2},$$

where $\begin{pmatrix} z \\ w \end{pmatrix} \coloneqq \lim_{u \to z} \lim_{v \to w} \frac{\Gamma(u+1)}{\Gamma(v+1)\Gamma(u-v+1)}$ Hence, for $1 \le p < 2$, we have $\operatorname{diam}_{\mathcal{S}_p}^p(\Omega_n) = 2^p n \cdot \frac{1}{n} \sum_{k=1}^n \sin^p \left(\frac{\pi k}{n}\right) \sim 2^p \binom{(p-1)/2}{p/2} n.$

The case for the Schatten 1-norm, also known as the *nuclear norm*, *trace norm*, or *Ky Fan norm*, is of marked interest. Using the trigonometric identity $\sum_{k=1}^{n} \sin\left(\frac{\pi k}{n}\right) = \cot\left(\frac{\pi}{2n}\right)$, Theorem 5.1 yields:

Corollary 5.3. The diameter of Ω_n relative to the nuclear norm is given by $\operatorname{diam}_{\mathcal{S}_1}(\Omega_n) = 2 \operatorname{cot}\left(\frac{\pi}{2n}\right)$.

Finally, note the argument presented in this section for the case $1 \le p \le 2$ holds just as true for p verifying $0 \le p \le 1$. For such p, though the function $\|\cdot\|_{S_p}$ defines only a quasi-norm, the function $d(x, y) = \|x - y\|_{S_p}^p$ is still a metric and the following holds true:

Proposition 5.4. For $0 \le p < 1$, the diameter of Ω_n relative to the metric $d(x, y) = ||x - y||_{S_n}^p$ is given by:

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2^p \sum_{k=1}^n \sin^p \left(\frac{\pi k}{n} \right).$$

5.2 Case p = 2

Recall that $\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = \operatorname{diam}_{\mathcal{S}_p}(\mathcal{P}_n)$. This implies that there exists a pair of permutation matrices P_1 and P_2 such that $\operatorname{diam}(\Omega_n) = ||P_1 - P_2||_{\mathcal{S}_p}$. For the particular case of the Schatten 2-norm, we can use some more precise knowledge about the norm of a doubly stochastic matrix to derive a stronger result.

Theorem 5.5. The diameter of Ω_n relative to the Schatten 2-norm is equal to $\sqrt{2n}$. Moreover, it is realized by a pair $D_1, D_2 \in \Omega_n$ if and only if $D_1, D_2 \in \mathcal{P}_n$ and $tr(D_1D_2^*) = 0$.

Proof. Let $D_1, D_2 \in \Omega_n$. Using Lemma 2.1, we have

$$\begin{aligned} \|D_1 - D_2\|_{S_2}^2 &= \|D_1\|_{S_2}^2 + \|D_2\|_{S_2}^2 - 2\mathrm{tr}(D_1D_2^*) \\ &\leq 2\|I_n\|_{S_2}^2 - 2\mathrm{tr}(D_1D_2^*) \leq 2n. \end{aligned}$$
(5.1)

Taking the supremum on each side yields $\dim_{S_2}(\Omega_n) \leq \sqrt{2n}$. We easily obtain the reverse inequality by taking the pair of doubly stochastic matrices I_n and Q, where Q is any permutation matrix with trace zero. Hence, $\dim_{S_2}(\Omega_n) = \sqrt{2n}$.

Note that we have equality in both inequalities of (5.1) if and only if $||D_1||_{S_2}^2 = ||D_2||_{S_2}^2 = n$ and $\operatorname{tr}(D_1D_2^*) = 0$. The former condition holds if and only if $\sigma_i(D_j) = 1$ for all i = 1, ..., n and for j = 1, 2. Hence, the SVD of D_j is given by $D_j = U_j I_n V_j^*$, where U_j and V_j are the unitary matrices. Thus, the D_j s are the unitary matrices and their eigenvalues must then all lie on the unit circle. It therefore follows from property (ii) mentioned in Section 2.3 that the D_j s are permutation matrices.

5.3 Case *p* > 2

Clearly, $\sin^p(x) \le \sin^2(x)$ for any $x \in [0, \pi]$ and p > 2. Moreover, it is easy to show (using Euler identity) that $\sum_{k=1}^{n} \sin^2\left(\frac{\pi k}{n}\right) = \frac{n}{2}$ for $n \ge 2$ and $\sum_{k=1}^{1} \sin^2\left(\frac{\pi k}{1}\right) = 0$. The combination of these basic facts gives us the following estimate:

$$\sum_{k=1}^{n_1} \sin^p \left(\frac{\pi k}{n_1} \right) + \dots + \sum_{k=1}^{n_r} \sin^p \left(\frac{\pi k}{n_r} \right) \le \sum_{k=1}^{n_1} \sin^2 \left(\frac{\pi k}{n_1} \right) + \dots + \sum_{k=1}^{n_r} \sin^2 \left(\frac{\pi k}{n_r} \right) \le \frac{n_1}{2} + \dots + \frac{n_r}{2} = \frac{n}{2}.$$

It follows that diam_{*S_p*(Ω_n) $\leq 2\left(\frac{n}{2}\right)^{\overline{p}}$ for p > 2. If *n* is even, the partition of *n* into 2s yields the reverse inequality, and thus,}

diam_{$$S_p$$}(Ω_n) = $2\left(\frac{n}{2}\right)^{\frac{1}{p}}$, ($p > 2$, n even).

If *n* is odd, the situation is trickier. Clearly, any partition of *n* must contain at least one odd term, say $n_r = m$. Proceeding as before, we have

$$diam_{\mathcal{S}_{p}}(\Omega_{n}) = 2\max_{\sum n_{j}=n} \left(\sum_{k=1}^{n_{1}} \sin^{p} \left(\frac{\pi k}{n_{1}} \right) + \dots + \sum_{k=1}^{n_{r-1}} \sin^{p} \left(\frac{\pi k}{n_{r-1}} \right) + \sum_{k=1}^{m} \sin^{p} \left(\frac{\pi k}{m} \right) \right)^{\frac{1}{p}}$$

$$\leq 2\max_{\sum n_{j}=n} \left(\frac{n_{1}}{2} + \dots + \frac{n_{r-1}}{2} + \sum_{k=1}^{m} \sin^{p} \left(\frac{\pi k}{m} \right) \right)^{\frac{1}{p}}$$

$$= 2\max_{\substack{1 \le m \le n \\ m \text{ odd}}} \left(\frac{n-m}{2} + \sum_{k=1}^{m} \sin^{p} \left(\frac{\pi k}{m} \right) \right)^{\frac{1}{p}}.$$

The reverse inequality is readily obtained by considering the partition (2, ..., 2, m), and thus,

$$\operatorname{diam}_{S_p}(\Omega_n) = 2 \max_{\substack{1 \le m \le n \\ m \text{ odd}}} \left(\frac{n-m}{2} + \sum_{k=1}^m \sin^p \left(\frac{\pi k}{m} \right) \right)^{\frac{1}{p}} = 2 \left(\frac{n}{2} + \max_{\substack{1 \le m \le n \\ m \text{ odd}}} S_p(m) \right)^{\frac{1}{p}},$$

where

$$S_p(m) = \sum_{k=1}^m \sin^p \left(\frac{\pi k}{m}\right) - \frac{m}{2}.$$

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We therefore seek to determine for which odd numbers m the term $S_p(m)$ (seen as a function of p) attains its maximum. To achieve this, we shall use the following trigonometric identity twice [32, Corollary 1]:

$$\sum_{k=1}^{m} \sin^{6}\left(\frac{\pi k}{m}\right) = \begin{cases} 0, & \text{if } m = 1, \\ \frac{27}{32}, & \text{if } m = 3, \\ \frac{5m}{16}, & \text{if } m \ge 5. \end{cases}$$
(5.2)

Let us first suppose that $p \ge 6$. Note that under this additional hypothesis, the fact that $0 \le \sin(x) \le 1$ for $x \in [0, \pi]$ implies that $S_p(m)$ decreases relative to p for any integer m. So,

$$S_p(1) \leq \max_{\substack{1 \leq m \leq n \\ m \text{ odd}}} S_p(m) \leq \max_{\substack{1 \leq m \leq n \\ m \text{ odd}}} S_6(m), \quad (p \geq 6).$$

The trigonometric identity (5.2) then ensures that

$$S_{6}(m) = \sum_{k=1}^{m} \sin^{6}\left(\frac{\pi k}{m}\right) - \frac{m}{2} = \begin{cases} -\frac{1}{2}, & \text{if } m = 1, \\ -\frac{21}{32}, & \text{if } m = 3, \\ -\frac{3m}{16}, & \text{if } m \ge 5. \end{cases}$$

But $-\frac{3m}{16} < -\frac{21}{32} < -\frac{1}{2}$ for every odd integer $m \ge 5$, and it follows that the maximum of $S_6(m)$ is realized when m = 1. Moreover, observe that $S_p(1) = -\frac{1}{2}$ for every $p \in \mathbb{R}$. Therefore, we have

$$S_p(1) \le \max_{\substack{1 \le m \le n \\ m \text{ odd}}} S_p(m) \le \max_{\substack{1 \le m \le n \\ m \text{ odd}}} S_6(m) = S_6(1) = S_p(1), \quad (p \ge 6).$$

Thus, the maximum of $S_p(m)$ when *m* is an odd integer and $p \ge 6$ is realized by m = 1.

Let us then go back to the case where 2 . By Hölder's inequality,

$$S_p(m) + \frac{m}{2} = \sum_{k=1}^m \sin^p \left(\frac{\pi k}{m}\right) = \sum_{k=1}^m \sin \left(\frac{\pi k}{m}\right)^{pt} \cdot \sin \left(\frac{\pi k}{m}\right)^{p(1-t)}$$
$$\leq \left(\sum_{k=1}^m \sin \left(\frac{\pi k}{m}\right)^{pta}\right)^{\frac{1}{a}} \cdot \left(\sum_{k=1}^m \sin \left(\frac{\pi k}{m}\right)^{p(1-t)b}\right)^{\frac{1}{b}},$$

for each $0 \le t \le 1$ and every $a, b \ge 1$ such that $\frac{1}{a} + \frac{1}{b} = 1$. By choosing $t = \frac{6-p}{2p}$ and $a = \frac{4}{6-p}$, we find that $0 \le t \le 1$ and $1 < a, b < \infty$ and we obtain

$$S_{p}(m) \leq \left(\sum_{k=1}^{m} \sin^{2}\left(\frac{\pi k}{m}\right)\right)^{\frac{b-p}{4}} \cdot \left(\sum_{k=1}^{m} \sin^{6}\left(\frac{\pi k}{m}\right)\right)^{\frac{p-2}{4}} - \frac{m}{2}$$
$$\leq \left(\frac{m}{2}\right)^{\frac{6-p}{4}} \cdot \left(\sum_{k=1}^{m} \sin^{6}\left(\frac{\pi k}{m}\right)\right)^{\frac{p-2}{4}} - \frac{m}{2} = T_{p}(m).$$

Once again, we use the trigonometric identity (5.2) to obtain

$$S_p(m) \le T_p(m) = \begin{cases} -\frac{1}{2}, & \text{if } m = 1, \\ 2\left(\frac{3}{4}\right)^{\frac{p}{2}} - \frac{3}{2}, & \text{if } m = 3, \\ \left(\left(\frac{5}{8}\right)^{\frac{p-2}{4}} - 1\right)^{\frac{p-2}{2}}, & \text{if } m \ge 5. \end{cases}$$

Note that $\left(\frac{5}{8}\right)^{\frac{p-2}{4}} - 1$ is a decreasing function of *p*, and thus,

$$\frac{5}{8}\right)^{\frac{p-2}{4}} - 1 \le \left(\frac{5}{8}\right)^{\frac{2-2}{4}} - 1 = 0.$$

Hence, $T_p(m)$ is decreasing relative to m for each p with $2 , and every odd integer <math>m \ge 5$. It follows that $T_p(5) \ge T_p(m)$ for any such p and every odd integer $m \ge 5$. Moreover,

$$T_p(3) \ge T_p(5) \iff 2 \ge 5 \left(\frac{5}{8}\right)^{\frac{p-2}{4}} - 4 \left(\frac{3}{4}\right)^{\frac{p}{2}}.$$

It is straightforward to verify that $5\left(\frac{5}{8}\right)^4 - 4\left(\frac{3}{4}\right)^2$ is a decreasing function of p whenever p > 2, and thus,

$$5\left(\frac{5}{8}\right)^{\frac{p-2}{4}} - 4\left(\frac{3}{4}\right)^{\frac{p}{2}} \le 5\left(\frac{5}{8}\right)^{\frac{d-2}{4}} - 4\left(\frac{3}{4}\right)^{\frac{d}{2}} = 2, \quad (p > 2).$$

Hence, $T_p(3) \ge T_p(5)$ for every *p* with 2 , and it follows that

$$S_p(m) \le T_p(m) \le \max\{T_p(1), T_p(3)\} = \max\left\{-\frac{1}{2}, 2\left(\frac{\sqrt{3}}{2}\right)^p - \frac{3}{2}\right\}, \quad (2$$

Moreover, one can readily verify that $S_p(1) = -\frac{1}{2}$ and $S_p(3) = 2\left(\frac{\sqrt{3}}{2}\right)^p - \frac{3}{2}$. Therefore, this upper bound on $S_p(m)$ is also realized by $S_p(1)$ and $S_p(3)$. Hence,

$$\max_{\substack{1 \le m \le n \\ m \text{ odd}}} S_p(m) = \max\{S_p(1), S_p(3)\} = \max\left\{-\frac{1}{2}, 2\left(\frac{\sqrt{3}}{2}\right)^p - \frac{3}{2}\right\}, \quad (2$$

It then follows from a few elementary computations that $S_p(1) \le S_p(3)$ if and only if $-\frac{1}{2} \le 2\left(\frac{\sqrt{3}}{2}\right)^p - \frac{3}{2}$, i.e., to

say if and only if $p \le \frac{\log(4)}{\log(4/3)} = c \approx 4.819$. Therefore, for p satisfying $2 , the maximum of <math>S_p(m)$ is reached for m = 3, whereas for p verifying $c \le p < 6$ (and thus on for $c \le p < \infty$), the maximum is reached for m = 1. Moreover, a direct calculation and some simplifications reveal that one can write the results of this section in the following closed form for every $n \in \mathbb{N}$:

Theorem 5.6. For p > 2, the diameter of Ω_n relative to the Schatten p-norm is

$$\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2 \left(\frac{n - \sin^2(\frac{n\pi}{2}) \min\{1, 3 - 4(\sqrt{3}/2)^p\}}{2} \right)^{\frac{1}{p}}.$$
(5.3)

In particular, if n is even, then $\operatorname{diam}_{\mathcal{S}_p}(\Omega_n) = 2(n/2)^{1/p}$.

5.4 Summary

The following theorem condenses the results derived in this section concerning the diameter of Birkhoff's theorem when the metric used is the one induced by Schatten's *p*-norms.

Theorem 5.7. Given p with $p \ge 1$, the diameter of Ω_n relative to the Schatten p-norm is given by:

$$\operatorname{diam}_{\mathcal{S}_{p}}^{p}(\Omega_{n}) = \begin{cases} 2^{p} \sum_{k=1}^{n} \sin^{p}\left(\frac{\pi k}{n}\right), & \text{if } 1 \le p \le 2, \\ \\ \frac{n - \sin^{2}\left(\frac{n\pi}{2}\right)\min(1, 3 - 4(\sqrt{3}/2)^{p})}{2}, & \text{if } 2 \le p < \infty. \end{cases}$$
(5.4)

In particular,

- (*i*) diam_{S₁}(Ω_n) = 2 cot $\left(\frac{\pi}{2n}\right)$,
- (*ii*) diam_{S₂}(Ω_n) = $\sqrt{2n}$,
- (iii) diam_{S_n}(Ω_n) = 2(n/2)^{1/p} if n is even and $p \ge 2$.

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