The asymptotic volume of diagonal subpolytopes of symmetric stochastic matrices

J. de Jong R. Wulkenhaar

WWU Münster, Germany

Mathematical Institute

j.dejong@uni-muenster.de raimar@math.uni-muenster.de

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Abstract

The asymptotic volume of the polytope of symmetric stochastic matrices can be determined by asymptotic enumeration techniques as in the case of the Birkhoff polytope. These methods can be extended to polytopes of symmetric stochastic matrices with given diagonal, if this diagonal varies not too wildly. To this end the asymptotic number of symmetric matrices with natural entries, zero diagonal and varying row sums is determined and a third order correction factor to this is examined.

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1 Introduction

Convex polytopes arise naturally in various places in mathematics. A fundamental problem is the computability of a polytope's volume. Some results are known for low-dimensional setups [1], polytopes with only a few vertices, or highly symmetric cases [2, 3]. This work belongs to the latter category.

Definition 1.1. A convex polytope p is the convex hull of a finite set $S_p = \{v_j \in \mathbb{R}^n\}$ of vertices.

Stochastic matrices are square matrices with nonnegative entries, such that every row of the matrix sums to one. The symmetric stochastic $N \times N$-matrices are an example of a convex polytope, which will be called $\mathcal{P}_N$. Its vertices are given by the symmetric permutation matrices. There are $\sum_{j=0}^{N/2} \binom{N}{2j}(2j-1)!!$ such matrices. It follows directly from the Birkhof-Von Neumann theorem that all symmetric stochastic matrices are of this form. A basis for this space is given by

$$\{I_N\} \cup \{B^{(jk)} | 1 \leq j < k \leq N\} \quad ,$$

where I_N is the $N \times N$ identity matrix and the matrix elements of $B^{(jk)}$ are given by

$$B^{(jk)}_{lm} = \begin{cases} B^{(jk)}_{lm} = 1 & \text{, if } \{l,m\} = \{j,k\} \quad ; \\ B^{(jk)}_{lm} = 1 & \text{, if } j \neq l = m \neq k \quad ; \\ B^{(jk)}_{lm} = 0 & \text{, otherwise} \end{cases} \quad .$$

All these vertices are linearly independent and it follows that the polytope is $\binom{N}{2}$-dimensional.

Definition 1.2. A convex subpolytope p' of a convex polytope p is the convex hull of a finite set $\{v'_j \in p\}$ of vertices in p.

Slicing a polytope yields a surface of section, which is itself a convex space and, hence, a polytope. Determining its vertices is in general very difficult.
Spaces of symmetric stochastic matrices with several diagonal entries fixed are examples of such slice subpolytopes of $\mathcal{P}_N$, provided that these entries lie between zero and one. The slice subpolytope of $\mathcal{P}_N$, obtained by fixing all diagonal entries $h_j \in [0,1]$, is called the diagonal subpolytope $P_N(h_1, \ldots, h_N)$. This is a polytope of dimension $N(N-3)/2$. These polytopes form the main subject of this paper.

To keep the notation light, vectors of N elements are usually written by a bold symbol. The diagonal subpolytope with entries $h_1, \ldots, h_N$ will thus be written by $P_N(\boldsymbol{h})$.

The main results are the following two theorems.

Theorem 1. *Let $V_N(\boldsymbol{t};\lambda)$ be the number of symmetric $N \times N$-matrices with an empty diagonal and entries in the natural numbers such that t_j is the j-th row sum. Let the total entry sum be $x = \sum_{j=1}^N t_j$ and the average entry $\lambda = x/(N(N-1))$ furthermore be bounded polynomially in N and the variance be given by $y = \sum_{j=1}^N (t_j - \lambda(N-1))^2$. If for some $\alpha \in (0, 1/2)$*

$$\lambda N^\alpha \to \infty \quad \text{and} \quad \frac{y}{\lambda^2 N^{2-2\alpha}} \to 0$$

hold as $N \to \infty$, then the number of matrices is asymptotically given by

$$V_N(\boldsymbol{t};\lambda) = \frac{\sqrt{2}(1+\lambda)^{\binom{N}{2}}}{(2\pi\lambda(\lambda+1)(N-2))^{\frac{N}{2}}}(1+\frac{1}{\lambda})^{\frac{x}{2}}\sqrt{\frac{N-2}{N-1}}\exp\Big[-\frac{\sum_{j=1}^N (t_j - \lambda(N-1))^2}{2\lambda(\lambda+1)(N-2)}\Big]\}$$
$$+ O((1+\lambda)^{\binom{N}{2}}(1+\frac{1}{\lambda})^{\frac{x}{2}}(2\pi\lambda(\lambda+1)(N-2))^{-\frac{N}{2}} N^{-N^{1-2\alpha}}) \quad .$$

Theorem 2. *Let $\boldsymbol{h} = h_1, \ldots, h_N$ with $h_j \in [0,1]$ and $\chi = \sum_{j=1}^N h_j$. If*

$$\lim_{N\to\infty} (\frac{N-1}{N-\chi})^2 \sum_{j=1}^N (h_j - \chi/N)^2 = 0 \quad ,$$

then the asymptotic volume of the polytope of symmetric stochastic $N \times N$-matrices with diagonal $\boldsymbol{h}$ is given by

$$\mathrm{vol}(P_N(\boldsymbol{h})) = \frac{\sqrt{2(N-2)}\, e^{\binom{N}{2}}}{\sqrt{N-1}(2\pi(N-2))^{\frac{N}{2}}}(\frac{N-\chi}{N(N-1)})^{\frac{N(N-3)}{2}}$$
$$\times \exp[-\frac{N^2(N-1)^2 \sum_{j=1}^N (h_j - \frac{\chi}{N})^2}{2(N-2)(N-\chi)^2}](1 + O(N^{-\sqrt{N}})) \quad .$$

The outline of this paper is as follows. In Paragraph 2 the volume problem is formulated as a counting problem and subsequently as a contour integral. Paragraph 3 is dedicated to a fundamental lemma to restrict the integration region for this integral. This is subsequently integrated in Paragraph 4. A correction factor to the counting result is discussed in Paragraph 5. The volume of the diagonal subpolytopes is extracted from the counting result in Paragraph 6.

2 Counting problem

The volume of a polytope p in $\mathbb{R}^n$ with basis $\{\mathcal{B}_j \in \mathbb{R}^n | 1 \leq j \leq d\}$ is obtained by

$$\int_{[0,1]^d} \mathrm{d}\boldsymbol{u}\, \mathbf{1}_p(\sum_{j=1}^{d} u_j \mathcal{B}_j) \quad ,$$

where $\mathbf{1}_p$ is the indicator function for the polytope p. If the polytope is put on a lattice $(a\mathbb{Z})^n$ with lattice parameter $a \in (0,1)$, an approximation of this volume is obtained by counting the lattice sites inside the polytope and multiplying this by the volume a^d of a single cell. This approximation becomes better as the lattice parameter shrinks. In the limit this yields

$$\mathrm{vol}(p) = \lim_{a \to 0} a^d \; |\{p \cap (a\mathbb{Z})^n\}| \quad . \tag{1}$$

This approach is formalized by the Ehrhart polynomial [4], which counts the number of lattice sites of $\mathbb{Z}^n$ in a dilated polytope. A dilation of a polytope p by a factor $a^{-1} > 1$ yields the polytope $a^{-1}p$, which is the convex hull of the dilated vertices $S_{a^{-1}p} = \{a^{-1}v | v \in S_p\}$. That the obtained volume is the same follows from the observation

$$|\{a^{-1}p \cap \mathbb{Z}^n\}| = |\{p \cap (a\mathbb{Z})^n\}| \quad .$$

The volume integral of the diagonal subpolytope $P_N(\boldsymbol{h})$ is

$$\mathrm{vol}(P_N(\boldsymbol{h})) = \Big\{ \prod_{1 \leq k < l \leq N} \int_0^1 \mathrm{d}u_{kl} \Big\} \quad \mathbf{1}_{P_N(\boldsymbol{h})}(I_N + \sum_{1 \leq k < l \leq N} u_{kl}(B^{(kl)} - I_N)) \quad .$$

To see that this integral covers the polytope, it suffices to see that the any symmetric stochastic matrix $A = (a_{kl})$ is decomposed in basis vectors as

$$A = (a_{kl}) = I_N + \sum_{k<l} a_{kl}(B^{(kl)} - I_N) \quad .$$

The next step is to introduce a lattice $(a\mathbb{Z})^{\binom{N}{2}}$ and count the sites inside the polytope. Each such site is a symmetric stochastic matrix with $h_1, \ldots, h_N$ on the diagonal.
Since the volume depends continuously on the extremal points, it can be assumed without loss of generality that all h_j are rational. This implies that a dilation factor a^{-1} exists, such that all $a^{-1}(1 - h_j) = t_j \in \mathbb{N}$ and that the matrices that solve

$$\begin{pmatrix} 0 & b_{12} & \cdots & b_{1N} \\ b_{12} & 0 & \cdots & b_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ b_{1N} & b_{2N} & \cdots & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{pmatrix}$$

with $t_j, b_{jk} \in \mathbb{N}$ are to be counted. This yields a number $V_N(\boldsymbol{t})$. The polytope volume is then given by

$$\mathrm{vol}(P_N(\boldsymbol{h})) = \lim_{a\to 0} a^{\frac{N(N-3)}{2}} V_N(\frac{1-h_1}{a}, \ldots, \frac{1-h_N}{a}) \quad ,$$

where

$$V_N(\boldsymbol{t}) = \oint_C \frac{\mathrm{d}w_1}{2\pi i w_1^{1+t_1}} \cdots \oint_C \frac{\mathrm{d}w_N}{2\pi i w_N^{1+t_N}} \prod_{1\le k<l\le N} \frac{1}{1-w_k w_l} \quad . \tag{2}$$

To see this, let the possible values m for the matrix element b_{jk} be given by the generating function

$$\frac{1}{1-w_j w_k} = \sum_{m=0}^{\infty} (w_j w_k)^m \quad .$$

Applying this to all matrix entries shows that $V_N(\boldsymbol{t})$ is given by the coefficient of the term $w_1^{t_1} w_2^{t_2} \ldots w_N^{t_N}$ in $\prod_{1\le j<k\le N} \frac{1}{1-w_j w_k}$. Formulating this in derivatives yields

$$V_N(\boldsymbol{t}) = \frac{1}{t_1!} \frac{\mathrm{d}}{\mathrm{d}w_1}\Big|_{w_1=0}^{t_1} \cdots \frac{1}{t_N!} \frac{\mathrm{d}}{\mathrm{d}w_N}\Big|_{w_N=0}^{t_N} \prod_{1\le k<l\le N} \frac{1}{1-w_k w_l} \quad . \tag{3}$$

By Cauchy's integral formula (2) follows from this.

The contour C encircles the origin once in the positive direction, but not the pole at $w_k w_l = 1$.
The next step is to parametrize this contour explicitly and find a way to compute the integral for $N \to \infty$. In practice this means that a combinatorial treatments must be avoided. A convenient choice is

$$w_j = \sqrt{\frac{\lambda}{\lambda+1}} e^{i\varphi_j} \qquad \text{, with } \lambda \in \mathbb{R}_+ \text{ and } \varphi_j \in [-\pi, \pi) \quad .$$

Later a specific value for λ will be chosen.
The counting problem has now been turned into an integral over the N-dimensional torus

$$V_N(\boldsymbol{t}) = (1+\frac{1}{\lambda})^{\frac{\sum_{j=1}^N t_j}{2}} \frac{(1+\lambda)^{\binom{N}{2}}}{(2\pi)^N} \int_{\mathbb{T}^N} \mathrm{d}\boldsymbol{\varphi}\, e^{-i\sum_{j=1}^N \varphi_j t_j} \prod_{1\le k<l\le N} \frac{1}{1-\lambda(e^{i(\varphi_k+\varphi_l)}-1)} \quad , \tag{4}$$

where we have written $\mathrm{d}\boldsymbol{\varphi}$ for $\mathrm{d}\varphi_1 \ldots \mathrm{d}\varphi_N$.

The notation

$$x = \sum_j t_j = \sum_{j=1}^N t_j$$

is used, when no doubt about N can exist. When no summation bounds are mentioned, these will always be 1 and N. The notation $a \ll b$ indicates that $a < b$ and $a/b \to 0$.

Such integrals appear in many counting problems and can be computed asymptotically by the saddle-point method [5, 6]. This method requires that all t_j are equal, which is not necessary in our case. We show that it suffices to demand that they do not deviate too much from the symmetric case.

3 Reduction of the integration region

Lemma 3.1. *For $a \in [0,1]$ there is a positive constant R_a such that for $n > R_a$ the estimates*

$$\frac{1}{2}\exp[na/e] \leq (1+a)^n \leq \exp[na]$$

hold.

Proof. The right-hand side follows from

$$(1+a)^n = \sum_{j=0}^{n} a^j \binom{n}{j} = \sum_{j=0}^{n} \frac{(na)^j}{j!} \frac{n!}{n^j(n-j)!} \leq \sum_{j=0}^{n} \frac{(na)^j}{j!} \leq \exp[na] \quad .$$

To prove the left-hand side, we apply Stirling's approximation to $n!$ and $(n-j)!$. It is then not difficult to see that there is a constant, say $\frac{1}{\sqrt{2}}$, such that

$$\begin{aligned}(1+a)^n &= \sum_{j=0}^{n} \frac{(na)^j}{j!} \frac{n!}{n^j(n-j)!} \geq \sum_{j=0}^{n-1} \frac{(na)^j}{j!} \frac{n!}{n^j(n-j)!} \\ &\geq \frac{1}{\sqrt{2}} \sum_{j=0}^{n-1} \frac{(na/e)^j}{j!} (\frac{n}{n-j})^{n-j+\frac{1}{2}} \quad .\end{aligned}$$

Approximating by the first n terms

$$e^{\frac{na}{e}} = \sum_{j=0}^{n-1} \frac{(na/e)^j}{j!}(1 + O(\sqrt{n}a^n))$$

shows that the error is small for large n. Choosing R_a such that $n > R_a$ guarantees $|(1 + O(\sqrt{n}a^n))| < 1/\sqrt{2}$ proves the statement. □

The integrals in (4) are too difficult to compute in full generality. A useful approximation can be obtained from the observation that the integrand

$$\left|\frac{1}{1-\lambda(e^{iy}-1)}\right|^2 = \frac{1}{1-2\lambda(\lambda+1)(\cos(y)-1)} \qquad \text{for } y \in (-2\pi, 2\pi) \tag{5}$$

is concentrated in a neighbourhood of the origin and the antipode $y = \pm 2\pi$, where it takes the value 1. This is plotted in Figure 1.
For small y and λy the absolute value of the integrand factor can be written as

$$\left|\frac{1}{1-\lambda(e^{iy}-1)}\right| = \sqrt{\frac{1}{1+\lambda(\lambda+1)y^2}}(1 + O(y^4)) \quad . \tag{6}$$

A crucial step is to introduce an essential bound, below which we lose accuracy. The aim is then to find the asymptotic number $V_N(\boldsymbol{t})$ for configurations $\boldsymbol{t}$, whenever this is larger than the essential bound.

Definition 3.1. *Essential bound*
For $N, x \in \mathbb{N}$, $\lambda \in \mathbb{R}_+$ and $\alpha \in (0, 1/2)$ we define the essential bound by

$$\mathcal{E}_\alpha = (2\pi\lambda(\lambda+1)(N-2))^{-\frac{N}{2}}(1+\lambda)^{\binom{N}{2}}(1+\frac{1}{\lambda})^{\frac{x}{2}} \exp[-N^{1-2\alpha}] \quad . \tag{7}$$

Lemma 3.2. *Let $(\zeta_k)_{k\in\mathbb{N}}$ and $\delta_N = \zeta_N \lambda^{-1} N^{-\alpha}$ be sequences such that the limits*

$$\zeta_N \to \infty \quad ; \quad \delta_N \to 0 \quad \textit{and} \quad \lambda < N^C \quad \textit{for some } C > 0$$

hold as $N \to \infty$ for some $\alpha \in (0, 1/2)$. The asymptotic integral (4) is then given by

$$V_N(\boldsymbol{t};\lambda) = 2(1+\frac{1}{\lambda})^{\frac{x}{2}}(1+\lambda)^{\binom{N}{2}}(2\pi)^{-N}$$
$$\times \int_{[-\delta_N,\delta_N]^N} \mathrm{d}\boldsymbol{\varphi}\, e^{-i\sum_{j=1}^N \varphi_j t_j} \prod_{1\le k<l\le N} \frac{1}{1-\lambda(e^{i(\varphi_k+\varphi_l)}-1)} + O(\mathcal{E}_\alpha \exp[-(\zeta_N^2-1)N^{1-2\alpha}]) \quad , \quad (8)$$

if this is larger than the essential bound $\mathcal{E}_\alpha$ (7).

Proof. The idea of the proof is to consider the integrand in a small box $[-\delta_N, \delta_N]^N$ and see what happens to it if some of the angles $\boldsymbol{\varphi}$ lie outside of it.
Because x is even, it follows that the integrand takes the same value at $\boldsymbol{\varphi}$ and $\boldsymbol{\varphi} + \boldsymbol{\pi} = (\varphi_1 + \pi, \ldots, \varphi_N + \pi)$. This means that only half of the space has to be considered and the result must be multiplied by 2.

It will be automatically proved in Paragraph 4 that

Claim 1.

$$\int_{[-\delta_N/2,\delta_N/2]^N} \mathrm{d}\boldsymbol{\varphi} \prod_{1\le k<l\le N} \frac{1}{1-\lambda(\exp[i(\varphi_k+\varphi_l)]-1)}$$
$$\le (\frac{2\pi}{\lambda(\lambda+1)(N-2)})^{\frac{N}{2}} \sqrt{\frac{N-2}{2(N-1)}}(1+O(2\delta_N^{-1}e^{-\frac{\lambda(\lambda+1)N\delta_N^2}{8}})) \quad .$$

Now we argue case by case why other configurations of the angles φ_j are asymptotically suppressed.
Case 1. All but finitely many angles lie in the box $[-\delta_N, \delta_N]^N$. A finite number of m angles lies outside of it. We label these angles $\{\varphi_1, \ldots, \varphi_m\}$. The absolute maximum of the integrand

$$f : (\varphi_{m+1}, \ldots, \varphi_N) \mapsto \prod_{1\le k<l\le N} \frac{1}{1-\lambda(\exp[i(\varphi_k+\varphi_l)]-1)}$$

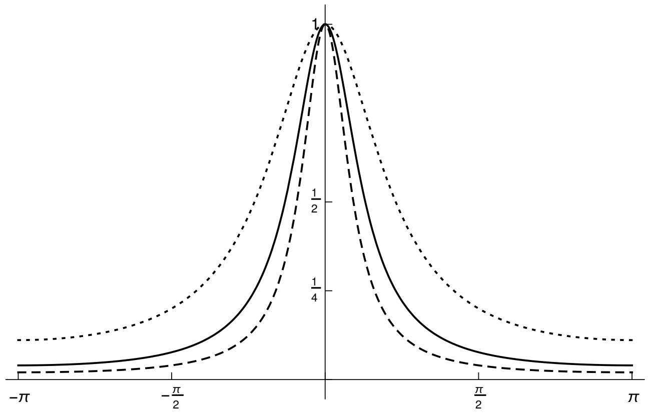


Figure 1: The absolute value squared of the integrand factor (5) for $\lambda = 1, 2$ and 3 in dotted, continuous and dashed lines respectively.

is given by the equations

$$0 = \partial_{\varphi_j}|f| = \sum_{k\neq j} \frac{\sin(\varphi_j + \varphi_k)}{1 - 2\lambda(\lambda+1)(\cos(\varphi_j+\varphi_k) - 1)} \qquad \text{for } j = m+1, \ldots, N \quad .$$

It is clear that the maximum is found for $\tilde{\varphi} = \varphi_{m+1} = \ldots = \varphi_N$. The first order solution to this is then

$$\tilde{\varphi} = \frac{-1}{2(N-m-1)} \sum_{k=1}^{m} \frac{\sin(\varphi_k)}{1 + 2\lambda(\lambda+1)(1-\cos\varphi_k)} \quad .$$

This shows that the maximum will lie in the box $[-\delta_N/2, \delta_N/2]^N$.

Applying the estimate (6) to pairs of angles at least a distance $\delta_N/2$ apart and afterwards Claim 1 to the remaining $N-m$ angles in the box $[-\delta_N/2, \delta_N/2]^{N-m}$ gives us an upper bound of

$$(\frac{2\pi}{\lambda(\lambda+1)(N-2)})^{\frac{N-m}{2}} \binom{N}{m} (2\pi)^{-N} (1+\lambda)^{\binom{N}{2}} (1 + \frac{1}{\lambda})^{\frac{x}{2}} (1 + \frac{(\lambda\delta_N)^2}{4})^{-\frac{Nm}{4}}$$

on the part of the integral in the small box $[-\delta_N/2, \delta_N/2]^N$. Because the maximum of the integrand lies in this small box, an upper bound for the integration box $[-\delta_N, \delta_N]^N$ is obtained by multiplying the above by 2^N. There are $\binom{N}{m}$ ways to select the m angles out of N.
Comparing this with the essential bound in combination with Lemma 3.1 shows that this may be neglected, if

$$2^N N^m (8\pi^3\lambda(\lambda+1)N)^{\frac{m}{2}} (\frac{\delta_N}{\pi})^{N-m} e^{N^{1-2\alpha}} e^{-\frac{Nm}{16e}(\lambda\delta_N)^2} \leq (2\delta_N \pi e^{N^{-2\alpha}})^N (\frac{\lambda\pi N^{\frac{3}{2}}}{\delta_N} e^{-N^{1-2\alpha}\frac{\zeta_N^2}{16e}})^m \to 0\,.$$

The sequence $\zeta_N \to \infty$ guarantees this. In fact, the same argument works for all m such that $m/N \to 0$.

Case 2. If the number $m = \rho N$ of angles outside the integration box $[-\delta_N, \delta_N]^N$ increases faster, another estimate is needed, because the maximum $\tilde{\varphi}$ may lie outside of $[-\delta_N/2, \delta_N/2]$. It is clear that $0 < \rho < 1$ in the limit.
To estimate the location $\varphi_j = \tilde{\varphi}$ of the maximum is much trickier now. We will nevertheless take the maximum value as the estimate for the integrand in the entire integration box. The smaller box $[-\delta_N/2, \delta_N/2]^N$ is considered once more. We distinguish two options.
-*Case 2a.* The maximum lies in $[-\delta_N/2, \delta_N/2]^N$, thus $\tilde{\varphi} \in [-\delta_N/2, \delta_N/2]$.
Applying the estimate (6) to this yields an upper bound

$$\binom{N}{\rho N} (2\delta_N)^{N(1-\rho)} (2\pi)^{\rho N} (1 + \frac{1}{\lambda})^{\frac{x}{2}} (1+\lambda)^{\binom{N}{2}} (1 + \frac{1}{4}\lambda^2\delta_N^2)^{-\frac{N^2\rho(1-\rho)}{4}} \quad .$$

Applying Lemma 3.1 to the last factor and dividing this by $\mathcal{E}_\alpha$ shows that

$$((\frac{\pi}{\delta_N})^{\frac{1-\rho}{\rho}} N \exp[\frac{N^{-2\alpha}}{\rho} - \frac{\lambda^2\delta_N^2 N(1-\rho)}{16e}])^{\rho N} \to 0$$

is a sufficient and satisfied condition.
-*Case 2b.* The maximum lies not in $[-\delta_N/2, \delta_N/2]^N$. This is the same as $\delta_N/2 < |\tilde{\varphi}| \leq$

δ_N.
Applying (6) only to the angles $\varphi_{\rho N+1}, \ldots, \varphi_{\rho N}$ in the integration box gives an upper bound

$$\binom{N}{\rho N}(2\delta_N)^{N(1-\rho)}(2\pi)^{\rho N}(1+\frac{1}{\lambda})^{\frac{x}{2}}(1+\lambda)^{\binom{N}{2}}(1+\frac{1}{4}\lambda^2\delta_N^2)^{-\frac{N^2(1-\rho)^2}{4}} \quad .$$

The same steps as in Case 2a. will do.
This shows that the integration can be restricted to the box $[-\delta_N, \delta_N]^N$. The error terms follow from *Case 1.*, since convergence there is much slower. □

Remark 1. The estimates in Lemma 3.2 caused the integral (8) to depend non-trivially on λ. For that reason λ is explicitly mentioned as an argument.

Lemma 3.2 shows that for every $\alpha \in (0, 1/2)$ and $N \in \mathbb{N}$ there is a box that contains most of the integral's mass. As N increases, this box shrinks and the approximation becomes better. The parameter α determines how fast this box shrinks. Smaller values of α lower the essential bound and, hence, increase the number of configurations within reach at the price of more intricate integrals and less accuracy.

4 Evaluation of the integral

In the previous paragraph the integration was restricted to a small box around the origin. The integral can now be cast into a simpler form, where the size of this box is used as an expansion parameter. The expansion used is

$$\frac{1}{1-\lambda(\exp[iy]-1)} = \exp[\sum_{j=1}^{k} A_j(iy)^j] + O(y^{k+1}(1+\lambda)^{k+1}) \quad . \tag{9}$$

The coefficients A_j are polynomials in λ of degree j with leading term λ^j/j. The first three are

$$A_1 = \lambda \quad ; \quad A_2 = \frac{\lambda}{2}(\lambda+1) \quad \text{and} \quad A_3 = \frac{\lambda}{6}(\lambda+1)(2\lambda+1) \quad . \tag{10}$$

Applying (9) produces the combinations

$$\begin{aligned}
&\sum_{1\le k<l\le N} \varphi_k + \varphi_l = (N-1)\sum_{j=1}^{N}\varphi_j \quad ; \\
&\sum_{1\le k<l\le N} (\varphi_k + \varphi_l)^2 = (N-2)\sum_{j=1}^{N}\varphi_j^2 + (\sum_{j=1}^{N}\varphi_j)^2 \quad ; \\
&\sum_{1\le k<l\le N} (\varphi_k + \varphi_l)^3 = (N-4)\sum_{j=1}^{N}\varphi_j^3 + 3(\sum_{j=1}^{N}\varphi_j)(\sum_{k=1}^{N}\varphi_k^2) \quad \text{and} \\
&\sum_{1\le k<l\le N} (\varphi_k + \varphi_l)^n = (N-2^{n-1})(\sum_{j=1}^{N}\varphi_j^N) + \sum_{m=1}^{\lfloor \frac{n}{2}\rfloor}\binom{n}{m}(\sum_{j=1}^{N}\varphi_j^m)(\sum_{i=1}^{N}\varphi_i^{n-m}) \quad \text{for } n \in \mathbb{N} \quad .
\end{aligned} \tag{11}$$

The error in (9) with $|y| \le \delta_N$ is $(\lambda+1)^{k+1}\delta_N^{k+1} \sim N^{-\alpha(k+1)}$. There are $\binom{N}{2}$ such factors, which suggests that we must choose $k = \lceil 2\alpha^{-1} \rceil$ to ensure convergence. The following lemma shows that this is not necessary.

Lemma 4.1. *Under the conditions of Lemma 3.2 the asymptotic integral (8) is given by*

$$V_N(\boldsymbol{t};\lambda) = \frac{2(1+\lambda)^{\binom{N}{2}}}{(2\pi)^N}(1+\frac{1}{\lambda})^{\frac{x}{2}} \int_{[-\delta_N,\delta_N]^N} \mathrm{d}\boldsymbol{\varphi}\, \exp[i\sum_j \varphi_j(\lambda(N-1)-t_j)]$$
$$\times \exp[-A_2((N-2)\sum_j \varphi_j^2 + (\sum_j \varphi_j)^2)] + O(\mathcal{E}_\alpha \exp[-N^{2-2\alpha}]) \quad .$$

Proof. The formula follows directly from the application up to second order of (9) with (10) and (11) to (8). It is sufficient to show that the difference divided by the essential bound (7)

$$2e^{N^{1-2\alpha}}(2\pi)^{-N}(2\pi\lambda(\lambda+1)(N-2))^{\frac{N}{2}}$$
$$\times \int_{[-\delta_N,\delta_N]^N} \mathrm{d}\boldsymbol{\varphi} \prod_{1\le k<l\le N}\Big(\frac{1}{1-\lambda(\exp[i(\varphi_k+\varphi_l)]-1)} - \exp[\sum_{j=1}^{1+2\alpha^{-1}} A_j i^j(\varphi_k+\varphi_l)^j]\Big) \to 0 \,. \quad (12)$$

Because there are $\binom{N}{2}$ factors, it follows that terms in this sum with j larger than $1+2\alpha^{-1}$ are irrelevant. We will demonstrate this identity for $\alpha = 2$. This means that we show that the third order may be ignored. It follows than automatically that this holds for smaller values $\alpha \in (0, 1/2)$.
The crucial observation is that

$$\max_{\boldsymbol{\varphi}\in[-\delta_N,\delta_N]^N} \Big| \exp[iA_1(N-1)\sum_j \varphi_j] \exp[-A_2((N-2)\sum_j \varphi_j^2 + (\sum_j \varphi_j)^2)]$$
$$\times (\exp[-iA_3((N-4)\sum_j \varphi_j^3 + 3(\sum_j \varphi_j^2)(\sum_j \varphi_j))] - 1)\Big|$$
$$\le \max_{\boldsymbol{\varphi}\in[-\delta_N,\delta_N]^N} 2\exp[-A_2((N-2)\sum_j \varphi_j^2 + (\sum_j \varphi_j)^2)]$$
$$\times \exp[A_3((N-4)\sum_j |\varphi_j^3| + 3(\sum_j \varphi_j^2)(\sum_j |\varphi_j|))]$$
$$\le 2\exp[-\lambda(\lambda+1)\delta_N^2 N(N-1)(1-\frac{2(2\lambda+1)}{3}\delta_N)] \quad .$$

Multiplying this by the volume of the box $(2\delta_N)^N$ and comparing it with the essential bound shows that the difference (12) vanishes as $\exp[-N^{2-2\alpha}] \to 0$.
Including higher order terms changes the estimate to

$$2\exp[-\lambda(\lambda+1)\delta_N^2 N(N-1)(1-\frac{2(2\lambda+1)}{3}\delta_N + O(\lambda^2\delta_N^2))] \quad ,$$

but leaves the rest of the argument unchanged. □

The result of Lemma 4.1 is the integral

$$V_N(\boldsymbol{t};\lambda) = \frac{2}{(2\pi)^N}(1+\frac{1}{\lambda})^{\frac{x}{2}}(1+\lambda)^{\binom{N}{2}}\int_{[-\delta_N,\delta_N]^N}\mathrm{d}\boldsymbol{\varphi}\ \exp[i\sum_{j=1}^N\varphi_j(\lambda(N-1)-t_j)]$$
$$\times\exp[-A_2((\sum_{j=1}^N\varphi_j)^2+(N-2)\sum_{j=1}^N\varphi_j^2)] \tag{13}$$
$$=\frac{2}{(2\pi)^N}(1+\frac{1}{\lambda})^{\frac{x}{2}}(1+\lambda)^{\binom{N}{2}}\int_{-\infty}^{\infty}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}x'\int_{[-\delta_N,\delta_N]^N}\mathrm{d}\boldsymbol{\varphi}\ \exp[2\pi i\tau(x'-\sum_{j=1}^N t_j)]$$
$$\times\exp[i\sum_{j=1}^N\varphi_j(\lambda(N-1)-t_j)]\exp[-A_2(x'^2+(N-2)\sum_{j=1}^N\varphi_j^2)] \quad ,$$

where we have used the Fourier representation of the Dirac delta to seperate the dependence on x and $\boldsymbol{t}$. Integrating respectively $\boldsymbol{\varphi}$, x' and τ now yields

$$V_N(\boldsymbol{t};\lambda) = \frac{\sqrt{2}(1+\lambda)^{\binom{N}{2}}}{(2\pi\lambda(\lambda+1)(N-2))^{\frac{N}{2}}}(1+\frac{1}{\lambda})^{\frac{x}{2}}\sqrt{\frac{N-2}{N-1}}\exp[\frac{(x-\lambda N(N-1))^2}{4\lambda(\lambda+1)(N-1)(N-2)}]$$
$$\times\exp[-\frac{\sum_j(t_j-\lambda(N-1))^2}{2\lambda(\lambda+1)(N-2)}] \quad . \tag{14}$$

The expansion parameter δ_N has disappeared from this result, as was to be expected. The error in the $\boldsymbol{\varphi}$-integration is $O(N^\alpha\exp[-\zeta_N^2N^{2-2\alpha}])$ and thus much smaller than that of Lemma 3.2. This also proves Claim 1.

Integrating this over $\boldsymbol{t}$, while keeping $x=\sum_{j=1}^N t_j$ fixed, gives an estimate of the total number $\mathcal{V}_N(x;\lambda)$ of symmetric matrices with zero diagonal and natural entries summing to x. Because it is assumed that $\lambda(N-1)\to\infty$, the integral is a simple gaussian. It follows that

$$\mathcal{V}_N(x;\lambda) = \int_{\mathbb{R}_+^N}\mathrm{d}\boldsymbol{t}\ \delta_N(x-\sum_j t_j)\,V_N(\boldsymbol{t};\lambda)$$
$$=\frac{(1+\lambda)^{\binom{N}{2}}}{\sqrt{\pi\lambda(\lambda+1)N(N-1)}}(1+\frac{1}{\lambda})^{\frac{x}{2}}\exp[-\frac{(x-\lambda N(N-1))^2}{4\lambda(\lambda+1)N(N-1)}] \quad . \tag{15}$$

Substituing $x=\lambda N(N-1)$ here and integrating x from 0 to $\mathcal{X}$ would yield the asymptotic number of symmetric matrices with natural entries and uniform row sums $\mathcal{X}/N$. However, it is simpler and more accurate to compute this number from scratch using the same methods as above.
Methods to treat such multi-dimensional combinatorical Gaussian integrals in more generality have been discussed in [7].

4.1 Parameter choice

It was mentioned before, that such integrals can be computed asymptotically by the saddle-point method. This requires all t_j to be equal and λ to be the average matrix entry for infinitely large matrices. Because (14) covers also this case, a similar result is expected. It follows from Lemma 3.2 that these formulas are accurate, when they are large compared to the essential bound (7). This means that

$$\exp[\frac{(x-\lambda N(N-1))^2}{8A_2(N-1)(N-2)}]\exp[-\frac{\sum_{j=1}^N(t_j-\lambda(N-1))^2}{4A_2(N-2)}]\exp[N^{1-2\alpha}]$$
$$=\exp[-\frac{(x-\lambda N(N-1))^2}{8A_2N(N-1)}]\exp[-\frac{y}{4A_2(N-2)}]\exp[N^{1-2\alpha}]\to\infty \quad ,$$

where the parameters x and y are defined by

$$x=\sum_{j=1}^N t_j \qquad ; \qquad y=\sum_{j=1}^N(t_j-\frac{x}{N})^2 \quad . \tag{16}$$

The asymptotic choice of λ is thus given by the average matrix entry

$$\lambda=\frac{x}{N(N-1)}(1+O(N^{-\frac{1}{2}-\alpha})) \quad . \tag{17}$$

It follows, furthermore, that convergence is expected for $y \ll \lambda^2N^{2-2\alpha}$ and that the rate of convergence α depends essentially on y.
The observation that $\zeta_N=\log(N)$ satisfies all the demands proves Theorem 1.

5 Corrections

It was shown in Lemma 4.1 that the third order term in (9) can be ignored. This simplified the integration considerably. However, it might be possible to retrieve a part of the contribution from the A_3-term.
The basis of (14) is the integral

$$\mathcal{F}_2=\int_{[-\delta_N,\delta_N]^N}\mathrm{d}\varphi\,\exp[i\sum_{j=1}^N\varphi_j(\lambda(N-1)-t_j)]\exp[-A_2((\sum_{j=1}^N\varphi_j)^2+(N-2)\sum_{j=1}^N\varphi_j^2)] \quad .$$

Formulating the third term as differentials with respect to $\boldsymbol{t}$ gives a purely asymptotic correction

$$\sum_{k=0}^\infty\frac{(-A_3)^k}{k!}[(N-4)\sum_j\partial_{t_j}^3-3A_3(\sum_j\partial_{t_j}^2)(\sum_l\partial_{t_l})]^k\mathcal{F}_2 \quad .$$

Selecting only dominant contribution yields the factor

$$\mathcal{F}_3=\sum_{k=0}^\infty\frac{(-A_3)^k}{k!}[\{(N-4)\sum_j\partial_{t_j}^3-3A_3(\sum_j\partial_{t_j}^2)(\sum_l\partial_{t_l})\}\mathcal{F}_2]^k$$
$$=\exp[\frac{A_3(x-\lambda N(N-1))^3}{16A_2^3N^2(N-1)^2}]\times\exp[-3A_3\frac{(2N-3)(x-\lambda N(N-1))}{8A_2^2(N-1)^2}]$$
$$\times\exp[\frac{3A_3(x-\lambda N(N-1))y}{8A_2^3N(N-1)(N-2)}]\times\exp[\frac{A_3(N-4)z}{8A_2^3(N-2)^3}] \quad . \tag{18}$$

The parameter

$$z=\sum_j(t_j-x/N)^3 \tag{19}$$

obtains an upper bound in the same way as y did. Asymptotically this factor should tend to one, which implies that $y\ll\lambda^2N^{\frac{3}{2}+\alpha}$ and $|z|\ll\lambda^3N^2$.
An idea of the accuracy of these formulas can be obtained from Table 1 and Table 2.

6 Polytope volume

Now that the counting statementis in place, it is time to return to the polytopes. The pivotal observation is that (14) yield asymptotically correct results for $y \ll \lambda^2 N^{2-2\alpha}$. The volume of the space of $N \times N$-matrices with entry sum x satisfying

$$\frac{y}{4A_2(N-2)} < M \ll N^{1-2\alpha}$$

is estimated by

$$\frac{N\pi^{\frac{N}{2}}}{\Gamma(\frac{N}{2}+1)} \int_0^M \mathrm{d}t\, e^{-t^2} t^{N-1} = \frac{N\pi^{\frac{N}{2}}}{2\Gamma(\frac{N}{2}+1)} \int_0^{M^2} \mathrm{d}y\, e^{-y} y^{\frac{N}{2}-1} \quad .$$

This is a fraction

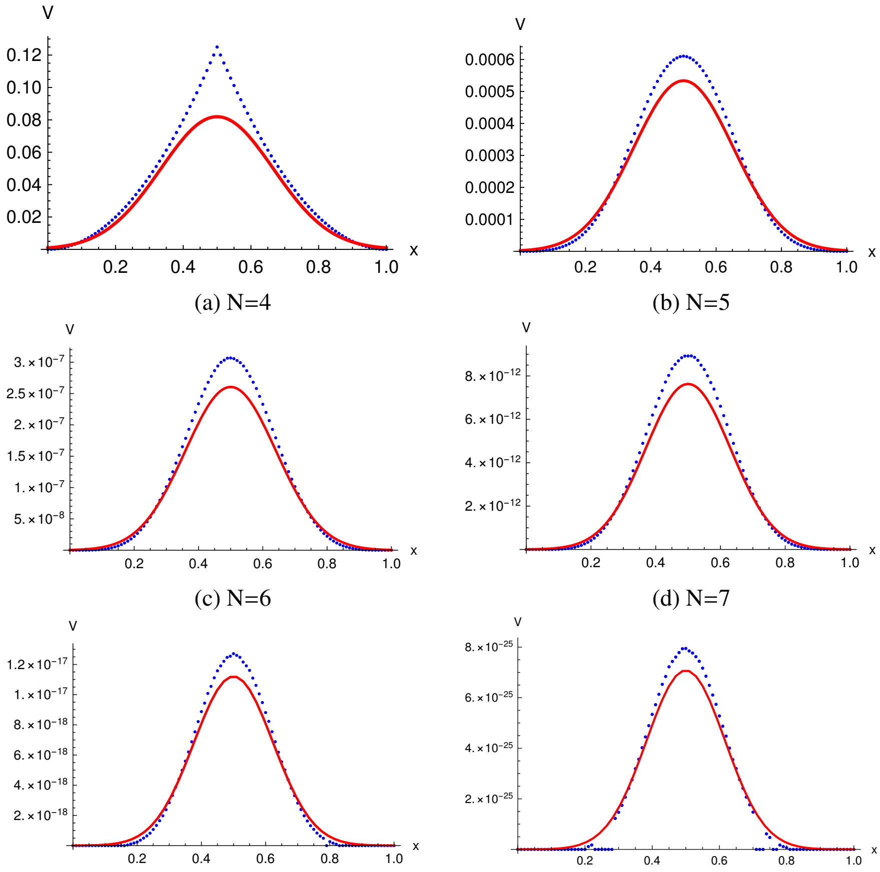
$$\frac{1}{\Gamma(\frac{N}{2})} \int_0^{M^2} \mathrm{d}y\, e^{-y} y^{\frac{N}{2}-1}$$

t_1	t_2	t_3	t_4	t_5	t_6	t_7	#	y	z	$V_N(\boldsymbol{t};\boldsymbol{\lambda})$	$(\mathcal{F}_3 V_N)(\boldsymbol{t};\boldsymbol{\lambda})$
8	8	8	8	8	8	8	5.42E7	0	0	4.77E7	4.77E7
7	7	8	8	8	9	9	4.75E7	4	0	4.19E7	4.19E7
7	7	7	8	8	9	10	4.18E7	8	6	3.69E7	3.72E7
7	7	7	7	8	9	11	3.48E7	14	24	3.04E7	3.15E7
6	7	7	7	7	11	11	2.44E7	26	42	2.07E7	2.20E7
6	7	7	7	8	8	13	2.01E7	32	114	1.70E7	2.03E7
6	6	6	6	6	13	13	8.10E6	70	210	5.02E6	6.91E6
5	8	8	8	9	9	9	3.53E7	12	-24	3.24E7	3.13E7
5	7	7	7	7	9	14	1.17E7	50	186	9.56E6	1.27E7
5	5	7	7	8	8	16	4.26E6	84	456	3.20E6	6.39E6
5	5	5	6	6	8	21	1.08E5	204	2100	6.77E4	1.63E6
4	6	7	7	8	10	14	7.92E6	62	150	6.50E6	8.16E6
4	6	7	7	8	8	16	3.88E6	86	438	3.00E6	5.83E6
3	7	8	8	9	9	12	1.09E7	44	-60	1.16E7	1.06E7
3	3	6	6	6	16	16	5.50E5	190	750	1.06E5	3.31E5
2	4	4	10	10	11	15	6.97E5	134	42	6.42E5	6.84E5
2	2	4	4	4	19	21	2.06E4	410	2904	9.01E1	7.34E3
2	2	2	3	5	14	28	1	578	7416	0.41	3.09E4

Table 1: The number (#) of symmetric 7×7-matrices with zero diagonal and natural entries summing to $x = 56$ such that the j-th row sums to t_j and the asymptotic estimates for this number by $V_N(\boldsymbol{t};\lambda)$ (14) and $(\mathcal{F}_3 V_N)(\boldsymbol{t};\lambda)$ (18) with λ given by (17). The parameters y and z are defined in (16) and (19) respectively. The notation $1.0E6 = 1.0 \times 10^6$ is used here.

N	x	$\lambda(N-1)$	#	$\#_c$	$\mathcal{V}_N(x;\lambda)$
5	80	16	2.25E09	2.03E09	2.07E09
6	72	12	1.07E12	9.60E11	9.44E11
7	56	8	2.07E13	1.78E13	1.68E13
8	40	5	1.36E13	1.04E13	9.82E12
9	30	3.33	3.61E12	2.26E12	2.26E12
10	32	3.2	2.50E14	1.47E14	1.50E14

Table 2: The number (#) of symmetric $N \times N$-matrices with zero diagonal and natural entries summing to x and the asymptotic estimate for this number by $\mathcal{V}_N(x;\lambda)$ (15) with λ given by (17). The corrected number $\#_c$ is given by $(\int_0^{x/2} \mathrm{d}t\, \exp[-(\frac{(t-\lambda(N-1))^2}{4A_2(N-2)})^2])^N$ times #. The notation $1.0E06 = 1.0 \times 10^6$ is used here.

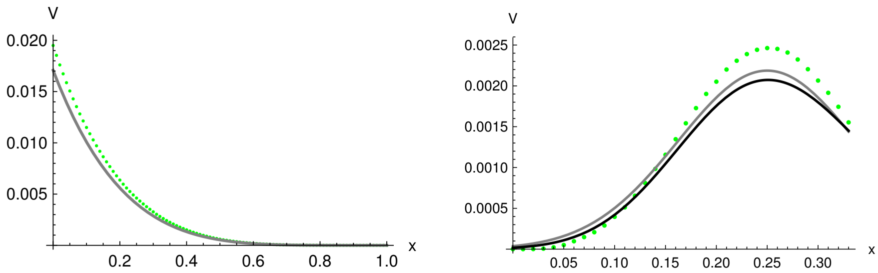


(a) N=4 (b) N=5

(c) N=6 (d) N=7

(e) N=8 (f) N=9

Figure 2: The volume result (20) (red) and the volume of $P_N(0.5, \ldots, 0.5, x, 1-x)$ (blue) for $N = 4, 5, 6, 7, 8, 9$. The latter were determined by a numerical integration algorithm for convex multidimensional step functions on the basis of Monte Carlo integration.



(a) $\mathrm{vol}(P_5(x, x, x, x, x))$ (b) $\mathrm{vol}(P_5(0.5, x, x, x, 1-3x))$

Figure 3: The volume result (20) (gray), the corrected volume result (black) and the volume for two functions (green) for $N = 5$. The latter were determined by straightforward Monte Carlo integration.

of the total volume. This ratio tends to one, if $M^2/N \to \infty$. Asymptotically, almost all matrices are covered by (14) provided that $\alpha \in (0, 1/4)$.

This shows that the polytope volume can be determined by (1). This is done on the basis of Theorem 1. In terms of the variables

$$t_j = \frac{1-h_j}{a} \quad \text{and} \quad \chi = \sum_j h_j$$

the volume of of the diagonal subpolytope is calculated by

$$\begin{aligned}
\mathrm{vol}(P_N(\boldsymbol{h})) &= \lim_{a\to 0} a^{\frac{N(N-3)}{2}} V_N(\frac{\mathbf{1}-\boldsymbol{h}}{a}; \frac{N-\chi}{aN(N-1)}) \\
&= \lim_{a\to 0} \sqrt{\frac{2(N-2)}{N-1}}(1+\frac{aN(N-1)}{N-\chi})^{\frac{N-\chi}{2a}}(a+\frac{N-\chi}{N(N-1)})^{\binom{N}{2}} \\
&\times (2\pi\frac{N-\chi}{N(N-1)}(a+\frac{N-\chi}{N(N-1)})(N-2))^{-\frac{N}{2}} \exp[-\frac{N(N-1)\sum_{j=1}^N (h_j-\frac{\chi}{N})^2}{2(N-2)(N-\chi)(a+\frac{N-\chi}{N(N-1)})}] \\
&= \frac{\sqrt{2(N-2)}\, e^{\binom{N}{2}}}{\sqrt{N-1}(2\pi(N-2))^{\frac{N}{2}}}(\frac{N-\chi}{N(N-1)})^{\frac{N(N-3)}{2}} \exp[-\frac{N^2(N-1)^2\sum_{j=1}^N (h_j-\frac{\chi}{N})^2}{2(N-2)(N-\chi)^2}] \quad . \qquad (20)
\end{aligned}$$

The error is given by the surface of the dilated polytope.

$$\begin{aligned}
&\lim_{a\to 0} a^{\frac{N(N-3)}{2}}\Big(-a^2\frac{\mathrm{d}}{\mathrm{d}a}\Big)V_N(\frac{\mathbf{1}-\boldsymbol{h}}{a}; \frac{N-\chi}{aN(N-1)}) \\
&\quad = \lim_{a\to 0} -\frac{N(N-3)a}{2}\; a^{\frac{N(N-3)}{2}}\; V_N(\frac{\mathbf{1}-\boldsymbol{h}}{a}; \frac{N-\chi}{aN(N-1)}) \quad .
\end{aligned}$$

It inherits furthermore the relative error $O((e/N)^{N^{1-2\alpha}})$ from Theorem 1.
The essential bound criterion becomes

$$\lim_{a\to 0} \frac{y}{\lambda^2 N^{2-2\alpha}} = (\frac{N^\alpha(N-1)}{N-\chi})^2 \sum_{j=1}^N (h_j - \frac{\chi}{N})^2 \quad .$$

Because all α-dependence has fallen out, it is safe to set $\alpha = 0$ here. This proves Theorem 2.

N	$V_N(0.5,\dots,0.5)$	vol$P_N(0.5,\dots,0.5)$	*ratio*
4	8.19E-02	1.25E-01	1.53
5	5.34E-04	6.11E-04	1.14
6	2.60E-07	3.07E-07	1.18
7	7.63E-12	8.92E-12	1.17
8	1.12E-17	1.27E-17	1.13
9	7.08E-25	7.95E-25	1.12

Table 3: The volume result $V_N(0.5,\dots,0.5)$ (20), the volume of $P_N(0.5,\dots,0.5)$ and the ratio between them for $N = 4,5,6,7,8,9$. The volumes of $P_N(\frac{\mathbf{1}}{\mathbf{2}})$ were determined by a numerical integration algorithm for convex multidimensional step functions on the basis of Monte Carlo integration.

Examples of this formula at work are given in Figure 2 and 3. It is not difficult to include the correction factor (18) in this. However, this would not result in a visible difference in Figure 2. In each of these figures a constant factor seems to be missing. In fact, this factor is already missing in the matrix counting, see the first entry of Table 1. This constant should tend to 1 and Table 3 suggests it does.

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