

A note on higher-dimensional magic matrices

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Abstract

We provide exact and asymptotic formulae for the number of unrestricted, respectively indecomposable, d -dimensional matrices where the sum of all matrix entries with one coordinate fixed equals 2.

1 Introduction

We begin by recalling the notion of a *magic matrix*:¹ this is a square matrix $m = (m_{i,j})_{1 \leq i,j \leq n}$ with non-negative integral entries such that all row and column sums

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¹Strictly speaking, the correct term here would be “ s -semi-magic,” since we do not require diagonals to sum up to the same number as the rows and columns, see e.g. [4]. However, here and in what follows we prefer the term “magic” for the sake of brevity.

are equal to the same non-negative integer. If this non-negative integer is s , then we call such a matrix *s-magic*. The enumeration of *s-magic* squares has a long history, going back at least to MacMahon [15, §404–419]. A good account of the enumerative theory of magic squares can be found in [18, Sec. 4.6], with many pointers to further literature. For more recent work, see for instance [4, 8].

Let $[n]$ denote the standard n -set $\{1, 2, \dots, n\}$. There are two obvious ways of generalising *s-magic* matrices to higher dimensions:

- (G1) *All line sums are equal.* Given a positive integer d , a d -dimensional matrix $m : [n]^d \rightarrow \mathbb{N}_0$ (where \mathbb{N}_0 denotes the set of non-negative integers) is called *s-magic* if

$$\sum_{\omega_i \in [n]} m(\omega_1, \omega_2, \dots, \omega_d) = s \quad (1.1)$$

for all fixed $\omega_1, \dots, \omega_{i-1}, \omega_{i+1}, \dots, \omega_d \in [n]$, and all $i = 1, 2, \dots, d$.

- (G2) *All hyperplane sums are equal.* Given a positive integer d , a d -dimensional matrix $m : [n]^d \rightarrow \mathbb{N}_0$ is called *s-magic* if

$$\sum_{\omega_1, \dots, \omega_{i-1}, \omega_{i+1}, \dots, \omega_d \in [n]} m(\omega_1, \omega_2, \dots, \omega_d) = s \quad (1.2)$$

for all fixed $\omega_i \in [n]$, and all $i = 1, 2, \dots, d$.

Generalisation (G1) appears already in the literature, see e.g. [1, 4]. For $d = 3$ and $s = 1$, these objects are equivalent to Latin squares counted up to isotopy: the roles of rows, columns, and symbols of the corresponding Latin square are played by the first, second, and third coordinate, respectively, and the entry in position (ω_1, ω_2) of the Latin square is ω_3 if and only if $m(\omega_1, \omega_2, \omega_3) = 1$.

Generalisation (G2) appears in the literature (in more general form) as *contingency tables* in statistics; there are Markov chain methods for approximate counting of these, as well as some remarkable asymptotic estimates, see [11, 9, 13, 19, 10]. Indeed, these results suggest that the counting problem for (G2) is much easier than for (G1). (We are grateful to a referee for this information and the references.)

The present note focusses on the second generalisation. Hence, from now on, whenever we use the term “*s-magic*,” this is understood in the sense of (G2).

Counting higher-dimensional magic matrices is made more difficult (than the already difficult case of 2-dimensional magic matrices) by the fact that the analogue of Birkhoff’s Theorem (cf. [5] or [2, Corollary 8.40]; it says that any 2-dimensional *s-magic* matrix can be decomposed in a sum of permutation matrices, that is, 1-magic matrices) fails for them. For example, the 3-dimensional 2-magic matrix with ones in positions $(1, 1, 1), (1, 2, 3), (2, 1, 2), (2, 2, 1), (3, 3, 2)$ and $(3, 3, 3)$ is not the sum of two 1-magic matrices.

As we demonstrate in this note, it is however possible to count the 2-magic matrices of any dimension. Our first result is a recurrence relation for the number

$u_n(d)$ of indecomposable d -dimensional 2-magic matrices of size n (see Corollary 3 in Section 4). This recurrence is used in Proposition 4 to derive, for fixed $d \geq 3$, an asymptotic formula for $u_n(d)$. In order to go from indecomposable matrices to unrestricted ones, we observe that the d -dimensional 2-magic matrices may be viewed as a d -sort species in the sense of Joyal [14] which obeys the (d -sort) exponential principle. Let $w_n(d)$ denote the number of all d -dimensional 2-magic matrices of size n . The exponential principle can then be applied to relate the numbers $w_n(d)$ to the numbers $u_n(d)$, see (3.5) (for $d = 2$) and (6.1) (for $d \geq 2$). This relation is used in Theorem 5 to find, for fixed $d \geq 3$, an asymptotic estimate for the numbers $w_n(d)$ as well. Exact and asymptotic formulae for $u_n(d)$ and $w_n(d)$ for $d = 2$ are presented in Section 3. We remark in passing that a simple counting argument shows that the obvious interpretation of the matrices in Generalisation (G1) as a d -sort species does *not* satisfy the exponential principle, not even under the—in a sense—minimal axiomatics of [7].

2 Indecomposable 2-magic matrices and fixed-point-free involutions

A d -dimensional matrix $m : [n]^d \rightarrow \mathbb{N}_0$ is called *decomposable*, if there exist non-empty subsets $B_1^{(1)}, B_2^{(1)}, B_1^{(2)}, B_2^{(2)}, \dots, B_1^{(d)}, B_2^{(d)}$ of $[n]$ with

$$B_1^{(1)} \amalg B_2^{(1)} = B_1^{(2)} \amalg B_2^{(2)} = \dots = B_1^{(d)} \amalg B_2^{(d)} = [n]$$

(\amalg denoting disjoint union) and

$$|B_1^{(1)}| = |B_1^{(2)}| = \dots = |B_1^{(d)}|,$$

such that $m(\omega_1, \omega_2, \dots, \omega_d) \neq 0$ only if either

$$(\omega_1, \omega_2, \dots, \omega_d) \in B_1^{(1)} \times B_1^{(2)} \times \dots \times B_1^{(d)}$$

or

$$(\omega_1, \omega_2, \dots, \omega_d) \in B_2^{(1)} \times B_2^{(2)} \times \dots \times B_2^{(d)},$$

otherwise it is called *indecomposable*.² (In less formal language: there exist reorderings of the lines of the matrix such that m attains a block form.) The integer n is called the *size* of m .

Let $u_n(d)$ denote the number of indecomposable d -dimensional 2-magic matrices of size n . Note that an indecomposable 2-magic matrix with an entry 2 has size 1. So it is enough to consider zero-one matrices.

²We warn the reader that for $d = 2$ this does not reduce to the notion of decomposability of matrices in linear algebra since there rows and columns are reordered by the *same* permutation. Yet another definition of indecomposability occurs in [1].

The purpose of this section is to relate the numbers $u_n(d)$ to another sequence of numbers $v_n(d)$ counting certain tuples of fixed-point-free involutions on a set with $2n$ elements. More precisely, let

$$t_1 = (1, 2)(3, 4) \cdots (2n-1, 2n) \quad (2.1)$$

be the standard fixed-point-free involution on the set $[2n]$. Then we define $v_n(d)$ to be the number of choices of $d - 1$ fixed-point-free involutions t_2, \dots, t_d on $[2n]$ such that the group $G = \langle t_1, t_2, \dots, t_d \rangle$ generated by t_1, t_2, \dots, t_d is transitive. (For example, when $n = 2$, there are just three fixed-point-free involutions on $\{1, 2, 3, 4\}$, viz., $(1, 2)(3, 4)$, $(1, 3)(2, 4)$ and $(1, 4)(2, 3)$, any two of which generate a transitive group. So $v_2(d) = 3^{d-1} - 1$.)

We have the following relation.

Lemma 1 *For all integers $n, d > 1$, we have*

$$u_n(d) = 2^{-n}(n!)^{d-1}v_n(d). \quad (2.2)$$

Proof. Let m be an indecomposable d -dimensional 2-magic matrix of size n , where $n > 1$. Then m is a zero-one matrix, and it contains $2n$ entries equal to 1, the rest being zero. Number the positions of the 1's in m from 1 to $2n$ in such a way that the positions with first coordinate j are numbers $2j - 1$ and $2j$ for $j = 1, \dots, n$. (There are 2^n ways to do this, since for each j we can choose arbitrarily which of the two 1's has number $j - 1$.) Then, for $i = 1, \dots, d$, let t_i be the fixed-point-free involution whose cycles are the pairs of numbers in $\{1, \dots, 2n\}$ indexing positions of 1's with the same i -th coordinate. Note that t_1 is the involution defined in (2.1).

We claim that the subgroup G of S_{2n} generated by t_1, \dots, t_d is transitive if and only if the matrix m is indecomposable. For this, note that the 1's whose labels belong to a cycle of t_i have the same i -th coordinate. So, if m is decomposable, and the 1 with label 1 belongs to $B_1^{(1)} \times \cdots \times B_1^{(d)}$, then an easy induction shows that any 1 whose label is in the same orbit belongs to this set, so that G is intransitive. Conversely, if G is intransitive, then the coordinates of the 1's whose labels belong to a G -orbit give rise to a decomposition of m .

So each matrix gives rise to 2^n such d -tuples of involutions. Thus, the number of pairs consisting of a matrix and a corresponding sequence of permutations is $2^n u_n(d)$.

For instance, the example of a matrix failing the analogue of Birkhoff's Theorem given in the Introduction, with the entries numbered in the order given, produces the three permutations $(1, 2)(3, 4)(5, 6)$, $(1, 3)(2, 4)(5, 6)$ and $(1, 4)(2, 6)(3, 5)$.

Conversely, let t_1, \dots, t_d be fixed-point-free involutions on the set $\{1, \dots, 2n\}$ which generate a transitive group, where t_1 is the standard involution defined in (2.1). Number the cycles of each t_i from 1 to n such that the cycle $(2j - 1, 2j)$ of t_1 has number j . (There are $(n!)^{d-1}$ such numberings.) Now construct a d -dimensional matrix m as follows: for $k = 1, \dots, 2n$, if k lies in cycle number ω_i of t_i , then $m(\omega_1, \omega_2, \dots, \omega_d) = 1$; all other entries are zero. Then m is 2-magic. Consequently,

each sequence of permutations gives rise to $(n!)^{d-1}$ matrices; and the number of pairs consisting of a matrix and a corresponding sequence of permutations equals $(n!)^{d-1} v_n(d)$.

Comparing these two expressions, we obtain (2.2), as required. \square

Remark. We note that $u_1(d) = v_1(d) = 1$ for all d . Hence, Formula (2.2) is false for $n = 1$.

3 Computation of $u_n(2)$ and $w_n(2)$

The number $w_n(2)$ of 2-dimensional 2-magic matrices of size n has been addressed earlier by Anand, Dumir and Gupta in [3, Sec. 8.1]. They found the generating function formula

$$\sum_{n \geq 0} w_n(2) \frac{z^n}{(n!)^2} = (1 - z)^{-1/2} e^{z/2}. \quad (3.1)$$

This gives the explicit formula

$$w_n(2) = \sum_{k=0}^n \binom{2k}{k} \frac{(n!)^2}{2^{n-k}(n-k)!}. \quad (3.2)$$

Singularity analysis (cf. [12, Ch. VI]) applied to (3.1) then yields the asymptotic formula

$$w_n(2) = (n!)^2 \sqrt{\frac{e}{\pi n}} \left(1 + \mathcal{O}\left(\frac{1}{n}\right) \right), \quad \text{as } n \rightarrow \infty. \quad (3.3)$$

The number $u_n(2)$ of *indecomposable* 2-dimensional 2-magic matrices of size n can also be computed explicitly. One way is to observe that, by Birkhoff's Theorem (cf. [5] or [2, Corollary 8.40]), a 2-magic matrix m is the sum of two permutation matrices, say p_1 and p_2 . If m is indecomposable, then the pair $\{p_1, p_2\}$ is uniquely determined. Premultiplying by p_1^{-1} , we obtain a situation where p_1 is the identity; indecomposability forces p_2 to be the permutation matrix corresponding to a cyclic permutation, since a cycle of p_2 not containing all points would provide a decomposition of m . So there are $n!(n-1)!$ choices for (p_1, p_2) , and half this many choices for m (assuming, as we may, that $n > 1$). Note that this formula gives half the correct number for $n = 1$. So we have

$$u_n(2) = \begin{cases} 1, & \text{if } n = 1, \\ \frac{1}{2}n!(n-1)!, & \text{if } n > 1. \end{cases} \quad (3.4)$$

Alternatively, we may observe that 2-dimensional 2-magic matrices may be seen as a 2-sort species in the sense of Joyal [14] (see also [6, Def. 4 on p. 102]), with the row indices and the column indices forming the two set on which the functor defining the

species operates. Hence, by the exponential principle for 2-sort species [14, Prop. 20] (see also [6, Sec. 2.4]), we have

$$\sum_{n \geq 0} w_n(2) \frac{z^n}{(n!)^2} = \exp \left(\sum_{n \geq 1} u_n(2) \frac{z^n}{(n!)^2} \right). \quad (3.5)$$

Combining this with (3.1), we find that

$$\sum_{n \geq 1} u_n(2) \frac{z^n}{(n!)^2} = \frac{z}{2} + \frac{1}{2} \log \left(\frac{1}{1-z} \right).$$

Extraction of the coefficient of z^n then leads (again) to (3.4).

4 A recurrence relation for $v_n(d)$

In this section we prove a recurrence relation for the numbers $v_n(d)$ (see Section 2 for their definition). By Lemma 1, this affords as well a recurrence relation for the numbers $u_n(d)$.

Proposition 2 *The numbers $v_n(d)$ satisfy $v_1(d) = 1$ and*

$$\sum_{k=1}^n \binom{n-1}{k-1} ((2n-2k-1)!!)^{d-1} v_k(d) = ((2n-1)!!)^{d-1}, \quad n > 1. \quad (4.1)$$

Here, $(2n-1)!! = 1 \cdot 3 \cdot 5 \cdots (2n-1)$ is the product of the first n odd positive integers for $n > 0$, and, by convention, $(-1)!! = 1$.

Proof. Recall that $(2n-1)!!$ is the number of fixed-point-free involutions on a set of size $2n$. (This is a special case of the general formula

$$\frac{n!}{\prod_{i=1}^n i^{a_i} a_i!}$$

for the number of permutations in S_n with a_i cycles of length i for $i = 1, \dots, n$.) The number of choices of involutions t_1, t_2, \dots, t_d , where t_1 is as in (2.1), such that the orbit containing 1 of the group they generate has size $2k$ is

$$\binom{n-1}{k-1} ((2n-2k-1)!!)^{d-1} v_k(d),$$

since we can choose in order

- (i) $k-1$ of the $n-1$ cycles of t_1 other than $(1, 2)$ such that the elements not fixed by all of these $k-1$ transpositions together with $\{1, 2\}$ form the desired orbit, O say;

- (ii) $d - 1$ fixed-point-free involutions on O which, together with the restriction of t_1 to O , generate a transitive group;
- (iii) $d - 1$ arbitrary fixed-point-free involutions on the complement of O .

Summing these values shows that the numbers $v_n(d)$ satisfy the desired recurrence. \square

Corollary 3 *For all integers $d > 1$, the numbers $u_n(d)$ satisfy $u_1(d) = 1$ and*

$$((2n-3)!!)^{d-1} + \sum_{k=2}^n \binom{n-1}{k-1} \left(\frac{(2n-2k-1)!!}{k!} \right)^{d-1} 2^k u_k(d) = ((2n-1)!!)^{d-1},$$

$n > 1.$

Remarks. (1) In the case $d = 2$, we have seen in (3.4) that $u_n(2) = n!(n-1)!/2$ for $n > 1$, so that

$$v_n(2) = 2^{n-1} (n-1)! = (2n-2)!!,$$

where $(2n-2)!!$ is the product of the even integers up to $2n-2$ (with $0!! = 1$ by convention). Substituting this in (4.1), we have proved the somewhat curious looking identity

$$\sum_{k=1}^n \binom{n-1}{k-1} (2n-2k-1)!! (2k-2)!! = (2n-1)!!$$

for $n > 1$.

We remark that this identity has an interpretation in terms of hypergeometric functions, for which we refer to [16], in particular, (1.7.7), Appendix (III.4). The left-hand side is

$$2^{n-1} (1/2)_{n-1} \cdot {}_2F_1 \left[\begin{matrix} -n+1, 1 \\ -n+\frac{1}{2} \end{matrix}; 1 \right],$$

and the identity is an instance of the Chu–Vandermonde identity.

(2) For $d > 2$, we have not been able to solve the recurrence explicitly. However, it is easy to calculate terms in the sequences, and we can describe their asymptotics (see Sections 5 and 6).

Table 1 gives counts of all indecomposable matrices, all zero-one matrices, and all non-negative integer matrices, with dimension d and hyperplane sums 2. The sequences for $d = 2$ are numbers A010796, A001499, and A000681 in the On-Line Encyclopedia of Integer Sequences [17]. For $d = 3$, they are A112578, A112579 and A112580.

d		$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$
2	indec	1	1	6	72	1440	43200
	0-1	0	1	6	90	2040	67950
	all	1	3	21	282	6210	202410
3	indec	1	8	900	359424	370828800	820150272000
	0-1	0	8	900	366336	378028800	833156928000
	all	1	12	1152	431424	427723200	920031955200

Table 1: Indecomposable, zero-one and arbitrary d -dimensional 2-magic matrices of size n

5 Asymptotics of the numbers $u_n(d)$

This section provides the preparation for the determination of the asymptotics of the numbers $w_n(d)$ for $d \geq 3$ in the next section. Our goal here is to establish an asymptotic estimate for the sequence $u_n(d)$ with fixed $d \geq 3$.

Proposition 4 *For fixed $d \geq 3$, we have*

$$u_n(d) \sim 2^{-dn} ((2n)!)^{d-1}, \quad \text{as } n \rightarrow \infty.$$

Proof. By Lemma 1, we have $u_n(d) = (n!)^{d-1} v_n(d)/2^n$ for $n > 1$, so it suffices to show that

$$v_n(d) \sim ((2n-1)!!)^{d-1}.$$

We will use the estimates

$$\sqrt{2(n+1)} \leq \frac{2^n n!}{(2n-1)!!} \leq 2\sqrt{n}$$

for $n \geq 1$. With $c_n = 2^n n!/(2n-1)!!$, we have $c_{n+1}/c_n = (2n+2)/(2n+1)$, and both inequalities are easily proved by induction. From these estimates, we obtain the inequality

$$\frac{(2n-1)!!}{(2k-1)!! (2n-2k-1)!!} \geq \binom{n}{k} \left(\frac{(k+1)(n-k+1)}{n} \right)^{1/2}. \quad (5.1)$$

To simplify our formulae, we denote the left-hand side of this inequality by $\binom{\binom{n}{k}}{k}$.

Now, by Proposition 4.1, $v_n(d)$ satisfies the recurrence

$$v_n(d) = ((2n-1)!!)^{d-1} - \sum_{k=1}^{n-1} \binom{n-1}{k-1} ((2n-2k-1)!!)^{d-1} v_k(d), \quad n > 1.$$

Clearly $v_n(d) \leq ((2n-1)!!)^{d-1}$. We show that $v_n(d) \geq ((2n-1)!!)^{d-1}(1 - O(1/n))$, an estimate which, in view of the above recurrence, follows if we can show that

$$L := \sum_{k=1}^{n-1} \binom{n-1}{k-1} \binom{\binom{n}{k}}{k}^{-(d-1)} = O\left(\frac{1}{n}\right).$$

Using (5.1), we have

$$\begin{aligned} L &\leq \frac{n}{(2n-1)^{d-1}} + \sum_{k=2}^{n-2} \binom{n-1}{k-1} \binom{n}{k}^{-(d-1)} \left(\frac{n}{(k+1)(n-k+1)} \right)^{(d-1)/2} \\ &\leq \frac{n}{(2n-1)^{d-1}} + \sum_{k=2}^{n-2} \frac{k}{n} \binom{n}{k}^{-(d-2)} \left(\frac{n}{(k+1)(n-k+1)} \right)^{(d-1)/2}. \end{aligned}$$

Since $k/n < 1$, $n/(k+1)(n-k+1) < 1/2$, and $\binom{n}{k} \geq \binom{n}{2}$, and there are fewer than $n-1$ terms in the sum, the second term is at most

$$n^{-(d-2)}(n-1)^{-(d-3)} \cdot 2^{d-2} \cdot 2^{-(d-1)/2} \leq \frac{1}{n},$$

as required. \square

6 Asymptotics of the numbers $w_n(d)$

Recall that $w_n(d)$ and $u_n(d)$ are the numbers of unrestricted, respectively indecomposable, d -dimensional 2-magic matrices of size n . Using the exponential principle, we can relate the sequence $(w_n(d))_{n \geq 0}$ to the sequence $(u_n(d))_{n \geq 0}$ for each fixed d , see (6.1) below. This relationship combined with the fact that the sequence $(u_n(d))_{n \geq 0}$ grows sufficiently rapidly for $d \geq 3$ (Proposition 4 says that it grows very roughly like $((2n)!)^{d-1}$) allows us to conclude that, for $d \geq 3$, $w_n(d)$ and $u_n(d)$ grow at the same rate.

Theorem 5 *For fixed $d \geq 3$, we have*

$$w_n(d) \sim 2^{-nd} ((2n)!)^{d-1}, \quad \text{as } n \rightarrow \infty.$$

Proof. Generalising the argument at the end of Section 3, we observe that d -dimensional 2-magic matrices may be seen as a d -sort species in the sense of Joyal [14] (see also [6, Def. 4 on p. 102]), with the row indices and the column indices forming the two sets on which the functor defining the species operates. Hence, by the exponential principle for d -sort species [14, Prop. 20] (see also [6, Sec. 2.4]), we have

$$\sum_{n \geq 0} w_n(d) \frac{z^n}{(n!)^d} = \exp \left(\sum_{n \geq 1} u_n(d) \frac{z^n}{(n!)^d} \right).$$

If we now differentiate both sides of this equation with respect to z and subsequently multiply both sides by z , then we obtain

$$\begin{aligned} \sum_{n \geq 0} nw_n(d) \frac{z^n}{(n!)^d} &= \left(\sum_{n \geq 1} nu_n(d) \frac{z^n}{(n!)^d} \right) \exp \left(\sum_{n \geq 1} u_n(d) \frac{z^n}{(n!)^d} \right) \\ &= \left(\sum_{n \geq 1} nu_n(d) \frac{z^n}{(n!)^d} \right) \left(\sum_{n \geq 0} w_n(d) \frac{z^n}{(n!)^d} \right). \end{aligned}$$

Comparison of coefficients of z^n on both sides then leads to the relation

$$w_n(d) = u_n(d) + \sum_{k=1}^{n-1} \frac{k}{n} \binom{n}{k}^d u_k(d) w_{n-k}(d). \quad (6.1)$$

As we said at the beginning of this section, our goal is to show that $w_n(d)$ grows asymptotically at the same rate as $u_n(d)$. Hence, putting $w_n(d) = u_n(d) + x_n(d)$, we have to show that $x_n(d) = o(u_n(d))$. We assume inductively that

$$x_m(d) \leq 2^{-m} ((2m-1)!!)^{d-1} (m!)^{d-1}$$

for all m between 2 and $n-1$; the induction starts since we have $x_1(d) = x_2(d) = 0$.

Now, using the inductive hypothesis with the recurrence relation (6.1), we have

$$\begin{aligned} \frac{x_n(d)2^n}{((2n-1)!!)^{d-1}(n!)^{d-1}} &\leq 2 \sum_{k=1}^{n-1} \frac{k}{n} \binom{n}{k}^d \left(\binom{n}{k} \right)^{-(d-1)} \binom{n}{k}^{-(d-1)} \\ &\leq 2 \sum_{k=1}^{n-1} \frac{k}{n} \binom{n}{k}^{-(d-2)} \left(\frac{n}{(k+1)(n-k+1)} \right)^{(d-1)/2} \\ &\leq (2^{1/2} n)^{-(d-3)}, \end{aligned}$$

which establishes the result if $d > 3$. For $d = 3$, this inequality gives the inductive step (that is, that the left-hand side is at most 1); the fact that it is $o(1)$ for large n is proved by an argument like that in the proof of Proposition 4. \square

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