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On a family of tridiagonal matrices

Roland Bacher

September 8, 2008

Abstract¹: We show that certain integral positive definite symmetric tridiagonal matrices of determinant n are in one to one correspondence with elements of $(\mathbb{Z}/n\mathbb{Z})^$. We study some properties of this correspondence.*

In a somewhat unrelated second part we discuss a construction which associates a sequence of integral polytopes to every integral symmetric matrix.

1 Introduction

Let $\alpha_1, \dots, \alpha_n$ be a finite sequence of elements in a commutative ring. We denote by $T(\alpha_1, \dots, \alpha_n)$ the symmetric tridiagonal matrix

$$\begin{pmatrix} \alpha_1 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & \alpha_2 & 1 & & 0 & 0 & 0 \\ 0 & 1 & \alpha_3 & & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & & \alpha_{n-2} & 1 & 0 \\ 0 & 0 & 0 & & 1 & \alpha_{n-1} & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & \alpha_n \end{pmatrix}$$

of size $n \times n$ with diagonal entries $\alpha_1, \dots, \alpha_n$ and sub and super diagonals consisting only of ones.

Leighton and Newman discovered in [2] the remarkable fact that the number of such matrices of size $n \times n$ which are unimodular, integral and positive definite is given by the n -th Catalan number $\binom{2n}{n}/(1+n)$, see also Exercice 6.19 nnn in [5] and [4]. One should mention that this result was already implicitly contained in [1], see the solution to problem (18).

In the present paper, we are interested in the number of such matrices of arbitrary size and determinant N which are integral and have diagonal entries in $\{2, 3, 4, \dots\}$. Such matrices are always positive definite, the case $\alpha_1 = \alpha_2 = \dots = \alpha_n = 2$ defining the root lattice of type A_n .

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Theorem 1.1. *The number of finite symmetric tridiagonal integral matrices of the form $T(\alpha_1, \alpha_2, \dots)$ with diagonal entries ≥ 2 and determinant N is given by Euler's totient function*

$$\Phi(N) = N \prod_{p|N} \left(1 - \frac{1}{p}\right)$$

(where the product is over all prime divisors of N) counting the number $\#((\mathbb{Z}/N\mathbb{Z})^*)$ of invertible elements of the ring $\mathbb{Z}/N\mathbb{Z}$.

The proof is bijective: Given (a, N) for a in $\{1, 2, \dots, N-1\}$ invertible modulo N , we construct a finite sequence $(\alpha_1, \alpha_2, \dots)$ giving rise to a matrix $T(\alpha_1, \alpha_2, \dots)$ with the desired properties. This construction is based on properties of $\mathrm{SL}_2(\mathbb{Z})$ related to Euclid's algorithm.

The organisation of the paper is as follows:

The next section exposes a few useful (and probably well-known) facts concerning $\mathrm{SL}_2(\mathbb{Z})$.

The proof of Theorem 1.1 is contained in Section 3.

Section 4 discusses some algorithmic aspects of the construction which associates to an element $a \in (\mathbb{Z}/N\mathbb{Z})^*$ the corresponding tridiagonal matrix of the form $T(\alpha_1, \dots)$.

Section 5 describes properties of the function $a \mapsto \mathrm{tr}(T) - \dim(T)$ for $a \in (\mathbb{Z}/N\mathbb{Z})^*$.

All matrices described by Theorem 1.1 are definite positive. Section 6 discusses briefly Euclidean lattices admitting the matrices of Theorem 1.1 as Gram matrices.

The final Section 7 is not closely related to the rest of the paper. It describes a construction of a sequence of integral polytopes associated to a symmetric integral matrix and discusses some easy properties of this construction. The first polytope obtained by applying this construction to tridiagonal matrices with 1's on the sub and super diagonal and zeros elsewhere yields for instance integral polytopes with vertices enumerated by Catalan numbers. These polytopes are however distinct from associahedrons (or Stasheff polytopes).

2 SL_2 and the determinant of $T(\alpha_1, \dots, \alpha_n)$

We consider the map

$$\alpha \mapsto M(\alpha) = \begin{pmatrix} 0 & -1 \\ 1 & \alpha \end{pmatrix}$$

extended to finite sequences by setting

$$M(\alpha_1, \alpha_2, \dots, \alpha_n) = M(\alpha_1)M(\alpha_2) \cdots M(\alpha_n) .$$

Denoting by

$$|T(\alpha_1, \dots, \alpha_n)| = \det(T(\alpha_1, \dots, \alpha_n))$$

the determinant of $T(\alpha_1, \dots, \alpha_n)$ we have the following result:

Proposition 2.1. *We have for all $n \geq 2$ the identity*

$$M(\alpha_1, \dots, \alpha_n) = \begin{pmatrix} -|T(\alpha_2, \dots, \alpha_{n-1})| & -|T(\alpha_2, \dots, \alpha_n)| \\ |T(\alpha_1, \dots, \alpha_{n-1})| & |T(\alpha_1, \dots, \alpha_n)| \end{pmatrix}$$

where we use the convention $|T(\alpha_2, \dots, \alpha_{n-1})| = 1$ for $n = 2$.

The proof is a straightforward computation left to the reader.

Proposition 2.1 implies easily the identity

$$|T((\alpha_1, \dots, \alpha_{n+1})| |T(\alpha_2, \dots, \alpha_{n-1})| = |T(\alpha_1, \dots, \alpha_n)| |T(\alpha_2, \dots, \alpha_{n+1})| - 1$$

which is a particular case of Dodgson's condensation formula.

Another useful result is the following "symmetry".

Proposition 2.2. *If*

$$M(\alpha_1, \alpha_2, \dots, \alpha_n) = \begin{pmatrix} -a & -b \\ c & d \end{pmatrix}$$

then

$$M(\alpha_n, \dots, \alpha_2, \alpha_1) = \begin{pmatrix} -a & -c \\ b & d \end{pmatrix}.$$

Proof Introducing the involution $V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, a short computation shows $VM(\alpha)V = M(\alpha)^{-1}$. This yields

$$VM(\alpha_1, \dots, \alpha_n)^{-1}V = M(\alpha_n, \dots, \alpha_1)$$

which establishes the result by computing

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} d & b \\ -c & -a \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

□

The easy identity

$$M(x)M(y) = M(x+1)M(1)M(y+1) = \begin{pmatrix} -1 & -y \\ x & xy-1 \end{pmatrix}$$

shows that the set of integral positive definite matrices of the form $T(\alpha_1, \alpha_2, \dots)$ with given determinant is infinite without further conditions.

Leighton and Newman consider matrices of the form $T(\alpha_1, \dots, \alpha_n)$ which are integral, positive definite and have fixed size $n \times n$ in order to get finite sets. In the present paper, the size of the matrices $T(\alpha_1, \alpha_2, \dots)$ is arbitrary but the diagonal coefficients $\alpha_1, \alpha_2, \dots$ are restricted to the set $\{2, 3, 4, \dots\}$ of natural integers ≥ 2 . This restriction is motivated by the following result.

Proposition 2.3. *Let $\alpha_1, \alpha_2, \dots, \alpha_l$ be a sequence of $l \geq 1$ real numbers $\alpha_i \geq 2$ for $i = 1, \dots, l$. Consider*

$$M(\alpha_1, \alpha_2, \dots, \alpha_l) = \begin{pmatrix} -a & -b \\ c & d \end{pmatrix}.$$

We have then the inequalities

$$0 \leq a < \min(b, c), \quad \max(b, c) < d \quad \text{and} \quad c - a \leq d - b.$$

Corollary 2.4. *We have*

$$\det(T(\alpha_1, \alpha_2, \dots, \alpha_{l-1})) < \det(T(\alpha_1, \alpha_2, \dots, \alpha_{l-1}, \alpha_l))$$

if $\alpha_1, \dots, \alpha_l$ are real numbers ≥ 2 .

In particular, the number of matrices of the form $T(\alpha_1, \alpha_2, \dots)$ with determinant N and integral diagonal coefficients $\alpha_1, \alpha_2, \dots \in \{2, 3, 4, \dots\}$ is finite.

Proof The first part follows by applying Proposition 2.1 and the inequality $c < d$ of Proposition 2.3 to the matrix $M(\alpha_1, \dots, \alpha_l)$.

The second part follows also from Proposition 2.1 and from the observation that the number of integral matrices satisfying the inequalities of Proposition 2.3 with $d = N$ is finite. \square

Corollary 2.5. *A matrix of the form $T(\alpha_1, \alpha_2, \dots, \alpha_l)$ with $\alpha_i \geq 2$ for $i = 1, 2, \dots, l$ is positive definite.*

Remark 2.6. *Corollary 2.5 follows of course also from the well-known observation that $T(2, 2, \dots, 2)$ is a Gram matrix for a root lattice of type A and from the fact that real symmetric positive matrices form a convex cone.*

Proof of Proposition 2.3 By induction on l . The results hold obviously for $l = 1$ since

$$M(\alpha_1) = \begin{pmatrix} 0 & -1 \\ 1 & \alpha_1 \end{pmatrix}$$

satisfies all inequalities for $\alpha_1 \geq 2$.

For the induction step we consider

$$\begin{pmatrix} -a & -b \\ c & d \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & x \end{pmatrix} = \begin{pmatrix} -b & a - xb \\ d & -c + xd \end{pmatrix}.$$

We have obviously $0 < b, d$ and $d > b$ by induction. Since $0 \leq a < b$ we have

$$-a + xb > (x - 1)b \geq b > 0$$

for $x \geq 2$.

The inequalities $0 < c < d$ show similarly

$$-c + xd > (x-1)d \geq d > 0 .$$

The inequalities $c - a \leq d - b$ and $d > b$ imply

$$(xd - c) - (xb - a) = x(d - b) - (c - a) \geq (x-1)(d - b) \geq d - b > 0$$

for $x \geq 2$. □

3 Proof of Theorem 1.1

Theorem 3.1. *For every integral unimodular matrix*

$$A = \begin{pmatrix} -a & -b \\ c & d \end{pmatrix}$$

such that

$$0 \leq \min(a, b, c, d) \text{ and } \max(b, c) < d$$

there exists a unique integer $l \geq 1$ and a unique finite sequence $(\alpha_1, \dots, \alpha_l) \in \{2, 3, 4, \dots\}^l$ such that

$$A = M(\alpha_1)M(\alpha_2) \cdots M(\alpha_l) .$$

Theorem 1.1 is now implied by the following result.

Proposition 3.2. *Integral matrices of the form $T(\alpha_1, \dots, \alpha_n)$ with determinant N and diagonal coefficients ≥ 2 are in bijection with the subset of integers in $\{1, \dots, N\}$ which are invertible modulo N .*

Proof of Proposition 3.2 Given a pair (a, N) of natural integers with $a \in \{1, \dots, N-1\}$ such that a is invertible modulo N , we consider $b \in \{1, \dots, N-1\}$ such that $ab \equiv 1 \pmod{N}$ and we set $k = \frac{ab-1}{N} \in \mathbb{N}$. The matrix $A = \begin{pmatrix} -k & -b \\ a & N \end{pmatrix}$ satisfies the hypotheses of Theorem 3.1 and has thus a unique factorisation of the form

$$A = M(\alpha_1)M(\alpha_2) \cdots M(\alpha_l)$$

for some integer $l \geq 1$ and $\alpha_1, \alpha_2, \dots \in \{2, 3, \dots\}^l$.

Proposition 2.1 shows thus that the matrix $T(\alpha_1, \dots, \alpha_l)$ has determinant N .

This construction yields an injective map from $(\mathbb{Z}/N\mathbb{Z})^*$ into integral matrices of the form $T(\alpha_1, \alpha_2, \dots)$ with determinant N and diagonal coefficients $\alpha_i \geq 2$.

The fact that this map is onto follows by applying the unicity result of Theorem 3.1 to the matrix

$$\begin{pmatrix} -|T(\alpha_2, \dots, \alpha_{n-1})| & -|T(\alpha_2, \dots, \alpha_n)| \\ |T(\alpha_1, \dots, \alpha_{n-1})| & |T(\alpha_1, \dots, \alpha_n)| \end{pmatrix} = M(\alpha_1) \cdots M(\alpha_l)$$

associated to a suitable tridiagonal matrix $T(\alpha_1, \alpha_2, \dots)$. \square

Proof of Theorem 3.1 If $a = 0$ then unimodularity of A implies $b = c = 1$ and $A = M(d)$ for some integer $d \geq 2 > 1 = b = c$. Otherwise, the identity

$$bc = ad + 1$$

implies $bc \equiv 1 \pmod{d}$. This shows that the integers c, d are coprime and determine a, b uniquely by considering the unique integer $b \in \{1, \dots, d-1\}$ such that $bc \equiv 1 \pmod{d}$ and by setting $a = \frac{bc-1}{d} \geq 1$. Unimodularity of A and strict positivity of a imply that Defining $t \in \{1, \dots, b-1\}$ as the unique integer satisfying the congruence $t \equiv -d \pmod{b}$, the equality $\det(A) = -ad + bd = 1$ implies $at \equiv 1 \pmod{b}$ and we can thus consider the natural integer $s = \frac{at-1}{b} \geq 0$. The computation

$$\begin{pmatrix} -a & -b \\ c & d \end{pmatrix} \begin{pmatrix} b & t \\ -a & -s \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & ct - sd \end{pmatrix}$$

and the inequality

$$b \left(ct - \frac{at-1}{b} d \right) = bct - adt + d = t + d > b$$

show thus

$$\begin{pmatrix} -a & -b \\ c & d \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & ct - sd \end{pmatrix} \begin{pmatrix} -s & -t \\ a & b \end{pmatrix}$$

where $ct - sd \geq 2$. Since $a = \frac{bc-1}{d} < b$, the integral unimodular matrix

$$\begin{pmatrix} -s & -t \\ a & b \end{pmatrix}$$

satisfies again the hypotheses of Theorem 3.1. Induction on $d > b$ establishes the existence of a sequence $(\alpha_1, \alpha_2, \dots, \alpha_l)$ in $\{2, 3, 4, \dots\}^l$ such that $A = M(\alpha_1)M(\alpha_2) \cdots M(\alpha_l)$.

Unicity of the sequence α_1, \dots is obvious for $a = 0$ by Proposition 2.1. For $a > 0$ it follows from the observation that the inequalities $0 \leq \min(\tilde{s}, \tilde{t})$ and $\tilde{t} < b$ determine the integral unimodular matrix

$$\begin{pmatrix} -\tilde{s} & -\tilde{t} \\ a & b \end{pmatrix} = \begin{pmatrix} \tilde{\alpha}_1 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} -a & -b \\ c & d \end{pmatrix} = T(\tilde{\alpha}_2, \tilde{\alpha}_3, \dots)$$

uniquely. This shows $\tilde{\alpha}_1 = \alpha_1$ and by induction $\tilde{\alpha}_i = \alpha_i$ and $l' = l$ for $\tilde{\alpha}_1, \dots, \tilde{\alpha}_{l'} \in \{2, 3, \dots\}^{l'}$ such that $M(\alpha_1, \dots, \alpha_l) = M(\tilde{\alpha}_1, \dots, \tilde{\alpha}_{l'})$. \square

Remark 3.3. *Theorem 3.1 is equivalent to the assertion that the matrices $M(2), M(3), M(4), \dots$ generate a free submonoid of $\mathrm{SL}_2(\mathbb{Z})$. The subgroup generated by $M(2), M(3), \dots$ is however not free and coincides with $\mathrm{SL}_2(\mathbb{Z})$. Indeed, the identity*

$$M(\lambda)M(\lambda + \mu)^{-1}M(\lambda) = M(\lambda - \mu)$$

shows that the subgroup generated by two integral matrices $M(k)$ and $M(k+1)$ contains the generators

$$M(0) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \text{ and } M(1) = \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}$$

of $\mathrm{SL}_2(\mathbb{Z})$.

4 Algorithmic aspects

In the sequel, $x \pmod{y}$ denotes always the unique natural integer in $\{1, \dots, y\}$ representing the equivalence class of x in $\mathbb{Z}/y\mathbb{Z}$ for an integer x and a natural integer $y \geq 2$. Similarly, if x is invertible modulo y , then $x^{-1} \pmod{y}$ denotes the unique integer in $\{1, \dots, y-1\}$ such that $x(x^{-1} \pmod{y}) \equiv 1 \pmod{y}$.

Given a natural integer $N \geq 2$ and an integer $a \in \{1, \dots, N-1\}$ which is invertible modulo N , we denote by

$$W(a, N) = \alpha_1, \dots, \alpha_l$$

the unique finite sequence of natural integers $\alpha_i \geq 2$ such that

$$M(\alpha_1 \dots \alpha_l) = \begin{pmatrix} -x & -y \\ a & N \end{pmatrix} \in \mathrm{SL}_2(\mathbb{Z})$$

where $y \equiv a^{-1} \pmod{N}$ and $x = \frac{ay-1}{N}$, cf Theorem 3.1.

We denote by $l(a, N) = l$ the length of the word $W(a, N)$ and by $W(a, N)_i = \alpha_i$ the i -th element (for $i = 1, \dots, l$) of the sequence $W(a, N)$. We have thus

$$W(a, N) = W(a, N)_1, W(a, N)_2, \dots, W(a, N)_{l(a, N)} .$$

We have obviously

$$W(1, N) = W(1, N)_1 = N, \quad l(1, N) = 1 .$$

If $a, b \in \{1, \dots, N-1\}$ are invertible elements modulo N such that $ab \equiv 1 \pmod{N}$, Proposition 2.2 shows that we have

$$l(a, N) = l(b, N)$$

and

$$W(a, N)_i = W(b, N)_{l(a, N)+1-i} .$$

Otherwise stated, the matrices $T(W(a, N))$ and $T(W(b, N))$ are related to each other by conjugation with the antidiagonal involution of size $l(a, N) \times l(a, N)$.

We denote by $\lfloor x \rfloor$ the integral part of a real number x defined as the unique integer satisfying

$$x - 1 < \lfloor x \rfloor \leq x .$$

The following result allows computations:

Theorem 4.1. *For every integer $N \geq 2$ we have*

$$W(1, N) = N .$$

For an integer $a \in \{2, \dots, N-1\}$ invertible modulo N (with N a natural integer ≥ 3) we have

$$W(a, N) = W((-N) \pmod{a}, a), \left(1 + \left\lfloor \frac{N}{a} \right\rfloor\right)$$

or equivalently

$$W(a, N) = \left(1 + \left\lfloor \frac{N}{b} \right\rfloor\right), W((-N)^{-1} \pmod{b}, b)$$

where $b = (a^{-1} \pmod{N}) \in \{1, \dots, N-1\}$.

Remark 4.2. *The map $(a, N) \mapsto ((-N \pmod{a}), a)$ involved in the first equality for $W(a, N)$ for $a \geq 2$ coincides (up to the $-$ sign) with Euclid's celebrated algorithm for computing the greatest common divisor of a and N .*

Proof of Theorem 4.1 The assertion concerning $W(1, N)$ is obvious.

Set $k = \frac{ab-1}{N} \geq 1$ where $b = a^{-1} \pmod{N}$ is the inverse of a modulo N in $\{2, \dots, N-1\}$. Computing

$$\begin{pmatrix} -k & -b \\ a & N \end{pmatrix} \begin{pmatrix} 1 + \lfloor N/a \rfloor & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -k(1 + \lfloor N/a \rfloor) + b & -k \\ a(1 + \lfloor N/a \rfloor) - N & a \end{pmatrix} ,$$

the lower left coefficient of the last matrix is given by

$$a \left(1 + \frac{N - (N \pmod{a})}{a}\right) - N = a + N - (N \pmod{a}) - N = (-N) \pmod{a}$$

and is thus a strictly positive natural integer $< a$. Since

$$k(a(1 + \lfloor N/a \rfloor) - N) \equiv -kN \equiv 1 \pmod{a} ,$$

positivity of $k, a(1 + \lfloor N/a \rfloor) - N$, the obvious inequality $k < a$ and unimodularity of all involved matrices imply that the last matrix satisfies the conditions of Theorem 4.1. This implies the first equality for $a \geq 2$ by induction on N .

The second equality can be proven similarly. It follows also from the first equality and from Proposition 2.2. \square

For computing $W(a, N)$ with $a \in \{1, \dots, N-1\}$ invertible modulo N and very close to a huge integer N the following result is useful:

Proposition 4.3. *The sequence $W(N-1, N)$ is the constant sequence $2, 2, \dots, 2$ of length $N-1$.*

We have for $a \in \{2, \dots, N-2\}$ invertible modulo N the equality

$$W(a, N) = W((\lambda + 1)a - \lambda N, \lambda a - (\lambda - 1)N), 2, 2, 2, \dots, 2$$

where $\lambda = \lfloor a/(N-a) \rfloor$ and where $2, 2, 2, \dots, 2$ is the constant sequence of length λ .

Proof The assertion for the sequence $W(N-1, N)$ follows from the case $k = N-1$ of the identity

$$\begin{pmatrix} 0 & -1 \\ 1 & 2 \end{pmatrix}^k = \begin{pmatrix} 1-k & -k \\ k & k+1 \end{pmatrix}$$

which is easily established.

For $a \geq 2$ such that $a < N/2$ we have $a/(N-a) < 1$ yielding $\lambda = 0$ and the formula is trivial.

The case $a = N/2$ implies $(a, N) = (1, 2)$ corresponding to the case $(N-1, N)$ for $N = 2$.

The proof in the case $a > N/2$ is by induction on λ . If $\lambda = 1$ we have to prove

$$W(a, N) = W(2a - N, a), 2$$

where $\frac{1}{2}N < a < \frac{2}{3}N$. This boils down to the identity $W(a, N) = W((-N) \pmod{a}, a), (1 + \lfloor N/a \rfloor)$ of Theorem 4.1.

For $\frac{2}{3}N \leq a < N-1$ we have as above $W(a, N) = W(2a - N, a), 2$ by Theorem 4.1. The trivial identities

$$\frac{2a - N}{a - (2a - N)} = \frac{a}{N - a} - 1$$

and

$$k(2a - N) - (k - 1)a = (k + 1)a - kN$$

and induction on λ end the proof. \square

Theorem 4.1 and Proposition 4.3 give a fast algorithm for computing

$$\sum_{i=1}^{l(a, N)} (W(a, N)_i)^e$$

for arbitrary $e \in \mathbb{N}$ (or $e \in \mathbb{C}$). The case $e = 0$ corresponds to the length $l(a, N)$ of the sequence $W(a, N)$ and the case $e = 1$ yields the trace of the tridiagonal matrix T associated to $W(a, N)$. The details are as follows:

INPUT: (a, N) with $a \in \{1, \dots, N-1\}$ invertible modulo N (for $N \geq 2$) and an integer e .

Set $r = 0$.

LOOP:

IF $a = 1$, OUTPUT: $(r + N^e)$ and STOP ENDIF.

IF $a < (N/2)$, replace r by $r + (1 + \lfloor N/a \rfloor)^e$ and (a, N) by $((-N) \pmod{a}, a)$ where $(-N) \pmod{a}$ is the choosen in $\{1, \dots, a-1\}$ ENDIF.

IF $a = N-1$, OUTPUT: $r + (N-1)2^e$ and STOP ENDIF.

IF $a > N/2$, set $\lambda = \lfloor a/(N-a) \rfloor$, replace r by $r + \lambda 2^e$ and (a, N) by $((\lambda+1)a - \lambda N, \lambda a - (\lambda-1)N)$ ENDIF.

END OF LOOP.

5 A function with an additional symmetry

Set $\sigma(a, N) = \sum_{k=1}^{l(a, N)} (W(a, N)_k - 1) = \text{tr}(T(W(a, N))) - \dim(T(W(a, N)))$ for $a \in \{1, \dots, N-1\}$ invertible modulo N .

Proposition 2.2 shows that the function σ satisfies $\sigma(a, N) = \sigma((a^{-1} \pmod{N}), N)$.

The following result shows that σ satifies an additional symmetry.

Theorem 5.1. *We have*

$$\sigma(a, N) = \sigma(N-a, N)$$

for every $a \in \{1, \dots, N-1\}$ which is invertible modulo N .

Proof We have $\sigma(1, N) = N-1$ and $\sigma(N-1, N) = (N-1)(2-1) = N-1$.

Consider now a such that $2 \leq a < \frac{N}{2}$. Setting $\lambda = \lfloor (N-a)/a \rfloor = \frac{N-(N \pmod{a})}{a} - 1$, Proposition 4.3 shows

$$\sigma(N-a, N) = \sigma(N - (\lambda+1)a, N - \lambda a) + \lambda$$

implying

$$\sigma(N-a, N) = \sigma(a, N - \lambda a) + \lambda$$

by induction on N . Theorem 4.1 yields thus

$$\begin{aligned} \sigma(N-a, N) &= \sigma((-N) \pmod{a}, a) + \frac{N - \lambda a - (N \pmod{a})}{a} + \lambda \\ &= \sigma((-N) \pmod{a}, a) + \lfloor N/a \rfloor \end{aligned}$$

which establishes the result since we have also

$$\sigma(a, N) = \sigma((-N) \pmod{a}, a) + \lfloor N/a \rfloor$$

by Theorem 4.1. □

A few values of $\sigma(a, N)$ are given by the following Table:

| | | | | | | | | | | | | | | | | |
|------------|----|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|
| $a =$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| $N = 2 :$ | 1 | | | | | | | | | | | | | | | |
| $N = 3 :$ | 2 | 2 | | | | | | | | | | | | | | |
| $N = 4 :$ | 3 | | 3 | | | | | | | | | | | | | |
| $N = 5 :$ | 4 | 3 | 3 | 4 | | | | | | | | | | | | |
| $N = 6 :$ | 5 | | | | 5 | | | | | | | | | | | |
| $N = 7 :$ | 6 | 4 | 4 | 4 | 4 | 6 | | | | | | | | | | |
| $N = 8 :$ | 7 | | 4 | | 4 | | 7 | | | | | | | | | |
| $N = 9 :$ | 8 | 5 | | 5 | 5 | | 5 | 8 | | | | | | | | |
| $N = 10 :$ | 9 | | 5 | | | | 5 | | 9 | | | | | | | |
| $N = 11 :$ | 10 | 6 | 5 | 5 | 6 | 6 | 5 | 5 | 6 | 10 | | | | | | |
| $N = 12 :$ | 11 | | | | 5 | | 5 | | | | 11 | | | | | |
| $N = 13 :$ | 12 | 7 | 6 | 6 | 5 | 7 | 7 | 5 | 6 | 6 | 7 | 12 | | | | |
| $N = 14 :$ | 13 | | 6 | | 6 | | | | 6 | | 6 | | 13 | | | |
| $N = 15 :$ | 14 | 8 | | 6 | | | 8 | 8 | | | 6 | | 8 | 14 | | |
| $N = 16 :$ | 15 | | 7 | | 7 | | 6 | | 6 | | 7 | | 7 | | 15 | |
| $N = 17 :$ | 16 | 9 | 7 | 7 | 6 | 7 | 6 | 9 | 9 | 6 | 7 | 6 | 7 | 7 | 9 | 16 |

5.1 Continued fraction expansions

Let $[\gamma_1, \gamma_2, \dots]$ be the continued fraction expansion of $x \in (0, 1)$ defined recursively by $x = \frac{1}{\gamma_1 + [\gamma_2, \dots]}$ where $\gamma_1 = \lfloor 1/x \rfloor$ and $[\gamma_2, \dots] = 1/x - \gamma_1$ (and $0 = [\emptyset]$ by convention).

Theorem 5.2. *We have*

$$1 + \sigma(a, N) = \sum_{i \geq 1} \gamma_i$$

where $\frac{a}{N} = [\gamma_1, \gamma_2, \dots]$ is the continued fraction expansion of the reduced rational fraction a/N in $(0, 1)$.

Proof The result holds obviously for $a = 1$. For $a > 1$, we have

$$\gamma_1 = \lfloor N/a \rfloor$$

and

$$[\gamma_2, \dots] = N/a - \lfloor N/a \rfloor = \frac{N - (N - (N \pmod{a}))}{a} = \frac{N \pmod{a}}{a}$$

The equality $\gamma_1 = \alpha_1$ and induction on N end the proof. □

Remark 5.3. *Theorem 5.1 follows also from Theorem 5.2 together with the easy continued fraction expansion*

$$1 - x = [1, \alpha_1 - 1, \alpha_2, \alpha_3, \dots]$$

for $x = [\alpha_1, \alpha_2, \alpha_3, \dots]$ in $(0, 1/2)$.

6 Lattices

Given d integers $\alpha_1, \dots, \alpha_d \in \{2, 3, \dots\}^d$, we denote by $\Lambda(\alpha_1, \dots, \alpha_d)$ the Euclidean lattice of rank d with scalar product given by the Gram matrix $T(\alpha_1, \dots, \alpha_d)$ (which is positive definite by Corollary 2.5. We say that such a lattice is of type T.

Proposition 6.1. *A lattice $\Lambda(\alpha_1, \dots, \alpha_d)$ of type T has minimal norm $\min(\alpha_1, \dots, \alpha_d) \geq 2$.*

Proof We work with a basis with Gram matrix $T(\alpha_1, \dots, \alpha_d)$. Replacing $\alpha_1, \dots, \alpha_d$ by 2 yields a root lattice Λ' of type A_d and the obvious map sending a vector $\lambda = (\lambda_1, \dots, \lambda_d)$ of the lattice $\Lambda(\alpha_1, \dots, \alpha_d)$ to the corresponding vector $\lambda' = (\lambda_1, \dots, \lambda_d)$ with the same coordinates in $\Lambda(2, 2, \dots, 2)$ is a linear map which is one-to-one and length-shrinking.

This proves the Proposition if $\min(\alpha_1, \dots, \alpha_d) = 2$. In the remaining case, apply the Proposition to the lattice $\Lambda' = \Lambda(\alpha_1 - \kappa, \alpha_2 - \kappa, \dots, \alpha_d - \kappa)$ where $\kappa = \min(\alpha_1, \dots, \alpha_d) - 2$ and observe that the obvious linear map from $\Lambda(\alpha_1, \dots, \alpha_d)$ onto Λ' is one-to-one and diminishes norms of non-zero elements at least by κ . \square

Proposition 6.2. *Blocks of adjacent 2's in the sequence $\alpha_1, \dots, \alpha_d$ are in bijection with irreducible root-sublattices in $\Lambda(\alpha_1, \dots, \alpha_d)$.*

The easy proof is left to the reader.

Theorem 6.3. *Two lattices $\Lambda(\alpha_1, \dots, \alpha_d)$ and $\Lambda(b_1, \dots, b_d)$ of type T are isomorphic if and only if either $\alpha_i = b_i$ for $i = 1, \dots, d$ or $\alpha_i = b_{d+1-i}$ for $i = 1, \dots, d$.*

Corollary 6.4. *The number of isomorphism classes of Euclidean lattices (of arbitrary dimension) of type T, determinant $N \geq 2$ and containing no elements of norm 1 is given by $(\Phi(N) + \nu_N)/2$ where ν_N equals the number of elements of order ≤ 2 in the multiplicative group $(\mathbb{Z}/N\mathbb{Z})^*$.*

Idea for the proof of Theorem 6.3 We show by induction on the dimension d that metric properties of a lattice $\Lambda(\alpha_1, \dots, \alpha_d)$ of type T determine the integer sequence $\alpha_1, \dots, \alpha_d$ uniquely, up to reversion of the order.

If $\min(\alpha_1, \dots, \alpha_d) = 2$, the root system \mathcal{R} of $\Lambda(\alpha_1, \dots, \alpha_d)$ is determined by the set of blocks of adjacent 2's in the sequence $\alpha_1, \alpha_2, \dots$. The sublattice $\tilde{\Lambda}$ orthogonal to the root lattice generated by \mathcal{R} corresponds to all terms α_i such that $\alpha_{i-1}, \alpha_i, \alpha_{i+1} \geq 2$ and is an orthogonal sum of lattices of type T. By induction on the rank, the lattice $\tilde{\Lambda}$ determines (up to reversion of the order) disjoint subsequences $\alpha_{i_j}, \alpha_{i_j+1}, \alpha_{i_j+d_j}$ containing no 2's and not adjacent to 2's in $\alpha_1, \dots, \alpha_d$. Terms adjacent to irreducible root lattices can essentially be recovered by considering minimal norms of sets of vectors not

contained and not orthogonal to such an irreducible root lattice. Orthogonality consideration allow then to glue all pieces together in an essentially unique way.

If $\min(\alpha_1, \dots, \alpha_d) > 2$ one can replace the root lattice by the lattice generated by the set of minimal vectors (corresponding to basis vectors $\pm e_i$ such that $\alpha_i = \min(\alpha_1, \dots, \alpha_d)$) and proceed as above. \square

Remark 6.5. *Lattices of type T have poor densities and are thus not interesting from the point of view of sphere-packings.*

7 Polytopes

Let A be an integral symmetric matrix of size $d \times d$. For every natural integer N , we denote by $\mathcal{L}_A(N)$ the set of integral diagonal matrices of size $d \times d$ such that $A + D$ is positive definite of determinant N for every matrix $D \in \mathcal{L}_A(N)$. We denote by $\text{Conv}(\mathcal{L}_A(N)) \subset \mathbb{R}^d$ the convex hull of $\mathcal{L}_A(N)$.

Theorem 7.1. *For all N , the set $\text{Conv}(\mathcal{L}_A(N))$ is a polytope whose set of integral elements is contained in*

$$\cup_{k=N}^{\infty} \mathcal{L}_A(k)$$

and whose vertices are given by the the integral elements $\mathcal{L}_A(N)$.

Proof The Brunn-Minkowski Theorem, see eg. Theorem 6.2 in [3] states that

$$\det(A + \sum_{D \in \mathcal{L}_A(N)} \lambda_D D)^{1/d} \geq \sum_{D \in \mathcal{L}_A(N)} \lambda_D \det(A + D)^{1/d}$$

if $\sum_{D \in \mathcal{L}_A(N)} \lambda_D = 1$ with λ_D positive real numbers. This shows that we have $\det(A + D') \geq N$ for all $D' \in \text{Conv}(\mathcal{L}_A(N))$ and the inequality is strict if $D' \notin \mathcal{L}_A(N)$. Finiteness of the set $\mathcal{L}_A(N)$ follows from the fact that given two elements $(\alpha_1, \dots, \alpha_d)$ and $(\beta_1, \dots, \beta_d)$ of $\mathcal{L}_A(N)$, there exists indices $i, j \in \{1, \dots, d\}$ such that $\alpha_i < \beta_i$ and $\alpha_j > \beta_j$. \square

The construction of the polytope $\text{Conv}(\mathcal{L}_A(N))$ has the following properties, given without proofs. (They are straightforward.)

The diagonal part of A is essentially irrelevant: If $\tilde{A} = A + D$ where D is integral diagonal and A is integral symmetric, then $\mathcal{L}_{\tilde{A}}(N) = \mathcal{L}_A(N) - D$. We suppose henceforth that A has zeroes along the diagonal.

Automorphisms of A (conjugations by signed permutation matrices commuting with A) act on the polytopes $\text{Conv}(\mathcal{L}_A(N))$ in the obvious way by permuting the coefficients according to the underlying ordinary permutation matrix.

If A is a “direct sum” $A = A_1 + A_2$ of disjoint diagonal blocks, then

$$\text{Conv}(\mathcal{L}_A(1)) = \text{Conv}(\mathcal{L}_{A_1}(1)) \times \text{Conv}(\mathcal{L}_{A_2}(1)) .$$

More generally,

$$\mathcal{L}_A(N) = \cup_{l|N} \mathcal{L}_{A_1}(l) \times \mathcal{L}_{A_2}(N/l)$$

where the union is over all natural integers dividing N .

The following construction yields a map from the permutation group on the d indices into the set $\mathcal{L}_A(1)$: Given a permutation matrix σ of size $d \times d$, we consider the unique integral diagonal matrix $D = D_\pi$ such that the submatrix formed by the first k rows and columns of $\sigma^{-1}(A + D_\sigma)\sigma$ is unimodular for every integer k in $\{1, \dots, d\}$. These special vertices are invariant under automorphisms of A (and their convex hull is a polytope contained in $\text{Conv}(\mathcal{L}_A(1))$ which is invariant under automorphisms of A).

If A is an adjacency matrix of a simple finite undirected graph which is connected, the above construction can be restricted to permutations such that the first k vertices form connected subgraphs for all k . The subset of these vertices is still invariant under automorphisms. There exists slight generalisations of this construction.

Examples The easiest case is given if the matrix A is the zero-matrix of size $d \times d$. For $d \geq 2$, the polytope $\text{Conv}(\mathcal{L}_A(N))$ is a $(d-1)$ -dimensional simplex if and only if N is a prime number. More interesting cases occur if N is highly composite.

A probably interesting example is given by considering the symmetric matrix A of size $d \times d$ with coefficients $A_{i,j} = 1$ if $|i-j| = 0$ and $A_{i,j} = 0$ otherwise. By [2], the set $\mathcal{L}_A(1)$ contains then exactly $C_d = \binom{2d}{d}/(d+1)$ elements forming the vertex set of an integral polytope P_d of dimension d if $d \geq 3$. The polytope P_3 for instance is the convex hull of the five vertices

$$\begin{aligned} v_1 &= (1, 2, 2) \\ v_2 &= (1, 3, 1) \\ v_3 &= (2, 1, 3) \\ v_4 &= (2, 2, 1) \\ v_5 &= (3, 1, 2) \end{aligned}$$

Its faces are defined by equalities of the five inequalities

$$\begin{array}{ll} y + z \leq 4 & \{v_1, v_2, v_3\} \\ x + y + z \geq 5 & \{v_1, v_2, v_4\} \\ x + 2y + z \geq 7 & \{v_1, v_3, v_4, v_5\} \\ 2x + 3y + 2z \leq 13 & \{v_2, v_3, v_5\} \\ x + y \leq 4 & \{v_2, v_4, v_5\} \end{array}$$

(with vertex-sets indicated for each face) and the polytope P_3 is thus a pyramid with summit v_2 over the planar polygon formed by the four vertices v_1, v_3, v_4, v_5 . The face $\{v_1, v_2, v_4\}$ contains all vertices associated to permutation matrices of size 3×3 . (This can easily be generalised to an arbitrary dimension d : Such special vertices are all of the form $(1, 2, 2, 2, \dots, 2, 1) + e_i$

where $e_i = (0, \dots, 0, 1, 0, \dots, 0)$ denotes the i -th basis vector and form a unique simplicial face of the of polytope $\text{Conv}(\mathcal{L}_A(1))$.)

It would perhaps be interesting to understand the polytopes P_d in general, in particular eventual connections with so-called Associahedrons (or Stasheff polytopes) whose vertices are also enumerated by Catalan numbers and whose dimensions are in general one less.

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