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Crystallographic Applications of the Elementary Divisor Theorem

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Abstract

A crystallographic interpretation of the elementary divisor theorem applied to square integral matrices is presented. The concept of a least multiplier of a rational square matrix is introduced and its properties are derived from the theorem. These topics are relevant in the formulation of a general theory of coincidence-site lattices.

1. Introduction

Mathematically, a lattice is a module of linear forms over the ring of integers. A linear mapping between an s-dimensional and an r-dimensional lattice can be expressed by an $s \times r$ matrix of rank equal to the smaller of r and s; this matrix is written in particular bases of the two lattices. We shall consider mostly matrices which contain only integral elements; they are termed integral or i matrices. Particular attention will be given to square i matrices. These matrices obviously define a relation between a lattice and a sublattice of the same dimension. A square i matrix will be termed a 1 matrix if the absolute value of its determinant is unity. A change of basis in a lattice is represented by a 1 matrix.

The purpose of this paper is twofold. First, we introduce the elementary divisor theorem of linear algebra (*e.g.* Van der Waerden, 1970) and give a crystallographic interpretation of the invariant set (related to the elementary divisors) of a square i matrix. We then apply the theorem to determine the least multiplier of a rational square matrix. This problem is relevant in the context of coincidence-site-lattice theory to find the degree of coincidence of two lattices. In the following paper (Fortes, 1983) these results are incorporated in a general theory of coincidence-site and related lattices. The elementary divisor theorem was previously applied by Grimmer (1976) to obtain the degree of coincidence between two crystal lattices. However, his results are not entirely correct as we will show in the following paper (Fortes, 1983).

2. The elementary divisor theorem

The elementary divisor theorem (Van der Waerden, 1970), which is central to the following discussion, states that given a square i matrix, N, it is always possible to find two 1 matrices S, T such that

$$SNT^{-1} = N_d, \tag{1}$$

where N_d is a diagonal matrix. Note that T^{-1} is also a 1 matrix. In other words, there are always bases for the two lattices related by N, such that the transformation is represented by an (equivalent) diagonal matrix. For a given N, there are in general several equivalent diagonal forms. Among these, there is a particular diagonal form, which we term the *principal diagonal form*, $\bar{N}_d$, with the following property: the diagonal elements (n_1, ..., n_s) of $\bar{N}_d$ (with $n_i > 0$) are such that n_{i-1} is a divisor of n_i. The n_i are termed the *elementary divisors* of N. It is clear that two i matrices with the same principal diagonal form are equivalent and *vice versa*.

The n_i can easily be determined in the following way (Van der Waerden, 1970). Let d_k be the greatest comon divisor (GCD) of the k-rowed subdeterminants of N. Clearly, $d_s = |\det N|$. Then

$$n_1 = d_1$$
$$n_i = d_i/d_{i-1}. \tag{2}$$

The d_i are therefore invariant on a change of bases, and will be called the *invariants* of N. The name 'determinant divisor' is also used for d_i. It is obvious that two i matrices with the same invariant set are equivalent.

Let n be the smallest positive integer such that nN^{-1} is an i matrix. It is easy to show that n is also an invariant. In fact, since $N^{-1} = \operatorname{adj} N/d_s$, it follows that $d_s = nd_{s-1}$, so that $n = n_s$ is an invariant.

The other diagonal forms of N can be obtained by combining the prime factors in $|\det N|$ in a different way. In the principal diagonal form the exponents of any prime factor appear in non-decrescent order in the successive elements. We give an example, for

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$$N = \begin{bmatrix} 6 & -8 & 0 \\ 9 & 8 & 9 \\ 18 & 8 & 18 \end{bmatrix}.$$

The invariants are $d_1 = 1$; $d_2 = 2 \times 3$; $d_3 = 2^4 \times 3^3$. The principal diagonal form is $(1; 2 \times 3; 2^3 \times 3^2)$ or (1, 6, 72). The other diagonal forms are (2, 3, 72), (1, 18, 24), (3, 8, 18), (2, 9, 24), (6, 8, 9) and all others obtained from these by changing the order and the sign of the integers.

It should be noted that the elementary divisor theorem can also be applied to rectangular i matrices. If the rank of the matrix is r, it can be put in a form which contains a square $r \times r$ principal diagonal submatrix and zeros (Van der Waerden, 1970). The diagonal elements are obtained in the same way, (2), from the invariant set.

3. Geometrical interpretation of the invariants

Consider an arbitrary s-dimensional lattice L with a vector basis $(\mathbf{e}_1 \dots \mathbf{e}_s)$. Any non-singular $s \times s$ i matrix N defines a sublattice L' of L, of the same dimension, and with a basis $(\mathbf{e}'_1 \dots \mathbf{e}'_2)$ given by

$$\mathbf{e}' = \mathbf{e}N, \tag{3}$$

where $\mathbf{e}$ and $\mathbf{e}'$ are to be regarded as row matrices with elements $\mathbf{e}_i$ and $\mathbf{e}'_i$, respectively. If we consider the lattice points of L, we may think that the points which belong to the sublattice L' are marked in some way that distinguishes them from the other points of L. The reciprocal fraction of marked points is $|\det N| = d_s$ since this is also the ratio of the volumes of unit cells in L and L'. The marked points are the points of lattice L in coincidence with points of lattice L'. Their reciprocal fraction, d_s, is accordingly called the degree of coincidence of lattice L with lattice L'.

We consider now the sublattices of lattice L of dimension $r < s$, which we term r *sublattices*. Each r sublattice can be defined by a rectangular i matrix C $(s \times r)$ such that the set $(\mathbf{f}_1 \cdots \mathbf{f}_r)$ obtained from

$$\mathbf{f} = \mathbf{e}C = \mathbf{e}' N^{-1} C \tag{4}$$

is a basis of the sublattice. The r sublattice is said to be *complete* if it contains all vectors of L that are parallel to any vector of the sublattice. In this case the matrix C is a prime matrix, that is, $CD^{-1} = (i)$, where (i) denotes an arbitrary i matrix, can only be satisfied by an i matrix D, if $|\det D| = 1$.

In each complete r sublattice there is a certain proportion of marked points relative to all points in that sublattice. We shall relate the reciprocal fraction of marked points (or degree of coincidence) in complete r sublattices to the invariants of N.

Theorem 1. The minimum reciprocal fraction of marked points or minimum degree of coincidence (maximum coincidence) in the various complete sublattices of dimension r is d_r $(r \le s)$.

The degree of coincidence in each r sublattice C is $|\det P|$, where P is an i matrix of order r with the least absolute value of its determinant and such that

$$N^{-1} CP = (i). \tag{5}$$

(i) is necessarily a prime matrix. This equation can be written as

$$C = N(i) P^{-1}. \tag{6}$$

N can always be put in its principal diagonal form (n_i) by a convenient change of bases in L and L'. Consider any prime factor p in n_i. Let α_i be the exponent of p in n_i, with $0 \le \alpha_1 \le \alpha_2 \dots \le \alpha_s$. We want to find the least value of $|\det P|$ for which $N(i) P^{-1}$ is an i matrix and (i) is an arbitrary prime matrix. Suppose first that (i) is a 1 matrix with 0,1 elements and with one element 1 in each line and column. Then the matricial products $N(i)$ are the set of all $r \times r$ submatrices of N. If we consider the determinants of such submatrices, we see that the minimum exponent of p in these determinants is $(\alpha_1 + \alpha_2 + \dots + \alpha_r)$ which is also the exponent of p in d_r. This happens for all prime factors in n_i; therefore, the minimum value of $|\det P|$ is d_r. If, instead of matrices (i) with 0,1 elements, we take arbitrary prime matrices (i) in (6), the least $|\det P|$ is obviously not changed.

In the example of § 2, the three-dimensional sublattice defined by N gives rise to a degree of coincidence $d_3 = 432$. The best coincidence in lattice planes (complete 2 sublattices) corresponds to a degree of coincidence $d_2 = 6$ and the best coincidence in lattice directions (complete 1 sublattices) corresponds to a degree of coincidence $d_1 = 1$ (that is, there are lattice directions in L which contain totally marked points).

The same geometrical interpretation of the invariants applies to rectangular i matrices.

4. Application to coincidence-site-lattice theory

As an application of the invariants of a square i matrix, we indicate a method of determining the value of the determinant of a least multiplier (LM) of a rational square matrix X, that is, a matrix with rational elements. This problem is relevant in the determination of the degree of coincidence between two lattices in a coincidence-site relation, which is in fact defined by a rational matrix (Grimmer, 1976).

A LM of the matrix X is an i matrix N with the least value of $|\det N|$ and such that XN is an i matrix N':

$$XN = N'. \tag{7}$$

This is the definition for a right multiplier. We shall find the least value of $|\det N|$ satisfying (7), which we denote by Σ.

The matrix X can be written in the form

$$X = \frac{t}{q} Q, \tag{8}$$

where t, q are positive coprime integers and Q is an i matrix with the invariant $d_1 = 1$; q is then the smallest integer such that qX is an i matrix. After finding the invariants $d_1 = 1, d_2, \ldots, d_s$ of Q, this matrix can be written in its principal diagonal form Q_d with elements $q_1, q_2, \ldots, q_s$, given by (2):

$$q_1 = 1; \quad q_i = d_i/d_{i-1}. \tag{9}$$

It is easily shown that Σ is not affected by diagonalization and is the same for left and right LM's. The value of Σ can be obtained immediately from the principal diagonal form. It is enough to find a diagonal matrix N_d with the least (positive) values of the diagonal elements, such that $(1/q)\,\bar{Q}_d N_d = (i)$. Then $\Sigma = \det N_d$ is the product of the diagonal elements of N_d.

Theorem 2. The absolute value Σ of the determinant of a least multiplier of a rational matrix is given by

$$\Sigma = q_{(1)} \cdot q_{(2)} \cdots q_{(s)}, \tag{10}$$

where

$$q_{(i)} = \frac{q}{\mathrm{GCD}\,(q, q_i)}. \tag{11}$$

Let us now take the matrix X^{-1} and determine the integers q', q'_i, $q'_{(i)}$ for this matrix $[X^{-1} = (r'/q')\,Q']$. Writing (7) in the form

$$X^{-1} N' = N, \tag{12}$$

it follows that the value of Σ' for the matrix X^{-1} is $|\det N'|$ and therefore

$$\Sigma'/\Sigma = |\det X|. \tag{13}$$

Using theorem 2 we may write

$$\frac{\Sigma |\det X|}{q'_{(1)} \cdots q'_{(s)}} = 1. \tag{14}$$

We now prove that Σ is coprime with $q'_{(s)}$. To simplify, assume that only one prime factor p appears in the principal diagonal form

$$\bar{X}_d = (r/p^{\alpha})\,(1, p^{\alpha_2}, p^{\alpha_3}, \ldots, p^{\alpha_s}),$$

with $\alpha_i \geq \alpha_{i-1}$. When $\alpha < \alpha_s$, an exponent α_c is defined such that $\alpha_c \leq \alpha$ and $\alpha_{c+1} > \alpha$. In this case the principal form of X^{-1} is

$$X_d^{-1} = \frac{1}{rp^{\alpha}\, s^{-\alpha}}\,(1, p^{\alpha_s - \alpha_{s-1}}, \ldots, p^{\alpha_s})$$

and $q'_{(i)} = r$ for $i > s - c$. The value of Σ is $\Sigma = p^{c\alpha - (\alpha_2 + \cdots + \alpha_c)}$ so that Σ is coprime with $q'_{(s)}$. When $\alpha \geq \alpha_s$ it is $\Sigma = p^{s\alpha - (\alpha_2 + \cdots + \alpha_c)}$ and the principal diagonal form of X^{-1} is

$$X_d^{-1} = \frac{p^{\alpha - \alpha_s}}{r}\,(1, \ldots, p^{\alpha_s}),$$

so that all $q'_{(i)} = r$. Therefore Σ and $q'_{(s)}$ are coprime in all cases. The same result holds if there is more than one prime factor in $\bar{X}_d$. Combining this result with (14), we may state Theorem 3.

Theorem 3. Σ is the smallest positive integer such that

$$\frac{\Sigma \det X}{q'_{(1)} \cdots q'_{(s-1)}}$$

is an integer.

Let us now consider $q'_{(s-1)}$. For $c > 1$, $q'_{(s-)} = r$ is coprime with Σ. For $c = 1$ it is $\Sigma = p^{\alpha} = q$.

Theorem 4. Σ is the smallest positive integer such that

$$\frac{\Sigma}{q} \quad \text{and} \quad \frac{\Sigma \det X}{q'_{(1)} \cdots q'_{(s-2)}}$$

are both integers.

This theorem is useful, because for third-order matrices $q'_{(s-2)} = q'_{(1)} = q'$.

Theorem 5. For third-order matrices, Σ is the smallest integer such that

$$\frac{\Sigma}{q} \quad \text{and} \quad \frac{\Sigma \det X}{q'}$$

are integers.

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