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Discrete tomography of Penrose model sets

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Various theoretical and algorithmic aspects of inverse problems in discrete tomography of planar Penrose model sets are discussed. These are motivated by the demand of materials science for the reconstruction of quasicrystalline structures from a small number of images produced by quantitative high resolution transmission electron microscopy.

1 Introduction

Discrete tomography is concerned with the inverse problem of retrieving information about some discrete object from (generally noisy) information about its incidences with certain query sets. A typical example is the reconstruction of a finite planar point set from its line sums in a small number of directions. More precisely, for a direction $u \in \mathbb{S}^1$ (the unit circle), the (discrete parallel) X -ray $X_u F$ of a finite subset F of the Euclidean plane \mathbb{R}^2 in direction u gives the number of points of the set on each line in \mathbb{R}^2 parallel to u , i.e., $X_u F$ is the function $X_u F : \mathcal{L}_u \longrightarrow \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, defined by

$$X_u F(\ell) := \text{card}(F \cap \ell) = \sum_{x \in \ell} \mathbb{1}_F(x),$$

where \mathcal{L}_u is the set of lines in direction u in \mathbb{R}^2 , with obvious generalization to higher dimensions. In the classical setting, motivated by crystals, the positions to be determined form a subset of a translate of the square lattice \mathbb{Z}^2 or, more generally, of arbitrary lattices L in \mathbb{R}^d , where $d \geq 2$. The cases $d = 2$ and $d = 3$ are practically relevant. In fact, many of the problems in discrete tomography have been studied on \mathbb{Z}^2 , the ‘classical planar setting’ of discrete tomography; see [1–4].

In the longer run, by also having other structures than perfect crystals in mind, one has to take into account wider classes of sets, or at least significant deviations from the lattice structure. As an intermediate step between periodic and random (or amorphous) Delone sets (defined below), we consider systems of aperiodic order, more precisely, of so-called model sets (or mathematical quasicrystals), which are commonly accepted as a reasonable mathematical model for quasicrystalline structures in nature [5].

The main motivation for our interest in the discrete tomography of model sets comes from the question how to reconstruct three-dimensional (quasi)crystals or planar layers of them from their images under quantitative high resolution transmission electron microscopy (HRTEM) in a small number of directions. In fact, in [6, 7] a technique called QUANTITEM (quantitative analysis of the information coming from transmission electron microscopy) is described, based on HRTEM, which can effectively measure the number of atoms lying on lines parallel to certain directions. In particular, with the growing importance of surface science, there is also increasing interest in additional methods for the reconstruction of planar structures which can supplement STM approaches. At present, the measurement of the number of atoms lying on a line can only be achieved for some crystals; see [6, 7]. However, it is reasonable to expect that

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Here, we restrict ourselves to an example, namely to the well-known class of planar model sets $\Lambda_P \subset \mathbb{R}^2$ that are associated with the well-known *Penrose tiling*, and present some results on the discrete tomography of these sets, with an emphasis both on reconstruction and uniqueness problems. Note that proofs are omitted; details will appear in [8, 9].

2 Penrose model sets

We always let $\zeta_5 = e^{\frac{2\pi i}{5}}$, a primitive 5th root of unity in \mathbb{C} . Then, $\mathbb{Q}(\zeta_5)$ is the corresponding cyclotomic field, an algebraic number field of degree 4 over \mathbb{Q} , and $\mathbb{Z}[\zeta_5]$ is its subring of cyclotomic integers.

Remark 1 Let C_5 denote the cyclic group of order 5, i.e., $C_5 = \mathbb{Z}/5\mathbb{Z}$. Moreover, C_5 is understood to be supplied with the discrete topology. It is well-known that every $z \in \mathbb{Z}[\zeta_5]$ can uniquely be written as $z = \sum_{j=0}^3 a_j(z) \zeta_5^j$, with $a_j(z) \in \mathbb{Z}$. Let σ_2 be the automorphism of the Galois extension $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ that is given by $\zeta_5 \mapsto \zeta_5^2$. Identifying \mathbb{R}^2 and \mathbb{C} in the canonical way, σ_2 gives rise to a map

$$\cdot^\sim : \mathbb{Z}[\zeta_5] \longrightarrow \mathbb{R}^2 \times (\mathbb{R}^2 \times C_5),$$

defined by $z \mapsto (z, (\sigma_2(z), \sum_{j=0}^3 (a_j(z) \pmod{5})))$. Via projection on the second factor, this induces a map $\cdot^* : \mathbb{Z}[\zeta_5] \longrightarrow \mathbb{R}^2 \times C_5$, defined by $z \mapsto (\sigma_2(z), \sum_{j=0}^3 (a_j(z) \pmod{5}))$. Then, $\mathbb{Z}[\zeta_5]^\sim$ is a lattice in $\mathbb{R}^2 \times (\mathbb{R}^2 \times C_5)$, i.e., a co-compact discrete subgroup. In fact, $\mathbb{Z}[\zeta_5]^\sim$ is the \mathbb{Z} -span of the set $\{1^\sim, (\zeta_5)^\sim, (\zeta_5^2)^\sim, (\zeta_5^3)^\sim\}$. Finally, note that $\mathbb{Z}[\zeta_5]^*$ is dense in $\mathbb{R}^2 \times C_5$; see [10].

It is well known by now that *model sets* arise from so-called *cut and project schemes*, compare [12, 13]. In particular, the class of *Penrose model sets* (PMS) arises as follows; cf. [14].

$$\begin{array}{ccccc} \mathbb{R}^2 & \xleftarrow{\pi} & \mathbb{R}^2 \times (\mathbb{R}^2 \times C_5) & \xrightarrow{\pi_{\text{int}}} & \mathbb{R}^2 \times C_5 \\ \cup \text{ dense} & & \cup \text{ lattice} & & \cup \text{ dense} \\ \mathbb{Z}[\zeta_5] & \xleftrightarrow{1-1} & \underbrace{\left\{ \left(z = \sigma_1(z), \left(\sigma_2(z), \sum_{j=0}^3 (a_j(z) \pmod{5}) \right) \right) \mid z \in \mathbb{Z}[\zeta_5] \right\}}_{= \mathbb{Z}[\zeta_5]^\sim} & \xleftrightarrow{1-1} & \mathbb{Z}[\zeta_5]^* \end{array} \quad (1)$$

Given any subset $W \subset \mathbb{R}^2 \times C_5$ with $\emptyset \neq W^\circ \subset W \subset \overline{W^\circ}$ and $\overline{W^\circ}$ compact, a so-called *window*, and any $t \in \mathbb{R}^2$, we obtain a planar model set $\Lambda(t, W) := t + \Lambda(W)$ relative to the above cut and project scheme (1) by setting $\Lambda(W) := \{z \in \mathbb{Z}[\zeta_5] \mid z^* \in W\}$.

Let P be the convex hull of the 5th roots of unity, which is a regular pentagon centred at the origin. Set $W^{(1)} := P$, $W^{(2)} := -P$, $W^{(3)} := \tau P$ and $W^{(4)} := -\tau P$, with $\tau = \frac{\sqrt{5}+1}{2}$ the golden ratio, and

$$W_P := \bigcup_{j=1}^4 \left(W^{(j)} \times \{j \pmod{5}\} \right) \subset \mathbb{R}^2 \times C_5.$$

Moreover, for $u \in \mathbb{R}^2$, set $W_P^u := (u, 0 \pmod{5}) + W_P$, $(W_P^u)^{(j)} := (u, 0 \pmod{5}) + (W^{(j)} \times \{j \pmod{5}\})$ and $\Lambda_P^u := \Lambda(W_P^u)$. If Λ_P^u is *generic*, i.e., if one has $W_P^u \cap \mathbb{Z}[\zeta_5]^* = \emptyset$, then all translates of Λ_P^u , meaning the sets $t + \Lambda_P^u$ with $t \in \mathbb{R}^2$, are called *Penrose model sets*.

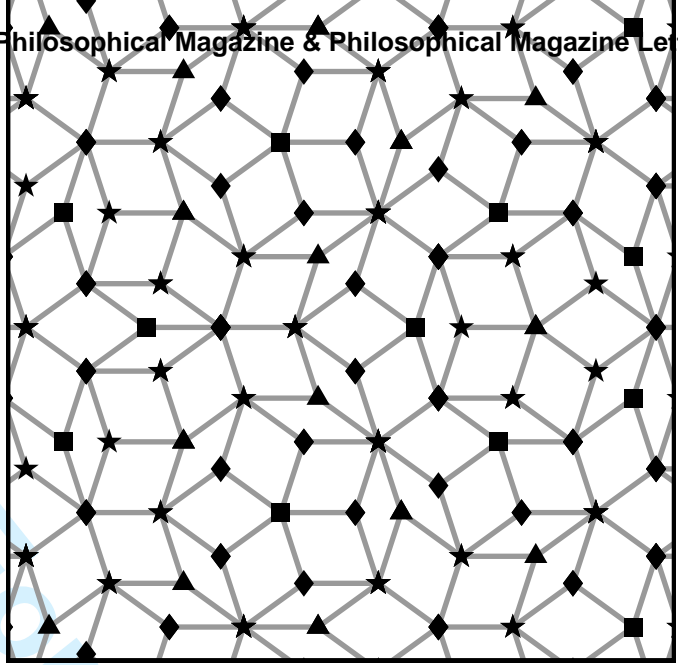


Figure 1. A patch of the fivefold symmetric Penrose tiling, with the four distinct classes of vertices indicated.

Remark 2 Λ_P^0 is not generic, while generic examples are obtained by shifting the window, i.e., Λ_P^u is generic for almost all $u \in \mathbb{R}^2$. Joining any two points with distance 1 in a generic Λ_P^u by edges results in a *Penrose tiling*, in particular, a tiling with two types of rhombi. See Figure 1 for a generic example; different generic choices of u result in locally indistinguishable (LI) Penrose tilings. Note that Penrose model sets $\Lambda_P \subset \mathbb{R}^2$ are aperiodic, meaning that they have no translational symmetries. Penrose model sets are Delone sets, i.e., they are uniformly discrete and relatively dense; cf. [12].

3 Problems in discrete tomography of Penrose model sets

Let Λ_P be a PMS, $k \in \mathbb{N}$ and $R > 0$. A finite subset C of Λ_P is called a *convex set in Λ_P* when its convex hull contains no new points of Λ_P , i.e., when one has $C = \text{conv}(C) \cap \Lambda_P$. We denote by $\mathcal{F}(\Lambda_P)$, $\mathcal{F}_{\leq k}(\Lambda_P)$, $\mathcal{D}_{<R}(\Lambda_P)$ and $\mathcal{C}(\Lambda_P)$ the set of finite subsets of Λ_P , the set of finite subsets of Λ_P having cardinality $\leq k$, the set of subsets of Λ_P with diameter less than R and the set of convex subsets of Λ_P , respectively.

Remark 1 The uniform discreteness of Penrose model sets Λ_P immediately implies the inclusion $\mathcal{D}_{<R}(\Lambda_P) \subset \mathcal{F}(\Lambda_P)$.

Clearly, in order to obtain electron microscopy images of high resolution, one should allow only directions which yield dense lines in Penrose model sets. These directions are clearly contained in the set of all directions, called $(\Lambda_P - \Lambda_P)$ -directions, which are parallel to a non-zero element of the difference set

$$\Lambda_P - \Lambda_P := \{\lambda - \lambda' \mid \lambda, \lambda' \in \Lambda_P\} \subset \mathbb{Z}[\zeta_5]$$

of Λ_P . Calling a direction $u \in \mathbb{S}^1$ a $\mathbb{Z}[\zeta_5]$ -direction when it is parallel to an element of $\mathbb{Z}[\zeta_5] \setminus \{0\}$, one has the following result.

PROPOSITION 3.1 *If Λ_P is a PMS, the set of $(\Lambda_P - \Lambda_P)$ -directions equals the set of $\mathbb{Z}[\zeta_5]$ -directions.*

Let us indicate the main *algorithmic problems* in discrete tomography of Penrose model sets. For a direction $u \in \mathbb{S}^1$, we denote by $\mathcal{L}_u^{\mathbb{Z}[\zeta_5]}$ the set of elements ℓ_u of \mathcal{L}_u that pass through a point of $\mathbb{Z}[\zeta_5]$.

CONSISTENCY.

Given functions $p_{o_i} : \mathcal{L}_{o_i} \rightarrow \mathbb{N}_0$, $i \in \{1, \dots, m\}$, whose supports are finite and satisfy $\text{supp}(p_{u_i}) \subset \mathcal{L}_{u_i}^{\mathbb{Z}[\zeta_5]}$, decide whether there is a finite set F which is contained in a PMS and satisfies $X_{u_i}F = p_{u_i}$, for all $i \in \{1, \dots, m\}$.

RECONSTRUCTION.

Given functions $p_{u_i} : \mathcal{L}_{u_i} \rightarrow \mathbb{N}_0$, $i \in \{1, \dots, m\}$, whose supports are finite and satisfy $\text{supp}(p_{u_i}) \subset \mathcal{L}_{u_i}^{\mathbb{Z}[\zeta_5]}$, in the case that CONSISTENCY is satisfied, construct a finite set F which is contained in a PMS and satisfies $X_{u_i}F = p_{u_i}$, for all $i \in \{1, \dots, m\}$.

UNIQUENESS.

Given a finite subset F of a PMS, decide whether there is a different finite set F' that is also a subset of a PMS and satisfies $X_{u_i}F = X_{u_i}F'$, for all $i \in \{1, \dots, m\}$.

In general, the above problem RECONSTRUCTION can have many solutions of rather different shape. Therefore, one is also interested in *uniqueness results*, e.g., the (unique) *determination* of the set

$$\bigcup_{\Lambda_P \text{ PMS}} \mathcal{F}(\Lambda_P)$$

or suitable subsets thereof by the X -rays in a small number of $\mathbb{Z}[\zeta_5]$ -directions. More precisely, we define the concept of *determination* and the interactive concept of *successive determination* as follows. Let \mathcal{E} be a collection of finite subsets of \mathbb{R}^2 and let $U \subset \mathbb{S}^1$ be a finite set of directions. We say that \mathcal{E} is *determined* by the X -rays in the directions of U if, for all $F, F' \in \mathcal{E}$, one has

$$(X_u F = X_u F', \quad \forall u \in U) \implies F = F'.$$

We say that \mathcal{E} is *successively determined* by the X -rays in the directions of $U = \{u_1, \dots, u_m\}$, if, for a given $F \in \mathcal{E}$, these can be chosen inductively, i.e., the choice of u_j depending on all $X_{u_k}F$ with $k \in \{1, \dots, j-1\}$, such that, for all $F' \in \mathcal{E}$, one has

$$(X_u F' = X_u F, \quad \forall u \in U) \implies F' = F.$$

We say that \mathcal{E} is *determined* (resp., *successively determined*) by m X -rays if there is a set U of m pairwise non-parallel directions such that \mathcal{E} is determined (resp., successively determined) by the X -rays in the directions of U .

4 Computational complexity and uniqueness results

Let us begin with a result on computational complexity, where we apply the real RAM-model of computation, see [15]. Here, each of the standard elementary operations on reals count only with unit cost. This leads to the following tractability result.

THEOREM 4.1 *When restricted to two $\mathbb{Z}[\zeta_5]$ -directions, the problems CONSISTENCY, RECONSTRUCTION and UNIQUENESS can be solved in polynomial time in the real RAM-model.*

Remark 1 It seems to be rather obvious from the results in [3] that one cannot expect a generalization of Theorem 4.1 to the case of three or more $\mathbb{Z}[\zeta_5]$ -directions. More precisely, we expect that, when restricted to three or more $\mathbb{Z}[\zeta_5]$ -directions, the problems CONSISTENCY, RECONSTRUCTION and UNIQUENESS are NP-hard.

Let us now present results dealing with the (successive) determination of finite subsets of Penrose model sets. Though we are not interested in non- $\mathbb{Z}[\zeta_5]$ -directions for practical reasons, we begin with the following

PROPOSITION 4.2 *If Λ_P is a PMS and $u \in \mathbb{S}^1$ is a non- $\mathbb{Z}[\zeta_5]$ -direction, the class of finite subsets $\mathcal{F}(\Lambda_P)$ is determined by the single X-ray in direction u .*

This last result immediately follows from the observation that, for all PMS Λ_P , each line in the plane in a non- $\mathbb{Z}[\zeta_5]$ -direction passes through at most one point of Λ_P , the latter being the reason for the practical irrelevance of this result. On the other hand, the next result shows that any fixed number of X-rays in $\mathbb{Z}[\zeta_5]$ -directions does not suffice to determine the whole class of finite subsets of a fixed PMS Λ_P .

PROPOSITION 4.3 *Let Λ_P be a PMS and $U \subset \mathbb{S}^1$ an arbitrary, but fixed finite set of pairwise non-parallel $\mathbb{Z}[\zeta_5]$ -directions. Then, the set $\mathcal{F}(\Lambda_P)$ is not determined by the X-rays in the directions of U .*

In order to obtain results on uniqueness, one has to restrict the class of finite sets under consideration. Within the class of finite subsets of a fixed PMS Λ_P with bounded cardinality, there is the following result.

PROPOSITION 4.4 *Let Λ_P be a PMS and $k \in \mathbb{N}$. Then, the set $\mathcal{F}_{\leq k}(\Lambda_P)$ is determined by any set of $k + 1$ pairwise non-parallel $\mathbb{Z}[\zeta_5]$ -directions, while any set of $1 + \lfloor \log_2 k \rfloor$ pairwise non-parallel X-rays in $\mathbb{Z}[\zeta_5]$ -directions is insufficient for this purpose.*

This last result is once again of limited relevance in practice, because typical atomic structures to be determined comprise about 10^6 to 10^9 atoms, and, in order not to damage or even destroy the examined structures, one has to make sure that one uses at most 4 or 5 X-rays.

PROPOSITION 4.5 *Let Λ_P be a PMS and $R > 0$. Then, the set $\mathcal{D}_{<R}(\Lambda_P)$ is determined by two X-rays in $\mathbb{Z}[\zeta_5]$ -directions.*

Though the last result seems to be more satisfactory, it is probably still pretty useless in practice. Here, the reason is that, in general, the second $\mathbb{Z}[\zeta_5]$ -direction can not be chosen in such a way that it yields dense lines in Penrose model sets Λ_P , in other words, one would have to deal with images of poor resolution. A deeper result is the following, which deals with the class of convex subsets of a fixed PMS Λ_P .

THEOREM 4.6 *There is a set $U \subset \mathbb{S}^1$ of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$ -directions such that, for all PMS Λ_P , the set $\mathcal{C}(\Lambda_P)$ is determined by the X-rays in the directions of U , while, for all PMS Λ_P and any set $U \subset \mathbb{S}^1$ of three or less pairwise non-parallel $\mathbb{Z}[\zeta_5]$ -directions, the set $\mathcal{C}(\Lambda_P)$ is not determined by the X-rays in the directions of U .*

For example, the set of $\mathbb{Z}[\zeta_5]$ -directions parallel to the elements of the following set U has the desired property to determine $\mathcal{C}(\Lambda_P)$ by the X-rays in its directions,

$$U := \{(1 + \tau) + \zeta_5, (\tau - 1) + \zeta_5, 2\tau - \zeta_5, -\tau + \zeta_5\}. \quad (2)$$

Remark 2 By a result of Pleasants [16], these directions can yield dense lines in Penrose model sets. It follows that, in the practice of quantitative HRTEM, the resolution coming from these directions is rather high, which makes Theorem 4.6 look promising.

Above, we restricted the class of finite subsets of a fixed Penrose model set Λ_P under consideration. In order to obtain positive uniqueness results, a second option is to consider the interactive technique of successive determination. One has the following positive results.

THEOREM 4.7 *If Λ_P is a PMS, the set $\mathcal{F}(\Lambda_P)$ is successively determined by two X-rays in $\mathbb{Z}[\zeta_5]$ -directions, while the set*

$$\bigcup_{\Lambda_P \text{ PMS}} \mathcal{F}(\Lambda_P)$$

is successively determined by three X-rays in $\mathbb{Z}[\zeta_5]$ -directions.

Unfortunately, this result is again somewhat limited in practice because, in general, one can not make sure that all the $\mathbb{Z}[\zeta_5]$ -directions which are used match dense lines in Penrose model sets.

For further details in this spirit, we refer to [2–4,18] for the lattice case and [17,18] for cyclotomic model sets which also provide a systematic generalization of the setting explained here for the PMS.

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