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How to cite:

Grimm, Uwe and Baake, Michael (2008). Homometric point sets and inverse problems. *Zeitschrift für Kristallographie*, 223(11-12) pp. 777–781.

For guidance on citations see [FAQs](#).

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Version: Accepted Manuscript

Link(s) to article on publisher's website:

<http://dx.doi.org/doi:10.1524/zkri.2008.1043>

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HOMOMETRIC POINT SETS AND INVERSE PROBLEMS

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ABSTRACT. The inverse problem of diffraction theory in essence amounts to the reconstruction of the atomic positions of a solid from its diffraction image. From a mathematical perspective, this is a notoriously difficult problem, even in the idealised situation of perfect diffraction from an infinite structure.

Here, the problem is analysed via the autocorrelation measure of the underlying point set, where two point sets are called homometric when they share the same autocorrelation. For the class of mathematical quasicrystals within a given cut and project scheme, the homometry problem becomes equivalent to Matheron's covariogram problem, in the sense of determining the window from its covariogram. Although certain uniqueness results are known for convex windows, interesting examples of distinct homometric model sets already emerge in the plane.

The uncertainty level increases in the presence of diffuse scattering. Already in one dimension, a mixed spectrum can be compatible with structures of different entropy. We expand on this example by constructing a family of mixed systems with fixed diffraction image but varying entropy. We also outline how this generalises to higher dimension.

1. INTRODUCTION

After 25 years of quasicrystal research, our understanding of the atomic structure of quasicrystalline alloys is still far from being complete [18]. The main reason for this is the difficult inverse problem of determining the structure at the atomic scale from the available information, which exists mainly in the form of diffraction intensities. Here, we discuss the non-uniqueness arising from *homometric* point sets, which is even present in the idealised situation of a perfect diffraction measurement from an infinite point set $\Lambda \subset \mathbb{R}^d$.

First, we consider the situation where Λ is a mathematical quasicrystal or model set. A perfect diffraction image of Λ , as described by the positive diffraction measure $\widehat{\gamma}_\Lambda$, uniquely determines its inverse Fourier transform, which is the autocorrelation (or Patterson) measure γ_Λ . The starting point is thus the (hypothetically complete) knowledge of γ_Λ , and the remaining task is then to determine Λ from this information. For a model set based on a known cut and project scheme, this amounts to determine the corresponding window W in internal space.

Beyond pure point diffraction, we reconsider the known homometry between the binary Rudin-Shapiro sequence and the Bernoulli (or coin flipping) chain [10]. We introduce a new process, called 'Bernoullisation', which provides a continuous isospectral transition between these two extremal cases. This method generalises to arbitrary dimension and shows that even a perfect diffraction image (of mixed type) may not be able to distinguish structures of different entropy.

2. HOMOMETRY

For finite point sets $F \subset \mathbb{R}^d$, homometry is defined in terms of their *difference sets* $F - F$, taking into account multiplicities. Two finite point sets are called *homometric* when they share the same weighted difference set (which is a multi-set), meaning that each difference vector occurs with the same cardinality in either set; see [16] for an early class of examples in one dimension.

A relatively simple homometric pair, realised as finite subsets $F_1 \neq F_2 \subset \mathbb{Z}^2$, was constructed in [9]. One choice of the coordinates results in

$$(1) \quad \begin{aligned} F_1 &= \left\{ \binom{0}{0}, \binom{1}{0}, \binom{1}{1}, \binom{1}{2}, \binom{1}{3}, \binom{2}{1}, \binom{2}{2}, \binom{2}{3}, \binom{2}{4}, \binom{2}{5}, \binom{3}{3}, \binom{3}{4}, \binom{3}{5}, \binom{4}{4}, \binom{4}{5} \right\}, \\ F_2 &= \left\{ \binom{0}{0}, \binom{0}{1}, \binom{1}{0}, \binom{1}{1}, \binom{1}{2}, \binom{1}{3}, \binom{1}{4}, \binom{2}{2}, \binom{2}{3}, \binom{2}{4}, \binom{2}{5}, \binom{3}{3}, \binom{3}{4}, \binom{3}{5}, \binom{4}{5} \right\}. \end{aligned}$$

One can explicitly check that $F_1 - F_1 = F_2 - F_2$, including multiplicities.

An appropriate generalisation to infinite point sets needs the concept of density. We call two infinite point sets *homometric* when their natural autocorrelation measures exist and coincide. Homometric point sets thus have the same density. Due to the volume averaging involved, two point sets related by adding or removing a point set of density 0 are homometric. This is also true of point sets related by translation or inversion (but not, in general, by rotation).

It is well known that two crystallographic (or fully periodic) point sets can only be homometric when they share the same lattice of periods. They are then mutually locally derivable (MLD) from each other [4, 2], which also implies that the associated dynamical systems (under the translation action [15]) are topologically conjugate [11]. The corresponding question for mathematical quasicrystals (model sets without any periodicity) is more difficult, as we shall demonstrate by an example.

2.1. Covariogram. There is an interesting connection between the homometry of model sets (with a Euclidean internal space) and the covariogram problem. For a non-empty, relatively compact subset $K \subset \mathbb{R}^d$, which is assumed to be Riemann measurable, the function

$$(2) \quad \text{cvg}_K(x) := \text{vol}(K \cap (x + K)),$$

defined for all $x \in \mathbb{R}^d$, is called the *covariogram* of K . The covariogram problem amounts to determine K from its covariogram $\text{cvg}_K(x)$; compare [6, 9]. This is sometimes also referred to as Matheron's problem, which was originally formulated as the question whether the covariogram determines a convex body, among all convex bodies, up to translation and inversion; see [12, 13, 6] for details. Since $\text{cvg}_K(x) = \text{cvg}_{t+K}(x)$ for any translation $t \in \mathbb{R}^d$ and $\text{cvg}_K(x) = \text{cvg}_{-K}(x)$, the covariogram cvg_K can determine K at best up to translations and inversion. We call two non-empty, relatively compact, Riemann measurable sets $K, K' \subset \mathbb{R}^d$ *homometric* when $\text{cvg}_K = \text{cvg}_{K'}$.

Denoting the characteristic function of K by 1_K , the function cvg_K is given by the convolution

$$(3) \quad \text{cvg}_K(x) = (1_K * 1_{-K})(x).$$

Its Fourier transform

$$(4) \quad \widehat{\text{cvg}_K}(k) = |\widehat{1_K}(k)|^2$$

is an analytic, positive function that vanishes in the limit as $|k| \rightarrow \infty$. This relation is the reason why, if K is itself inversion symmetric in the sense that $-K = t + K$ for a suitable translation $t \in \mathbb{R}^d$, the function 1_K (and hence K) can be reconstructed from the knowledge of cvg_K , up to translation and inversion [8].

If K is a convex polytope in dimension $d \leq 3$, it is determined by cvg_K ; see [5, 6, 1, 7] and references therein. In general, however, the reconstruction of K from the knowledge of cvg_K is a difficult problem. An interesting example of two polyominoes with the same covariogram [3] follows from the point set pair of Eq. (1) by adding the unit square $C = [-\frac{1}{2}, \frac{1}{2}]^2$, so that

$$(5) \quad P_1 = F_1 + C \quad \text{and} \quad P_2 = F_2 + C.$$

Their covariograms are equal as a consequence of the homometry of the finite point sets F_1 and F_2 , whence P_1 and P_2 are homometric (as are also any translates of $\pm P_1$ and $\pm P_2$). The polyominoes P_1, P_2 and their joint covariogram are displayed and discussed in more detail in [3]. Let us mention in addition that the scaled polyominoes αP_1 and αP_2 are homometric to each other for any choice of $\alpha \in \mathbb{R}$.

2.2. Homometry of model sets. Let us now consider the situation of regular model sets Λ that are defined via a cut and project scheme [14, 2] with Euclidean internal space

$$(6) \quad \begin{array}{ccccc} \mathbb{R}^d & \xleftarrow{\pi} & \mathbb{R}^d \times \mathbb{R}^m & \xrightarrow{\pi_{\text{int}}} & \mathbb{R}^m \\ \cup & & \cup & & \cup \text{ dense} \\ \pi(\mathcal{L}) & \xleftarrow{1-1} & \mathcal{L} & \longrightarrow & \pi_{\text{int}}(\mathcal{L}) \\ \parallel & & & & \parallel \\ L & \xrightarrow{\quad \star \quad} & & & L^\star \end{array}$$

by

$$(7) \quad \Lambda = t + \mathcal{A}(W) = t + \{x \in \pi(\mathcal{L}) \mid x^\star \in W\}.$$

Here, \mathcal{L} is a lattice in $\mathbb{R}^d \times \mathbb{R}^m$, the window $W \subset \mathbb{R}^m$ is a non-empty, relatively compact set with boundary of measure 0, and $t \in \mathbb{R}^d$ is an arbitrary translation.

The autocorrelation γ_Λ of the corresponding Dirac comb $\delta_\Lambda = \sum_{x \in \Lambda} \delta_x$ exists and has the explicit form $\gamma_\Lambda = \sum_{z \in \Lambda - \Lambda} \eta(z) \delta_z$, with coefficients

$$(8) \quad \eta(z) = \text{dens}(\Lambda) \frac{\text{vol}(W \cap (W - z^\star))}{\text{vol}(W)} = \text{dens}(\mathcal{L}) \text{cvg}_W(z^\star),$$

expressed in terms of the covariogram of the window W . Hence, two (Euclidean) model sets obtained from the same cut and project scheme are homometric if and only if the defining windows share the same covariogram. As a consequence, homometric model sets from the same cut and project scheme have the same diffraction measure. Conversely, kinematic diffraction cannot discriminate between homometric model sets.

A planar example is obtained by using the homometric pair of polyominoes P_1 and P_2 as windows for model sets in a cut and project scheme of type (6). For instance, we can use the Minkowski embedding $\mathcal{L}_8 \subset \mathbb{C}^2 \simeq \mathbb{R}^4$ of $L = \mathbb{Z}[\xi_8]$, where ξ_8 is a primitive 8th root of unity, and a \star -map defined by a suitable algebraic conjugation. The two model sets $\Lambda_1 := \mathcal{A}(P_1)$

and $\Lambda_2 := \lambda(P_2)$, with P_1 and P_2 as defined in (5), are then homometric by construction (the relative position of the windows, which is irrelevant for homometry, maximises their intersection). The two model sets Λ_1 and Λ_2 are *not* locally indistinguishable, and differ in points of positive density. In particular, the difference sets $\Lambda_1 \setminus \Lambda_2$ and $\Lambda_2 \setminus \Lambda_1$ are model sets themselves (but not homometric).

The diffraction measure $\widehat{\gamma}$ is the same for both Λ_1 and Λ_2 , and reads

$$\widehat{\gamma} = \sum_{k \in \frac{1}{2}L} I(k^*) \delta_k,$$

with intensity function $I(y) = |A_i(y)|^2$ derived from

$$A_i(y) = \text{dens}(\mathcal{L}_8) \widehat{1_{P_i}}(-y).$$

While the amplitudes depend on the window, their absolute squares do not. One can work out the explicit diffraction intensities; see [3] for details. The ratio of the (complex) amplitudes is given by

$$(9) \quad \frac{A_1(y)}{A_2(y)} = \frac{1 + e^{2\pi i y_2} + e^{2\pi i (y_1 + 2y_2)}}{1 + 2 e^{\pi i (2y_1 + 3y_2)} \cos(\pi y_2)} = 1 + \frac{1 - e^{2\pi i y_1}}{e^{2\pi i y_1} + e^{2\pi i (y_1 + y_2)} + e^{-2\pi i y_2}}$$

with $y = (y_1, y_2)$. This is a well-defined function on internal space \mathbb{R}^2 , with values in \mathbb{S}^1 , unless the denominator vanishes. The latter happens for $y_2 \in \mathbb{Z} + \{\frac{1}{3}, \frac{2}{3}\}$ together with $y_1 \in \mathbb{Z}$. One can check that the ratio has no continuous extension to these points. Writing the ratio as $\exp(2\pi i \chi(y))$, the phase function χ is not defined at these points. Moreover, as one can check explicitly, it does *not* satisfy the additivity property $\chi(y + y') = \chi(y) + \chi(y') \pmod{1}$, wherefore the ratio fails to be a character on \mathbb{R}^2 by violating both defining properties; compare [15] and references therein. Note that an analogous phenomenon already shows up in the comparison of P_i with $-P_i$, because these windows are not inversion symmetric up to translations.

The choice of the windows P_1 and P_2 is special in the sense that Λ_1 and Λ_2 turn out to be MLD, because the square C satisfies

$$C = P_1 \cap (-t + P_1) = P_2 \cap (-t + P_2)$$

with the translation $t = (4, 5)$, and each window is now the union of 15 integral (and hence admissible) translates of C according to Eq. (5); see [4] for details. In this case, the associated dynamical systems [15] are again topologically conjugate. As mentioned above, the two windows may be scaled (by the same factor) without affecting their mutual homometry. For almost all choices of the scaling factor, one loses the MLD property of the corresponding model sets, because the finite reconstruction property [4] is lost. Nevertheless, the associated dynamical systems will always be *metrically* isomorphic (due to the Halmos-von Neumann theorem). It is an interesting open question whether they are still also *topologically* conjugate, which is a weaker equivalence notion than MLD.

Independent of this conjugacy issues, our example illustrates that diffraction (hence auto-correlation) alone is generally insufficient to uniquely determine a regular model set. However, as discussed in [15], this ambiguity can be resolved with the knowledge of the 3-point correlations. This statement is immediate in our example (via the existence or non-existence of

certain patches), but holds in full generality for regular model sets; see [15] and references therein.

3. RANDOM DIRAC COMBS

The problem of reconstruction becomes even more involved in the case of mixed spectra. In this setting, a slight change in point of view is helpful to separate distinct spectral components. This is most easily achieved by considering *weighted* Dirac combs of point sets, with real (or even complex) weights. Below, generalising an example discussed in [10], we construct a family of one-dimensional homometric (weighted) point sets, based on the binary Rudin-Shapiro sequence, which cover the entire entropy range from 0 to $\log(2)$, the maximal possible entropy for a binary system. This shows that, in general, it is not even possible to determine the degree of long-range order of the weighted point set from diffraction data. The same conclusion also holds for the diffraction of the associated unweighted point sets.

3.1. Bernoulli versus Rudin-Shapiro. We start by re-considering the example of Ref. [10]. The first model is a Bernoulli system on \mathbb{Z} , with the stochastic Dirac comb

$$(10) \quad \omega_B = \sum_{m \in \mathbb{Z}} Y_m \delta_m,$$

where $(Y_m)_{m \in \mathbb{Z}}$ is a family of i.i.d. random variables that each take the values 1 and -1 , with probabilities p and $1 - p$, where $0 \leq p \leq 1$. For the stochastic Dirac comb ω_B , the autocorrelation measure γ_B and the diffraction measure $\widehat{\gamma}_B$ almost surely exist and read

$$(11) \quad \begin{aligned} \gamma_B &= (2p - 1)^2 \delta_{\mathbb{Z}} + 4p(1 - p) \delta_0, \\ \widehat{\gamma}_B &= (2p - 1)^2 \delta_{\mathbb{Z}} + 4p(1 - p) \lambda, \end{aligned}$$

where λ denotes Lebesgue measure on \mathbb{R} . Note that, in this stochastic situation, almost sure results are unavoidable. In particular, one has $\widehat{\gamma}_B = \lambda$ for $p = \frac{1}{2}$ and $\widehat{\gamma}_B = \delta_{\mathbb{Z}}$ for $p = 0$ or $p = 1$. The choices $p = 0$ and $p = 1$ correspond to the deterministic limiting cases $\omega_B = \pm \delta_{\mathbb{Z}}$, while $p = \frac{1}{2}$ describes a stochastic comb (coin tossing) with weights of average 0.

The binary Rudin-Shapiro sequence is defined in two steps as follows [17]. We start from the substitution rule

$$(12) \quad a \mapsto ac, \quad b \mapsto dc, \quad c \mapsto ab, \quad d \mapsto da,$$

on the four-letter alphabet $\mathcal{A} = \{a, b, c, d\}$. We choose a bi-infinite fixed point (under the square of the above substitution, with seed ba) and apply the morphism $\varphi : \mathcal{A} \rightarrow \{\pm 1\}$ defined by $\varphi(a) = \varphi(c) = 1$ and $\varphi(b) = \varphi(d) = -1$, extended to $\mathcal{A}^{\mathbb{Z}}$. The autocorrelation and diffraction measures of the resulting binary Rudin-Shapiro chain S_{RS} are

$$(13) \quad \gamma_{RS} = \delta_0 \quad \text{and} \quad \widehat{\gamma}_{RS} = \lambda.$$

This is an example with a purely absolutely continuous diffraction, despite the fact that the Rudin-Shapiro chain is deterministic and has entropy 0. In particular, it agrees with the diffraction measure of the Bernoulli comb with $p = \frac{1}{2}$, which has entropy $\log(2)$.

3.2. ‘Bernoullisation’. It is possible to impose the influence of chance on the order of a deterministic system, and thus interpolate between deterministic and random systems. Here, we focus on binary sequences and modify them by an i.i.d. family of Bernoulli variables.

Consider a bi-infinite binary sequence $S \in \{\pm 1\}^{\mathbb{Z}}$ which we assume to be uniquely ergodic (in the sense that its hull under the action of the shift map is a uniquely ergodic dynamical system). Then, the corresponding Dirac comb $\omega_S = \sum_{i \in \mathbb{Z}} S_i \delta_i$ possesses the (natural) autocorrelation $\gamma_S = \sum_{m \in \mathbb{Z}} \eta_S(m) \delta_m$ with autocorrelation coefficients $\eta_S(m)$, where $\eta_S(0) = 1$ by construction.

Let $(Y_i)_{i \in \mathbb{Z}}$ be an i.i.d. family of random variables that each take values $+1$ and -1 with probabilities p and $1 - p$. The ‘Bernoullisation’ of ω_S is the random Dirac comb

$$(14) \quad \omega_{S;p} := \sum_{i \in \mathbb{Z}} S_i Y_i \delta_i,$$

which emerges from ω_S by independently changing the sign of each S_i with probability $1 - p$. Setting $Z_i := S_i Y_i$ defines a new family of independent (though, in general, not identically distributed) random variables, with values in $\{\pm 1\}$. Despite this modification, the autocorrelation $\gamma_{S;p}$ of $\omega_{S;p}$ almost surely exists and can be determined via its autocorrelation coefficients $\eta_{S;p}(m)$ as follows. Since one always has $\eta_{S;p}(0) = \eta_S(0) = 1$, let $m \neq 0$ and consider, for large N , the sum

$$(15) \quad \frac{1}{2N+1} \sum_{i=-N}^N Z_i Z_{i-m} = \frac{1}{2N+1} \left(\sum_{(+,+)} + \sum_{(-,-)} - \sum_{(+,-)} - \sum_{(-,+)} \right) Y_i Y_{i-m},$$

which is split according to the value of (S_i, S_{i-m}) . Each of the four sums can be handled in the same way as for the Bernoulli comb, thus contributing $(2p - 1)^2$ times the frequency of the corresponding sign pair. Observing that the overall signs are the products $S_i S_{i-m}$, it is clear that, as $N \rightarrow \infty$, one obtains (almost surely)

$$(16) \quad \eta_{S;p}(m) = (2p - 1)^2 \eta_S(m)$$

for all $m \neq 0$. Thus, the autocorrelation $\gamma_{S;p}$ of $\omega_{S;p}$ almost surely exists and is given by

$$(17) \quad \gamma_{S;p} = (2p - 1)^2 \gamma_S + 4p(1 - p) \delta_0,$$

where γ_S is the unique autocorrelation of ω_S .

Consider now the Bernoullisation (with parameter p) of the binary Rudin-Shapiro sequence with random Dirac comb $\omega_{\text{RS};p}$. Its autocorrelation measure almost surely exists and reads $\gamma_{\text{RS};p} = \delta_0$, independently of p . This means that the random Dirac combs $\omega_{\text{RS};p}$, even for different values of p , are almost surely homometric, and share the purely absolutely continuous diffraction measure $\widehat{\gamma_{\text{RS};p}} = \lambda$.

3.3. Extension to higher dimension. Our above discussion has an immediate extension to Euclidean space of arbitrary dimension d . Consider d complex-valued sequences $(U_i^{(\ell)})_{i \in \mathbb{Z}}$ and define the weighted Dirac comb

$$\omega_U = U^{(1)} \delta_{\mathbb{Z}} \otimes \dots \otimes U^{(d)} \delta_{\mathbb{Z}} = \sum_{x \in \mathbb{Z}^d} \left(\prod_{\ell=1}^d U_{x_\ell}^{(\ell)} \right) \delta_x.$$

Here, $x = (x_1, \dots, x_d)$, and the weights (on \mathbb{Z}^d) are products of d elements of the individual sequences. Assuming that the natural autocorrelations of the individual sequences exist, the relevant observation is that the resulting autocorrelation of ω_U (and hence also the corresponding diffraction measure) factorises accordingly.

Each $U^{(\ell)}$ may be chosen as a member of our previous one-parameter family of (14), in particular as $U^{(\ell)} = S_{\text{RS}}$ for all ℓ . This results in a deterministic weighted Dirac comb on \mathbb{Z}^d with diffraction measure $\hat{\gamma} = \lambda$, where λ now denotes Lebesgue measure on \mathbb{R}^d . This represents a system of entropy 0.

The analogue of the Bernoullisation of (14) in d -space, with an i.i.d. family $(Y_x)_{x \in \mathbb{Z}^d}$, then results in an isospectral one-parameter family of random Dirac combs on \mathbb{Z}^d , which can realise any entropy between 0 and $\log(2)$. Similarly, using $\mathbb{Z}^d \simeq \mathbb{Z}^k \times \mathbb{Z}^{d-k}$ for some $0 \leq k \leq d$ and restricting the Bernoullisation to \mathbb{Z}^k , one obtains isospectral families with arbitrary entropy of rank k between 0 and $\log(2)$. This indicates that the variety of homometric structures grows with dimension.

4. CONCLUSIONS

The homometry problem for regular model sets in dimensions $d \leq 3$ appears to have a unique solution if one may assume that the window is convex [1, 7]. However, this favourable situation is not always met in real quasicrystals. Our example, with non-convex windows, illustrates the existence of distinct homometric structures. Since homometric model sets are always metrically isomorphic, but not necessarily MLD, it remains an interesting question how they are related as topological dynamical systems.

For the case of spectra with a continuous component, the Bernoullisation approach can explore the full entropy range: the Bernoulli case (with $p = \frac{1}{2}$) has entropy $\log 2$, the maximal value for a binary system, while Rudin-Shapiro has entropy 0, and the parameter p interpolates continuously between the two limiting cases. This gives an indication of how degenerate the inverse problem really is. Unless additional information is available, one possible strategy to proceed would employ an optimisation approach, for instance by choosing the structure which maximises the entropy, which singles out the Bernoulli comb here.

ACKNOWLEDGEMENTS

We are grateful to R.V. Moody for valuable discussions and comments on the manuscript. It is a pleasure to thank the School of Mathematics and Physics at the University of Tasmania for their kind hospitality during an extended stay in Hobart. This work was supported by the German Research Council, within the Collaborative Research Centre 701, and by EPSRC via Grant EP/D058465.

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