On the metric spaces of lattices and periodic point sets

based on a joint work with Nicolò Zava and Žiga Virk

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Motivation

Question

Given two point sets in $\mathbb{R}^d$, how close are they to each other?

- Usual mathematical answer: Hausdorff distance
- This approach does not work well if we want to think of point sets as atoms of some solids.

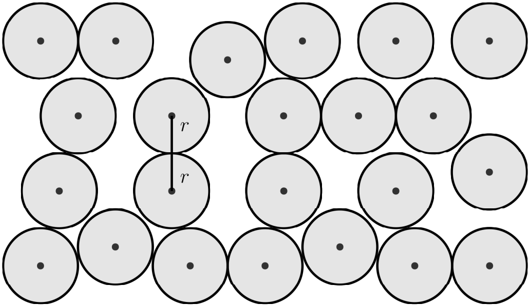
Additional requirement: make it “relevant” to the point sets that are used to model physical matter.

Delone sets

Definition

A set $X \subset \mathbb{R}^d$ is called a **Delone set** if it is uniformly discrete and relatively dense.

- There exists a **packing radius** $r > 0$ such that every open ball of radius r in $\mathbb{R}^d$ contains at most one point of X

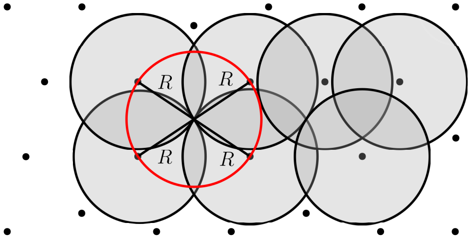


Delone sets

Definition

A set $X \subset \mathbb{R}^d$ is called a **Delone set** if it is uniformly discrete and relatively dense.

- There exists a **covering radius** $R < \infty$ such that every closed ball of radius R in $\mathbb{R}^d$ contains at least one point of X



Lattices

Definition

Given a basis $v_1, \dots, v_d$ in $\mathbb{R}^d$, the set of all **integer** linear combinations

$$\Lambda := \mathbb{Z}(v_1, \dots, v_d) = \left\{ \sum_{i=1}^{d} a_i v_i \mid a_i \in \mathbb{Z}, i = 1, \dots, d \right\}$$

is called a **lattice**.

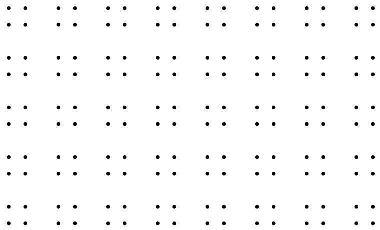
- **Unit cell** U of the lattice Λ is the parallelepiped

$$U := \left\{ \sum_{i=1}^{d} t_i v_i \mid t_i \in [0, 1), i = 1, \dots, d \right\}.$$

PERIODIC POINT SETS

Definition

For a lattice with the unit cell U and a finite subset $P \subset U$, called **motif**, the set $\Lambda + P$ is called a **periodic point set**.



Cut-and-project sets (simplified version)

Definition

$$\begin{array}{ccccc} G = \mathbb{R}^d & \xleftarrow{\pi_1} & G \times H & \xrightarrow{\pi_2} & H = \mathbb{R}^m \\ \cup & & \cup & & \cup \\ \Lambda & & \Gamma & & W \end{array}$$

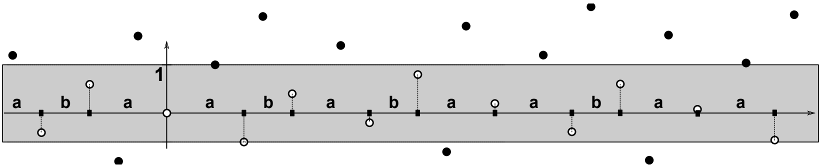
- G and H are locally compact abelian groups;
- Γ is a lattice in $G \times H$;
- W is a relatively compact set in H; and
- π_1 and π_2 are projections to G and to H respectively.

Then

$$\Lambda = \{\pi_1(x) \mid x \in \Gamma,\ \pi_2(x) \in W\}$$

is called a **cut-and-project set** (or **CPS**).

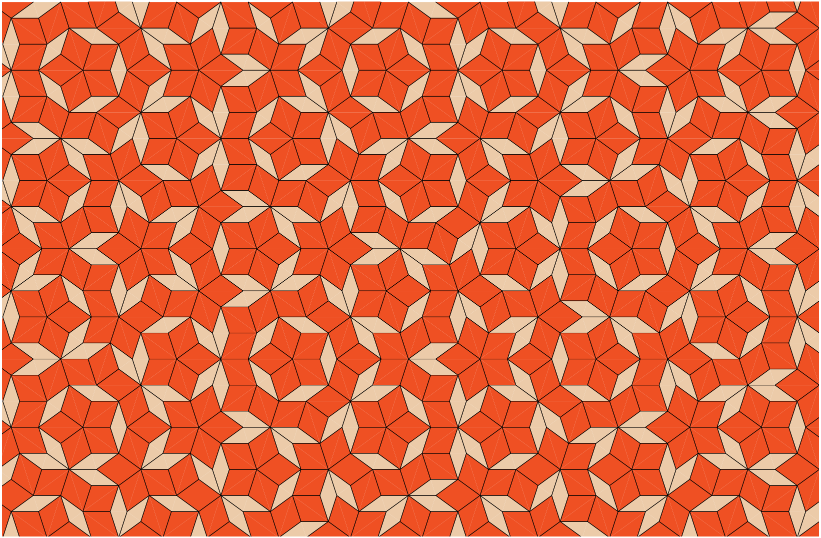
CPS: examples



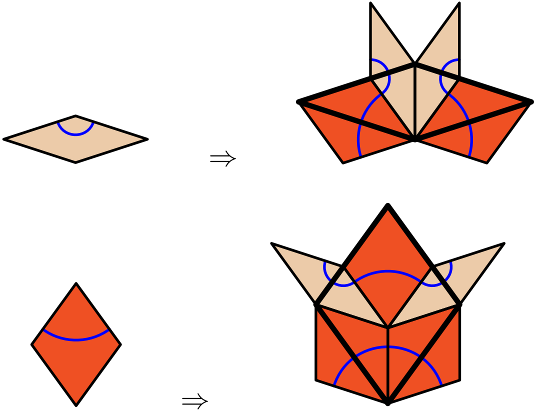
Fibonacci sequence is a CPS with

- $G = \mathbb{R}$ (**direct space**, horizontal) and $H = \mathbb{R}$ (**internal space**, vertical);
- The lattice Γ is spanned by the vectors $(1,1)$ and $(\tau, -\tau^{-1})$. Here $\tau = \frac{\sqrt{5}+1}{2}$;
- Both projections π_1 and π_2 are orthogonal projections on the corresponding spaces;
- The **window** $W = \left[-\tau^{-1}, 1\right)$.

CPS: examples

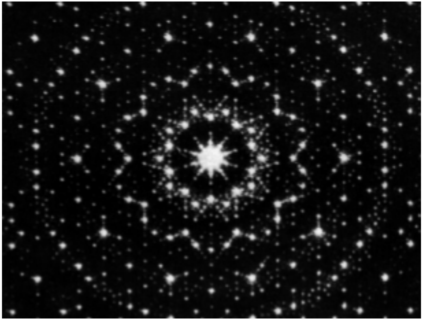


Substitution tilings



Why restrict to these sets?

- Lattices and PPS are usual models for **periodic crystals**;
- CPS and substitution tilings are frequently used as models for **aperiodic crystals**. Particularly, they usually have nice diffractive properties.



Which sets are close? Qualitative approach

Definition

Two (Delone) sets X and Y are called **bounded distance equivalent** (or **b.d.e.**) if there is bijection $f : X \longrightarrow Y$ such that

$$\sup_{x \in X} ||f(x) - x|| < \infty.$$

- This equivalence can also be given interpretation in terms of bounded transport.

Which sets are close? Quantitive approach

Definition

If X and Y are bounded distance equivalent, then we define the **bottleneck distance** d_B as

$$d_B(X,Y) := \inf \sup_{x \in X} ||x - f(x)||$$

where infimum is taken over all bijections $f : X \to Y$.

Definition

Similarly, we define the **Euclidean bottleneck distance** d_{EB} as

$$d_{EB}(X,Y) = \inf d_B(X, \psi(Y))$$

where infimum is taken over all isometries ψ of $\mathbb{R}^d$.

What are we looking for?

- Given two Delone sets X and Y, under what conditions are they bounded distance equivalent?
- For the whole family of Delone sets, what are the properties of the metric spaces defined by d_B and d_{EB}?
- Can we embed it into a "nice" and "familiar" metric space even if we need to "moderately" distort the distances?

B.d.e. to a lattice

Question

For a given X, does there exist a lattice Λ such that X is b.d.e. to Λ?

- Motivation: lattices are "well-distributed" so let's try to analyze the "simplest" case first.

Laczkovich criterion

Theorem (Laczkovich, 1992)

A Delone set X is b.d.e. to the scaled integer lattice $\alpha\mathbb{Z}^d$ if and only if there is a positive constant C such that for every bounded, measurable set $S \subset \mathbb{R}^d$ the inequality

$$\left| \#(X \cap S) - \frac{1}{\alpha^d} \lambda_d(S) \right| \leq C \cdot \lambda_d(p_1(S))$$

holds.

- λ_d is the d-dimensional Lebesgue measure, and
- $p_1(S)$ is the 1-neighborhood of the boundary of S.

Density

Definition

For given discrete set $X \subset \mathbb{R}^d$, its **density** is the limit

$$\mathrm{den}(X) = \#\text{ of points per unit volume } = \lim_{n\to\infty} \frac{\#(S_n \cap X)}{\lambda_d(S_n)}$$

where S_n is a **van Hove sequence**, provided the limit exists and does not depend on the choice of S_n.

- Van Hove (or Følner) sequence is any sequence of measurable sets S_n such that for every $\varepsilon > 0$,

$$\lim_{n\to\infty} \frac{\lambda_d(p_\varepsilon(S_n))}{\lambda_d(S_n)} = 0.$$

Density for lattices and PPS

- For lattice Λ with unit cell U,

$$\mathrm{den}(\Lambda) = \frac{1}{\mathrm{vol}_d U}.$$

- For PPS X with an underlying lattice Λ and motif P,

$$\mathrm{den}(X) = \frac{\#(P)}{\mathrm{vol}_d U}.$$

- Similarly, densities can be computed for large classes of cut-and-project sets and sets originating from substitution tilings.

B.d.e. for lattices and PPS

Theorem (Duneau, Oguey, 1991)

Two lattices Λ_1 and Λ_2 in $\mathbb{R}^d$ are b.d.e. if and only if

$$\mathrm{den}(\Lambda_1) = \mathrm{den}(\Lambda_2).$$

Corollary

Two periodic point sets X_1 and X_2 in $\mathbb{R}^d$ are b.d.e. if and only if

$$\mathrm{den}(X_1) = \mathrm{den}(X_2).$$

When is CPS b.d.e. to a lattice?

Theorem (Kesten, 1966)

A $\mathbb{R} \times \mathbb{R}$ CPS Λ with a window $W = [a, b]$ is b.d.e. to a lattice if and only if there is a vector $\mathbf{e} \in \Gamma$ such that $\pi_2(\mathbf{e}) = b - a$.

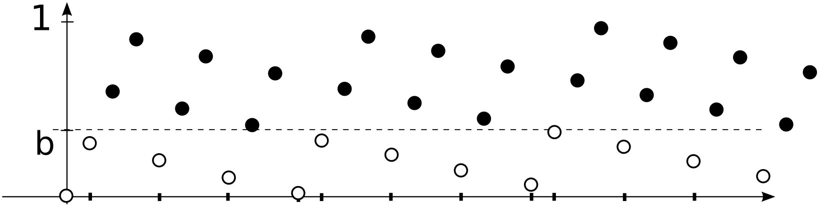
Theorem (Duneau, Oguey, 1990)

Let Λ be a $\mathbb{R}^d \times \mathbb{R}^n$ CPS. If the window of Λ is a π_2-projection of a fundamental domain of n-sublattice of Γ, then Λ is b.d.e. to a d-lattice.

Theorem (Grepstad, Lev, 2015)

Complete classifitcation of measurable windows of $\mathbb{R} \times \mathbb{R}^n$ that are b.d.e. to lattices. Includes some fractal windows too.

Proof of "if" part



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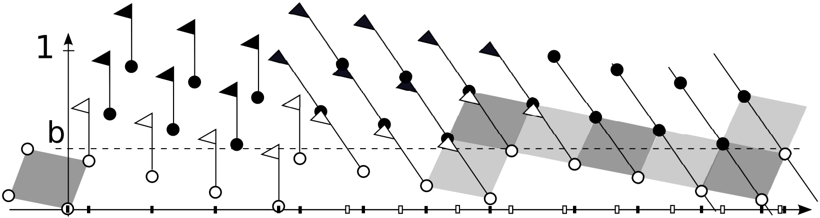
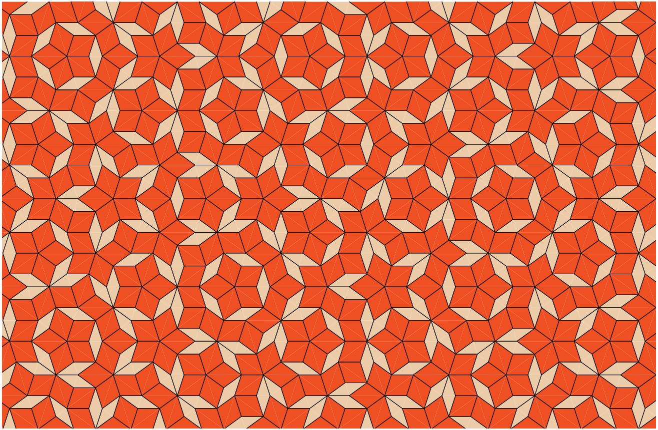


Penrose tiling is b.d.e. to a lattice



For Penrose tilings, the window is a rhombic triacontahedron, a union of several projections of unit cells, so every Penrose tiling is b.d.e. to a lattice.

When is substitution tiling b.d.e. to a lattice?

- For substitution tilings, the **substitution matrix** M encodes how many original tiles are needed to subdivide the inflated tiles.
- The leading eigenvalue of M, the Perron-Frobenius eigenvalue λ_1, helps to find the density.
- The eigenvalue λ_2 with the second largest absolute value shows when the tiling is b.d.e. to a lattice.

Theorem (Solomon, 2014)

- *If* $|\lambda_2| < \lambda_1^{\frac{d-1}{d}}$*, then the tiling is b.d.e. to a lattice;*
- *If* $|\lambda_2| > \lambda_1^{\frac{d-1}{d}}$*, then the tiling is not b.d.e. to a lattice.*

Why "b.d.e. to a lattice"?

- A Delone set X has **finite local complexity** (or **FLC**) if for every radius $R > 0$, there are only finitely many patches of radius R in X.

Theorem (Frettlöh, G., Sadun, 2022)

Suppose $X \subset \mathbb{R}^d$ is a Delone set with FLC. Then

- *either X is b.d.e. to a lattice, and then all sets that "look like" X are b.d.e. to the same lattice;*
- *or X is not b.d.e. to a lattice, and then there are* **uncountably** *many sets that "look like" X which represent uncountably many different b.d.e. classes.*

THE METRIC SPACES

- $\mathrm{PPS}(\mathbb{R}^d)$ is the space of PPS in $\mathbb{R}^d$;
- $\mathrm{PPS}_{\mathbf{r}}(\mathbb{R}^d)$ is the space of PPS with **packing radius greater than r**;
- $\mathrm{PPS}^{\mathbf{R}}(\mathbb{R}^d)$ is the space of PPS with **covering radius less than R**;
- $\mathrm{PPS}(\mathbb{R}^d, \kappa)$ is the space of PPS with **density** κ. By default, we use $\kappa = 1$ everywhere.

Or combined notations like

$$\mathrm{PPS}_r^R(\mathbb{R}^d), \quad \mathrm{PPS}_r(\mathbb{R}^d, \kappa), \quad \mathrm{PPS}^R(\mathbb{R}^d, \kappa), \quad \mathrm{PPS}_r^R(\mathbb{R}^d, \kappa).$$

And similar notations for the spaces of lattices based on $\mathrm{Latt}(\mathbb{R}^d)$ for the space of all lattices in $\mathbb{R}^d$.

WHAT ARE WE LOOKING FOR?

For every metric space X from the previous slide equipped with d_B or d_{EB}, we are looking for a function $f : X \longrightarrow Y$ where Y is a **Hilbert space with countable basis** and f is either bi-Lipschitz or coarse.

- **bi-Lipschitz**: there exists a constant L such that

$$\frac{1}{L} \cdot d(x_1, x_2) \leq d(f(x_1), f(x_2)) \leq L \cdot d(x_1, x_2).$$

- **coarse**: there exist two positive values functions ρ_-, ρ_+ such that $\lim \rho_-(t) = \infty$ and

$$\rho_-(d(x_1, x_2)) \leq d(f(x_1), f(x_2)) \leq \rho_+(d(x_1, x_2)).$$

Motivation: bi-Lipschitz or coarse embeddings into a Hilbert space allow us to approximate the bottleneck distances.

Bi-Lipschitz embeddings

Theorem (G., Virk, Zava, 2023+)

For sufficiently small r and for sufficiently large R, none of the PPS *or* Latt *spaces can be bi-Lipschitz embedded into a Hilbert space with countable basis.*

This also pertains to the PPS with bounded diameter of unit cells or with bounded cardinality of motifs.

Idea: the family of lattices Λ_α with bases $(1, 0)$ and $(\alpha, 1)$ for $\alpha \in [0, \frac{1}{2}]$ have pairwise distances bounded away from 0 for both d_B and d_{EB}.

Coarse embeddings: positive results

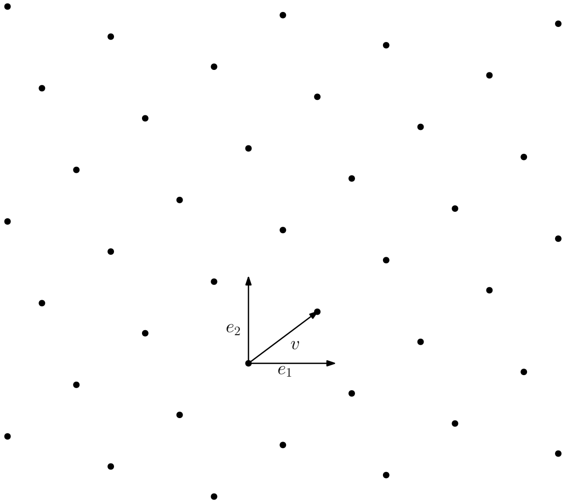
Theorem (G., Virk, Zava, 2023+)

For every fixed density, the spaces Latt_r, Latt^R, Latt_r^R *can be coarsely embedded into Hilbert space.*

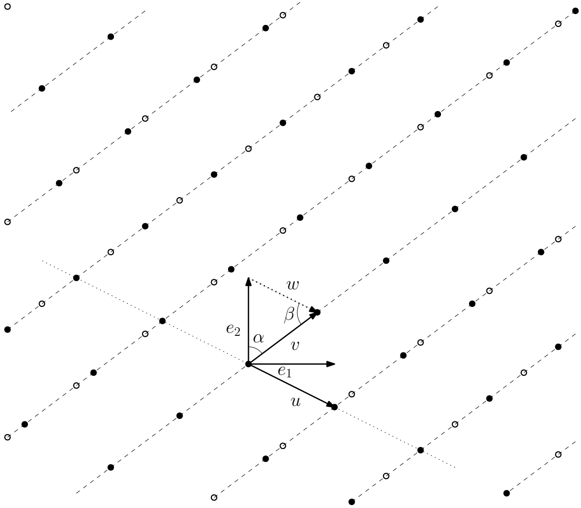
This also pertains to the spaces of lattices and PPS with bounded diameters of unit cells, and the space of PPS with bounded cardinality of motifs.

Idea: the family $\mathrm{Latt}_r(\mathbb{R}^d, 1)$ is bounded which can be tracked from the proof of Duneau and Oguey of b.d.e. for lattices of equal densities.

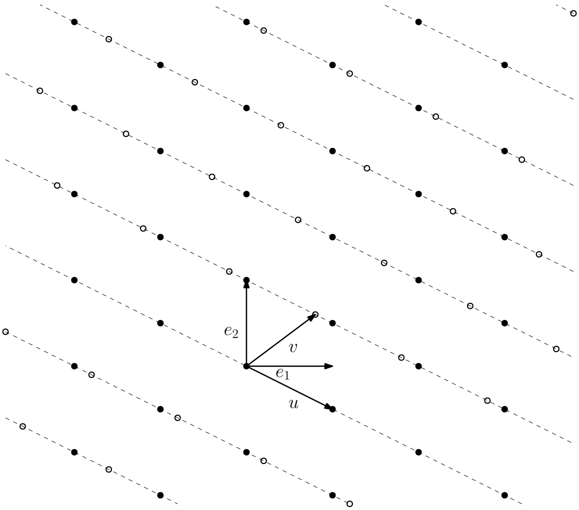
$\mathrm{Latt}_r(\mathbb{R}^d)$ is bounded



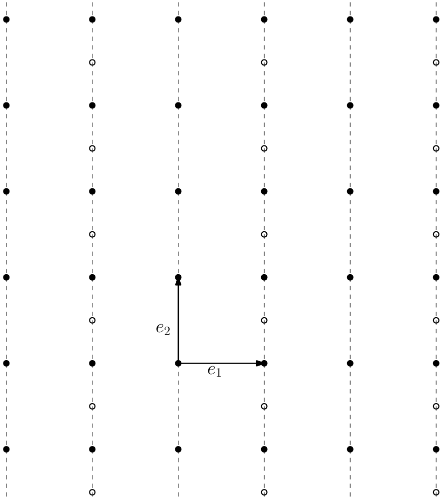
$\mathrm{Latt}_r(\mathbb{R}^d)$ is bounded



$\mathrm{Latt}_r(\mathbb{R}^d)$ is bounded



$\mathrm{Latt}_r(\mathbb{R}^d)$ is bounded



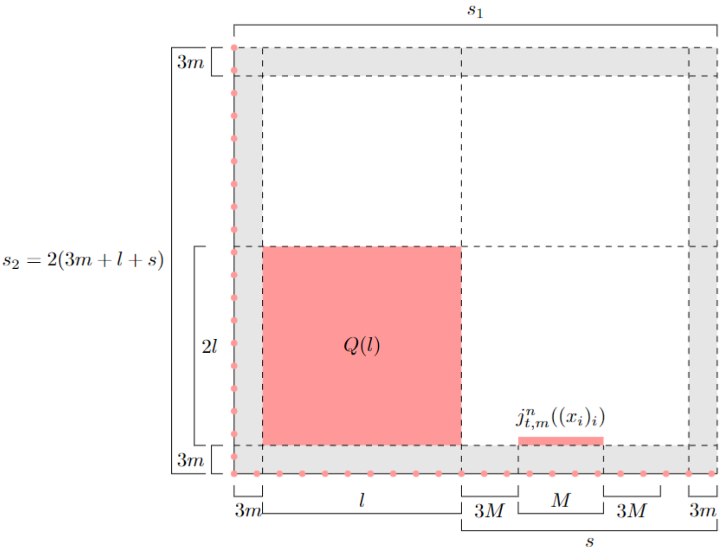
Coarse embeddings: negative results

Theorem (G., Virk, Zava, 2023+)

For every fixed density, the spaces PPS_r, PPS^R, PPS *cannot be coarsely embedded into Hilbert space.*

Idea: There is a known construction for coarse nonembeddability into Hilbert spaces using coarse embeddings of a sequence of Hamming cubes.

PPS_r cannot be coarsely embedded



Open question

- What about coarse embeddability of $\mathrm{Latt}(\mathbb{R}^d)$ and $\mathrm{PPS}_r^R(\mathbb{R}^d)$?

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THANK YOU!