Computing fundamental domains of crystallographic groups

With connections to topological interlocking

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Definition (Isometry)

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Lemma

Let $E(n)$ be the set of all isometries of a dimension $n \in \mathbb{N}$.
Then $E(n)$ is a group with the composition of homomorphisms as the group operation.
Further $E(n)$ operates on $\mathbb{R}^n$ by matrix vector multiplication.

Proposition ([4, Exa. 1.1, Prop. 1.6])

There is an isometry

$$E(n) \cong O(n) \ltimes \mathbb{R}^n.$$

We denote with φ_o the orthogonal part of φ and with φ_t the vector/translation part of φ.

Then the group operation of $\varphi, \psi \in E(n)$ is as follows:

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and the action of $E(n)$ on $\mathbb{R}^n$ extends to the action of $O(n) \ltimes \mathbb{R}^n$ on $\mathbb{R}^n$:

$$\mathbb{R}^n \times (O(n) \ltimes \mathbb{R}^n) \to \mathbb{R}^n : (v, (\varphi_o, \varphi_t)) \mapsto v^{(\varphi_o, \varphi_t)} = v^{\varphi_o} + \varphi_t.$$

Definition (System of representatives)

Let λ be a partition of $\mathbb{R}^n$ and let $\emptyset \neq V \subseteq \mathbb{R}^n$ be a set.

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(i) $\bigcup_{\gamma \in \Gamma} F^{\langle \gamma \rangle} = \mathbb{R}^n$,

(ii) there is a system of representatives $V \subseteq \mathbb{R}^n$ w.r.t. the partition given by the orbits of Γ acting on $\mathbb{R}^n$ such that

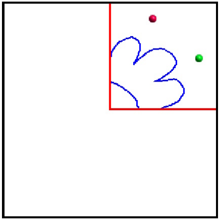
$$F^\circ \subseteq V \subseteq F.$$

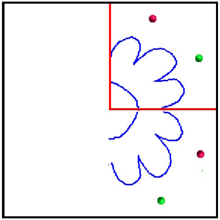
Definition (Crystallographic group)

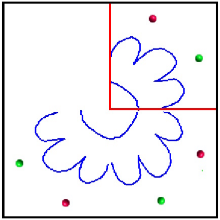
Let $\Gamma \leq E(n)$ be a subgroup. Γ is called a *crystallographic group* if Γ is discrete and there exists a compact fundamental domain for Γ.

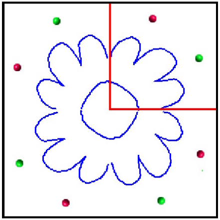
Example

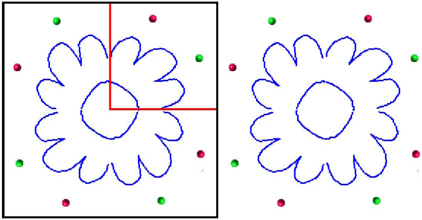
$$p4 := \left\langle \rho := \left(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix}^T \right), \right.$$
$$\tau_1 := \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T \right),$$
$$\left. \tau_2 := \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T \right) \right\rangle$$

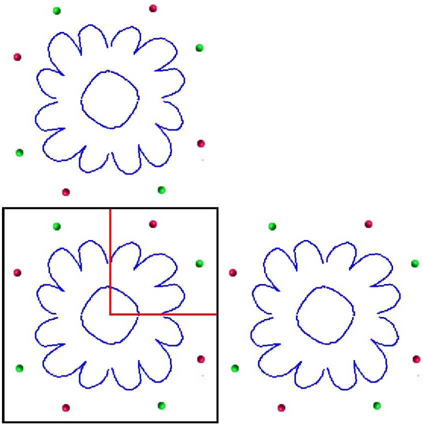


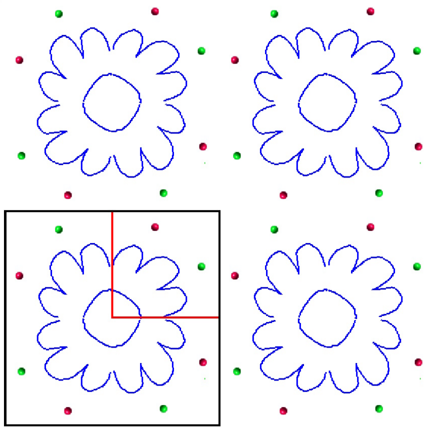


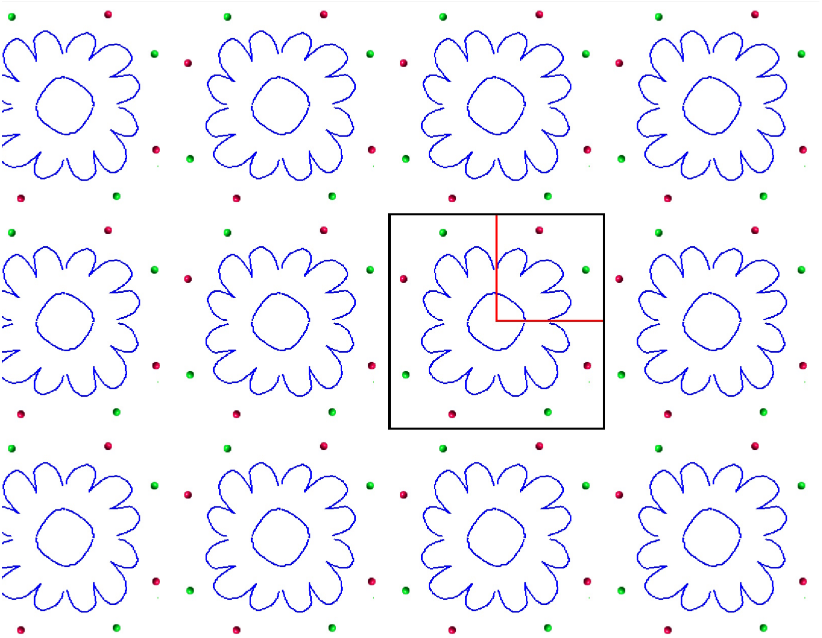












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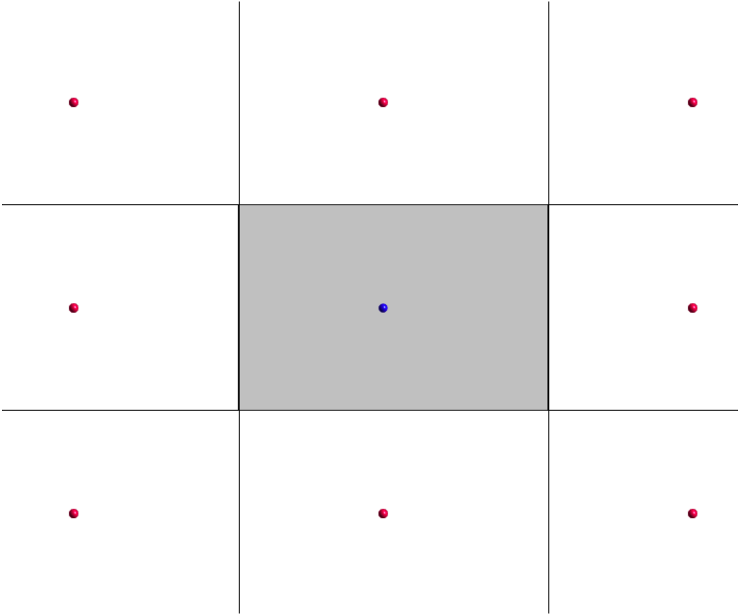
Definition

Dirichlet cell [[3, Def. III.1]] Let $O \subseteq \mathbb{R}^n$ be a discrete set and $u \in O$ be a point. We call

$$D(u, O) = \bigcap_{w \in O, w \neq u} H^+(u, w).$$

the *Dirichlet cell of u*.



Definition (Points in special/general position)

Let $\Gamma \leq E(n)$ be a crystallographic group and $v \in \mathbb{R}^n$ be a point. We say v is in *special position for* Γ if $\mathrm{Stab}_\Gamma(v) \neq \{Id\}$,

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Theorem ([2, Thm. III.11 (ii)])

Let $\Gamma \leq E(n)$ *be a crystallographic group and* $u \in \mathbb{R}^n$ *a point in general position.*

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Theorem ([2, Thm. III.11 (ii)])

Let $\Gamma \leq E(n)$ be a crystallographic group and $u \in \mathbb{R}^n$ a point in general position. Then the Dirichlet cell $D(u, u^\Gamma)$ is a fundamental domain for Γ.

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Theorem ([2, Thm. III.11 (ii)])

Let $\Gamma \leq E(n)$ be a crystallographic group and $u \in \mathbb{R}^n$ a point in general position. Then the Dirichlet cell $D(u, u^\Gamma)$ is a fundamental domain for Γ.

Example

Let $\Gamma \leq E(n)$ a crystallographic group and $u \in \mathbb{R}^n$ a point in general position. Then the following is a fundamental domain:

$$D(u, u^\Gamma) = \bigcap_{w^\gamma, \gamma \in \Gamma \setminus \{Id\}} H^+(u, w).$$

Definition (Volume)

Let $B \subset \mathbb{R}^n$ be a closed subset. We define the *volume* of B as the Lebesgue measure of B, so $\mathrm{vol}(B) := \lambda(B)$ in the notation of [1].

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It can be shown that all fundamental domains of crystallographic groups have the same volume.

Remark

For every crystallographic group Γ there is a certain subgroup called the translation subgroup that is denoted by

$$\mathcal{T}(\Gamma) \leq \Gamma.$$

Theorem

Let $\Gamma \leq E(n)$ be a crystallographic group with fundamental domain F and $u \in \mathbb{R}^n$ a point in general position. Then we choose a generating set for Γ and I, K finite index sets, such that

$$\Gamma = \langle \rho_i, \tau_k \mid i \in I, k \in K \rangle,$$

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with $\tau_k \in \mathcal{T}(\Gamma)$ for all $k \in K$ and $\{(\tau_k)_t \mid k \in K\}$ are a basis for the lattice induced by $\mathcal{T}(\Gamma)$. Furthermore, let $\rho_i \in \Gamma$ for $i \in I$ be chosen such that

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Then there is an $A \in \mathbb{N}$ such that the Dirichlet cell $D(u, u^\Gamma)$ is the intersection of halfspaces $H^+(u, w)$ for words w of length at most $A + 1$.

Algorithm 3.2: Dirichlet Cell

Data: a crystallographic group
$\Gamma = \langle \rho_i, \tau_k \mid i \in I, k \in K \rangle \leq E(n)$ such that
$\Gamma = \cup_{i \in I} \rho_i \mathcal{T}(\Gamma)$, a point u in general position w.r.t. Γ
and the maximal *length* of words in *gens* to check

Result: *triangularComplex*, a triangular complex that is a fundamental domain.

wordsOfLenghtL $\leftarrow$ all words in the generators *gens* of length at most *length*

for γ *in wordsOfLenghtL* **do**

  Add(elementsInOrbit, u^γ);

end

halfspaces $\leftarrow$ halfspaces $H_{u,v}$ for all $v \in$ *elementsInOrbit*;

fundDom $\leftarrow$ triangular complex given by intersection of *halfspaces* (done with polymake(ing));

return *fundDom*;

Time for some examples

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Motivation

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Definition

Topologically interlocking A block $B \subseteq \mathbb{R}^3$ is called topologically interlocking, if there is an assembly of it, such that by fixing a subset of the assembly there is no subset of the remaining blocks that can be moved without intersecting any blocks.

Thank you for your attention

References:

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