Energy minimization for periodic sets in Euclidean spaces

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Traditio et Innovatio

- A **lattice** $L \subset \mathbf{R}^n$ is a closed discrete subgroup of finite covolume, *i.e.*

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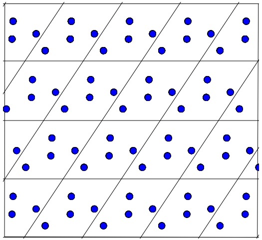
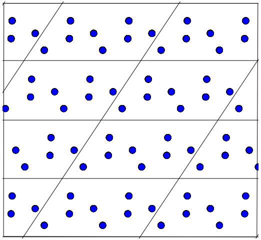
$$\Lambda + L = \Lambda.$$
$\Leftrightarrow \exists$ a lattice L and vectors $t_1, \ldots, t_m$ in $\mathbf{R}^n$, pairwise incongruent $\mod L$, such that
$$\Lambda = \bigcup_{i=1}^{m} (t_i + L)$$
In that case we say that Λ is m-periodic.

A given periodic set Λ admits infinitely many period lattices and representations $\Lambda = \bigcup_{i=1}^{m} (t_i + L)$, in which the number $m = |\Lambda / L|$ varies, but not the *point density* :

$$p\delta(\Lambda) := \frac{m}{\sqrt{\det L}}$$ "number of points per unit volume of space".

For instance one can replace L by any of its sublattice L' and obtain a representation as a union of $m\,[L : L']$ translates of L'





All period lattices are contained in

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Local maxima of packing density

- ***Lattice packings :*** Voronoi theory (1907).
  - Local maxima sit at the vertices of the *Ryshkov polyhedron*.
  - Algorithm to enumerate the vertices.

- ***Periodic packings :***
  - Schürmann (2004) : characterization of the local maxima.
  - Andreanov-Kallus(2017) : refinement in the case of 2-periodic sets + algorithm to enumerate the vertices.

Energy of periodic sets

Reminder : the energy of a finite configuration of points $\mathcal{C}$ in $\mathbf{R}^n$ *w.r.t.* a potential f is given by

$$E(f, \mathcal{C}) = \frac{1}{|\mathcal{C}|} \sum_{x,y \in \mathcal{C}, x \neq y} f(|x-y|^2).$$

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$\rightsquigarrow$ well-defined if Λ is periodic.

Energy of periodic sets

Cohn and Kumar (2007) define the energy of a m-periodic set $\Lambda = \bigcup_{i=1}^{m} (t_i + L)$ with respect to a potential f as

$$E(f, \Lambda) = \frac{1}{m} \sum_{1 \le i,j \le m} \sum_{\substack{w \in L \\ w + t_j - t_i \neq 0}} f(|w + t_j - t_i|^2)$$

$$= \frac{1}{m} \sum_{i=1}^{m} \sum_{u \in \Lambda \setminus \{t_i\}} f(|u - t_i|^2)$$

Fact : for a rapidly decreasing f, this agrees with the previous definition, namely $\lim_{R \to \infty} E(f, \Lambda_R)$ exists and equals $E(f, \Lambda)$.

Recall : $\Lambda_R := \Lambda \cap B(0, R)$.

Comments

The definition of the energy as

$$E(f,\Lambda) = \lim_{R\to\infty} \frac{1}{|\Lambda_R|} \sum_{x,y\in\Lambda_R, x\neq y} f(|x-y|^2)$$

involves only the set

$$"\Lambda - \Lambda" := \{x - y, x \in \Lambda, y \in \Lambda\}.$$

(no reference to a period lattice)

- If Λ is a lattice ($m = 1$), then $\Lambda - \Lambda = \Lambda$ (group structure).

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- Definitely more complicated if $m > 2$.

Automorphisms

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If $0 \in \Lambda$, then

$$\mathrm{Aut}\,\Lambda \supset \mathrm{Aut}_0\,\Lambda = \{\varphi \in \mathrm{Aut}\,L_{\mathrm{max}} \mid \varphi(\Lambda) = \Lambda\}\,.$$

Universal optimality

$$\Lambda = \bigcup_{i=1}^m (t_i + L),\ E(f,\Lambda) = \frac{1}{m} \sum_{1\le i,j\le m} \sum_{\substack{w\in L \\ w+t_j-t_i\neq 0}} f(|w+t_j-t_i|^2)$$

For the potential f, we restrict to *completely monotonic functions*, that is, real-valued, $\mathcal{C}^\infty$ on $(0,\infty)$, and such that

$$\forall k \ge 0, \forall x \in (0,\infty), \quad (-1)^k f^{(k)}(x) \ge 0.$$

The class of completely monotonic functions contains all the "reasonable functions" in the context of energy minimization, *e.g.* :

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Definition

Λ is *universally optimal* if it minimizes $E(f_c, \Lambda)$ for any $c > 0$.

Cohn and Kumar conjecture

Conjecture (Cohn-Kumar (2007))

The lattices A_2, D_4, E_8 and Λ_{24} are universally optimal.

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- The conjecture has been proved recently for E_8 and Λ_{24} by Cohn, Kumar, Miller, Radchenko and Viazovska.

A non lattice example : D_n^+.

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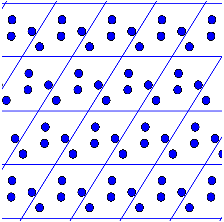
Cohn, Kumar, Schürmann : experimental study suggest that D_9^+ is universally optimal.

Local deformations



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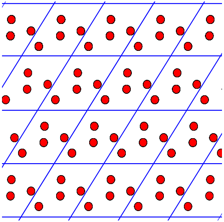

Purely translational deformation

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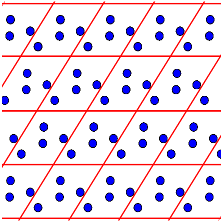

Purely lattice deformation

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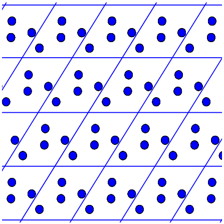

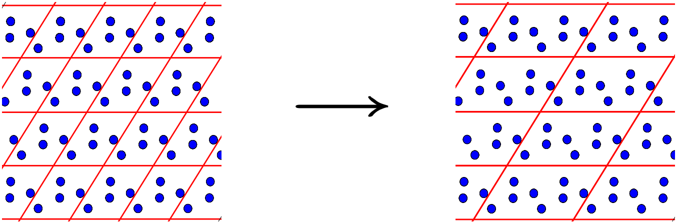

change m

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We say that Λ is *f-critical* if the gradient of the above map vanishes at Λ.

Necessary conditions for universal optimality

Let S be a sphere in $\mathbf{R}^n$ centered at 0.

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Definition

A finite set $\mathcal{D} \subset S$ is a *weighted spherical design of strength* t if there exists a function $\nu : \mathcal{D} \to (0, \infty)$ such that for all polynomial of degree $\leq t$ one has

$$\frac{1}{\mathrm{Vol}(S)} \int_S P(x)dx = \frac{1}{\nu(\mathcal{D})} \sum_{x \in \mathcal{D}} \nu(x)P(x).$$

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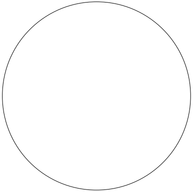
If $t = 1$ and $\nu \equiv 1$, this reduces to the condition that

$$\sum_{x \in \mathcal{D}} x = 0$$

which we refer to in the sequel as $\mathcal{D}$ being a *balanced* set.

Examples

In dimension 2, the set of vertices of a regular s-gone is a $(s-1)$-design.



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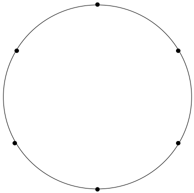

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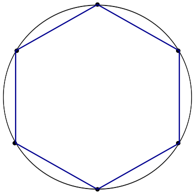

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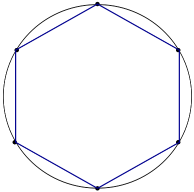

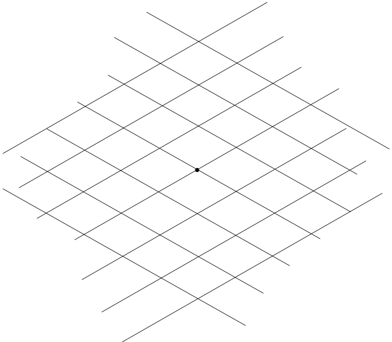

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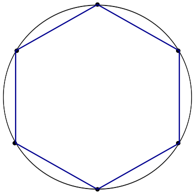

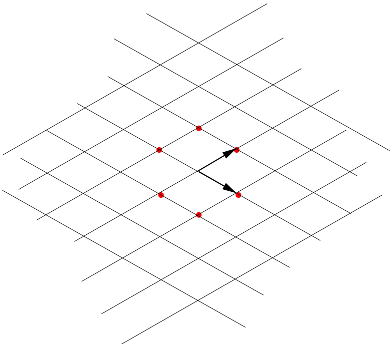

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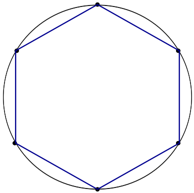

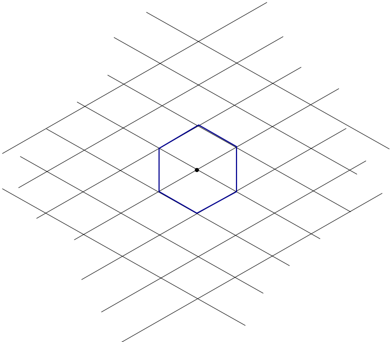

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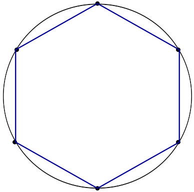

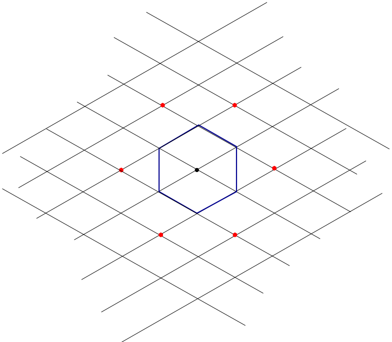

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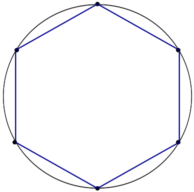

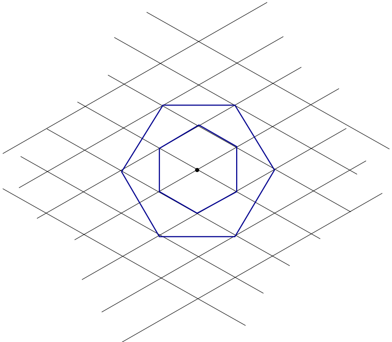

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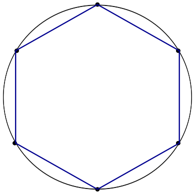

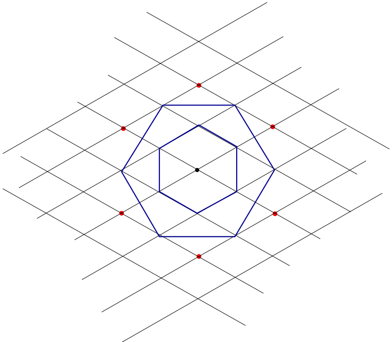

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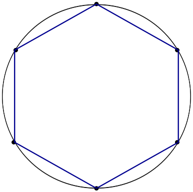

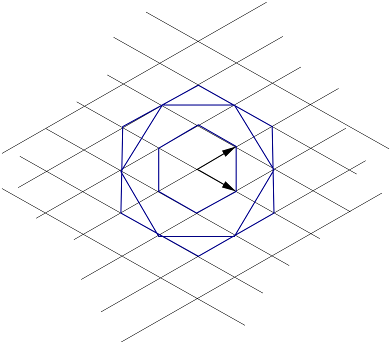

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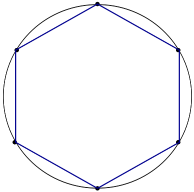

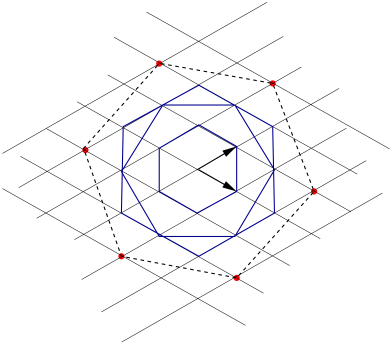

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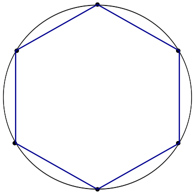

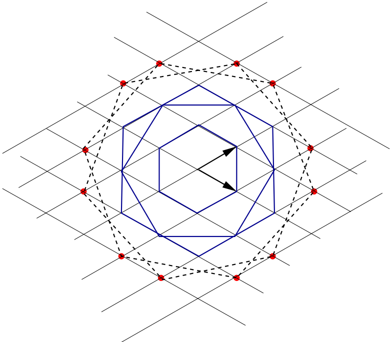

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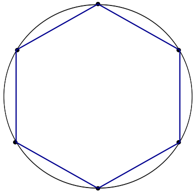

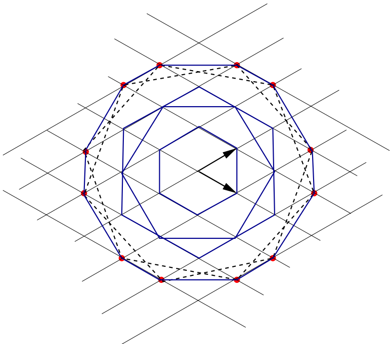

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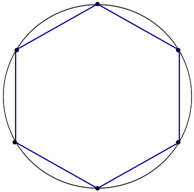

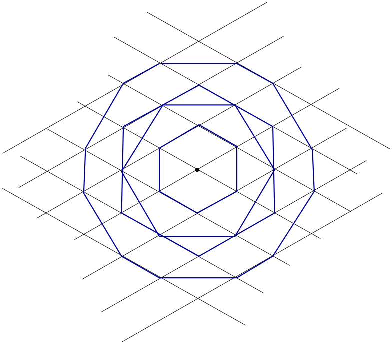

First order condition (gradient)

For $x \in \Lambda$ and $r > 0$ we define

$$\Lambda_x(r) \; = \; \{y - x \mid \|y - x\| = r, \; y \in \Lambda\} \text{ "pointed shell"}$$

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Theorem (C., Schürmann (2017))

A periodic set Λ in $\mathbf{R}^n$ is f_c-critical for all $c > 0$ if and only if the following two conditions are satisfied :

1. *All non-empty pointed shells $\Lambda_x(r)$ for $x \in \Lambda$ and $r > 0$ are balanced.*
2. *All non-empty shells $\Lambda(r)$ for $r > 0$ are weighted spherical 2-designs with respect to the following weight ν :*

$$\nu(w) = \frac{1}{m} \left| \{ i \mid w \in \Lambda_{t_i} \} \right| .$$

Proposition

If the automorphism group of Λ *acts* $\mathbf{R}$*-irreducibly, then* Λ *is* f_c*-critical for any* $c > 0$.

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$$\sum_{x \in \mathcal{D}} \nu(x) x = 0 \text{ and } \sum_{x \in \mathcal{D}} \nu(x) x x^t = c\, I_n$$

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Second order condition (Hessian)

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In the case of D_n^+, we obtain :

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Let n be an odd integer ≥ 9. Then there exists a constant c_n such that D_n^+ is locally f_c-optimal for any $c > c_n$.

In the computation of the "lattice part" of the Hessian for D_N^+, one has to estimate the quantities

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As for step 2 it does not really make sens in general, since there is no Poisson formula...but D_9^+ is formally self-dual !