Formally dual configurations in Euclidean space and in abelian groups

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Background: energy minimization

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$$E_f(x) = \sum_{y \in \mathcal{P}, y \neq x} f(|x - y|)$$

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Remark: We usually take f to be a completely monotonic function of squared distance.

Gradient descent

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[Cohn-K-Schürmann '09]: computer simulations for $f(r) = e^{-c\pi r^2}$ for various c, dimension $n \leq 8$, number of translates $N \leq 10$. Gradient descent on the space of periodic configurations with fixed number of translates.

We observed very interesting phenomena for $n \geq 5$. For instance, in dimensions 5 and 7, the limit of the energy minimizers for $c >> 0$ is not the densest lattice packing, but rather a periodic packing! (Disproving a conjecture of Torquato and Stillinger).

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For instance, let D_n^+ be $D_n \bigcup (D_n + (1/2, \ldots, 1/2))$, where D_n is the checkerboard lattice. Let $D_n^+(\alpha)$ be obtained by scaling the last coordinate of every point of D_n^+ by the positive real number α.

Then $D_n^+(\alpha)$ is **formally dual** to $D_n^+(1/\alpha)$.

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For $n = 5$, and for c not too close to 1, the global minimum seems to be some $D_5^+(\alpha)$.

Dual lattices and Poisson summation

For any lattice Λ, we have its dual lattice
$\Lambda^* = \{y \in \mathbb{R}^n \,|\, \langle x, y\rangle \in \mathbb{Z} \quad \forall\, x \in \Lambda\}$.

We know $\mathrm{vol}(\mathbb{R}^n/\Lambda^*) = 1/\mathrm{vol}(\mathbb{R}^n/\Lambda)$, $(\Lambda^*)^* = \Lambda$, etc.

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Poisson summation formula: For any nice function $f : \mathbb{R}^n \to \mathbb{R}$ (e.g. Schwartz function),

$$\sum_{x\in\Lambda} f(x) = \frac{1}{\mathrm{vol}(\mathbb{R}^n/\Lambda)} \sum_{y\in\Lambda^*} \widehat{f}(y)$$

where $\widehat{f}(y) = \int_{\mathbb{R}^n} f(x) e^{2\pi i \langle x,y\rangle} dx$

Formal duality I

Can the same hold for periodic configurations $\mathcal{P}$ and $\mathcal{Q}$? i.e. Can we have

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But we're really only interested in $\mathcal{P} - \mathcal{P} = \{x - y : x, y \in \mathcal{P}\}$, since if

$$\Sigma(f,\mathcal{P}) := \frac{1}{N} \sum_{i,j} \sum_{x\in\Lambda} f(x + v_i - v_j)$$

then $E_f(\mathcal{P}) = \Sigma(f,\mathcal{P}) - f(0)$.

Formal duality II

Say $\mathcal{P}$ and $\mathcal{Q}$ are formal duals if $\Sigma(f, \mathcal{P}) = \delta(\mathcal{P})\Sigma(\widehat{f}, \mathcal{Q})$ for every Schwartz function $f : \mathbb{R}^n \to \mathbb{R}$ (we do not omit the diagonal).

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For binary codes, the weight enumerators are related by MacWilliams identities.

For periodic configurations, the average theta functions are related by the modular transformation $z \to -1/z$. This follows by analytic continuation from

$$E_f(\mathcal{P}) + 1 = \delta \cdot (1 + E_{\widehat{f}}(\mathcal{Q}))$$

when $f(x) = \exp(-\pi c|x|^2)$, $\widehat{f}(y) = \exp(-\pi|y|^2/c)$

$D_n^+(\alpha)$

Theorem (Cohn-K-Schürmann)

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Corollary

$D_n^+(\alpha)$ is formally dual to an isometric copy of $D_n^+(1/\alpha)$.

So if f is radially symmetric, the Gaussian potential energies of these periodic configurations at parameters c and $1/c$ respectively are related.

Combinatorial description

Remark: if $\mathcal{P}$ and $\mathcal{Q}$ are formally dual, then so are $\phi(\mathcal{P})$ and $\phi^{-1}(\mathcal{Q})$ for any affine transformation ϕ of $\mathbb{R}^n$.

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So formal duality really is only a combinatorial property of the group structure and cosets involved. Namely, if $\mathcal{P} = \Lambda + \{v_1, \ldots, v_n\}$ and $\mathcal{Q} = \Gamma + \{w_1, \ldots, w_n\}$, we need for every $y \in \Lambda^*$:

$$\sum_{y \in \Lambda^*} \left| \frac{1}{N} \sum_{i=1}^{N} e^{2\pi i \langle v_j, y \rangle} \right|^2 = \frac{1}{M} \#\{(x, j, k) \in \Gamma \times [M] \times [M] : y = x + w_j - w_k\}.$$

Group-theoretic reformulation

We can reformulate everything now in terms of abelian groups. Letting $\mathcal{Q}$ be M translates $w_1, \ldots, w_M$ of a lattice Γ, it is not hard to check that $v_1, \ldots, v_N$ lie in Γ^*.

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Let $G = \Gamma^*/\Lambda$ and its dual $\widehat{G} = \Lambda^*/\Gamma$. We are then looking for subsets S of G and T of $\widehat{G} = Hom(G, \mathbb{C}^*)$ such that

$$\left| \sum_{v \in S} \langle v, y \rangle \right|^2 = \frac{N^2}{M} \#\{(w, w') \in T \times T : y = w - w'\}$$

for every $y \in \widehat{G}$.

It automatically follows that duality is a symmetric relation.

TITO

The simplest example is of course $G = \widehat{G} = \{0\}$ and $S = T = \{0\}$.

The next simplest example, from which D_n^+ arises by a taking a product with $n-1$ copies of the first example, is the following:

Take $G = \widehat{G} = \mathbb{Z}/4\mathbb{Z}$ and $S = T = \{0, 1\}$.

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The relevant calculations are:

$$
\begin{aligned}
|1+1|^2 &= 4 = 2 \cdot \#\{(0,0),(1,1)\} \\
|1+i|^2 &= 2 = 2 \cdot \#\{(1,0)\} \\
|1-i|^2 &= 2 = 2 \cdot \#\{(0,1)\} \\
|1-1|^2 &= 0 = 2 \cdot \#\{\}
\end{aligned}
$$

Call this example **TITO** (two-in-two-out).

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We can show that when $M = N$ is squarefree and odd, there only solutions are the trivial ones, i.e. $S = H$ a subgroup of G, and $T = H^{\perp}$ its annihilator in $\widehat{G}$.

Quadratic examples and Gauss sums

We will now give some examples with $G = \widehat{G} = (\mathbb{Z}/p\mathbb{Z})^2$, with the pairing

$$\langle (a, b), (c, d) \rangle = \zeta_p^{ac+bd},$$

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Recall that

$$\left|\sum_{n=1}^{p} \zeta_p^{cn^2+dn}\right|^2 = \begin{cases} p^2 & \text{if } p|c,d \\ 0 & \text{if } p|c, p\nmid d \\ p & \text{if } p\nmid c. \end{cases}$$

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Proof is an easy exercise using the basic Gauss sum $\left|\sum_{n=1}^{p} \zeta_p^{n^2}\right|^2 = p$ and completing squares.

Proposition

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Proof.

We need to show for every $(c, d) \in [p] \times [p]$ that

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For $p|c$ this is trivial.
For $p \nmid c$ it easily follows from the previous page that the LHS is p. So enough to show there is a unique solution (j, k) to $c = j - k, d = j^2 - k^2$. This is trivial once we observe that $j + k = d/c$. □

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- Conway and Sloane asked whether the Best packing in 10 dimensions has a formal dual. We can at least show it doesn't have a formal dual in our stronger sense.
- Understanding which Barlow packings may have a formal dual (work in progress).

Thank you!