Computing Delaunay polytopes of lattices

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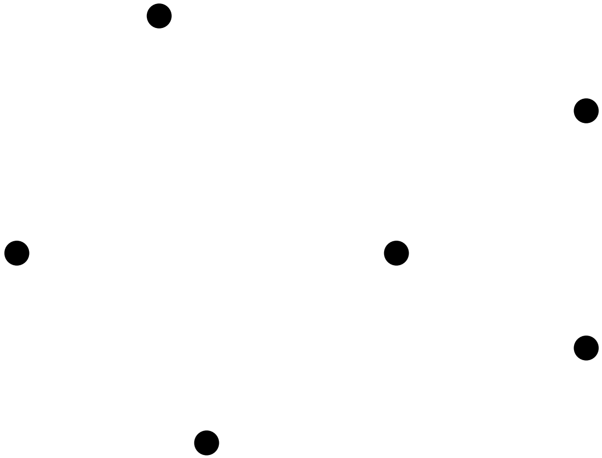
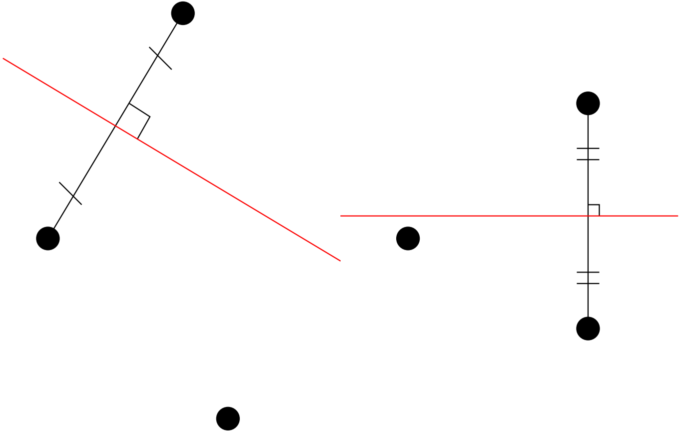
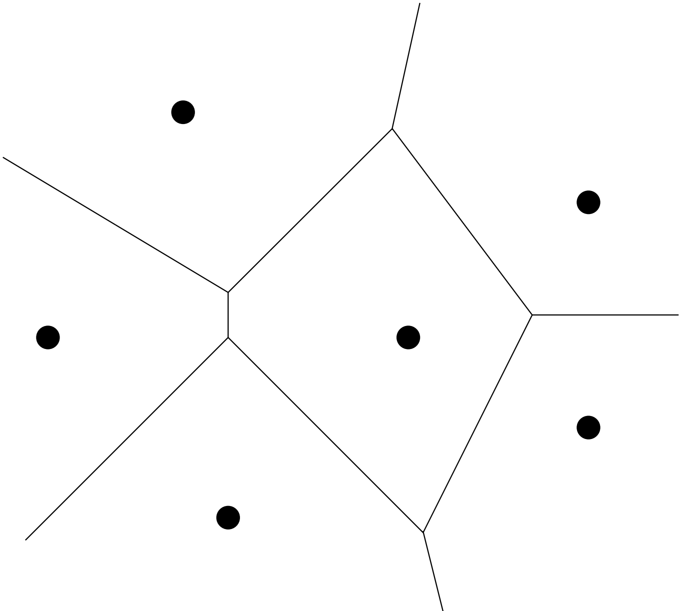
A finite set of points



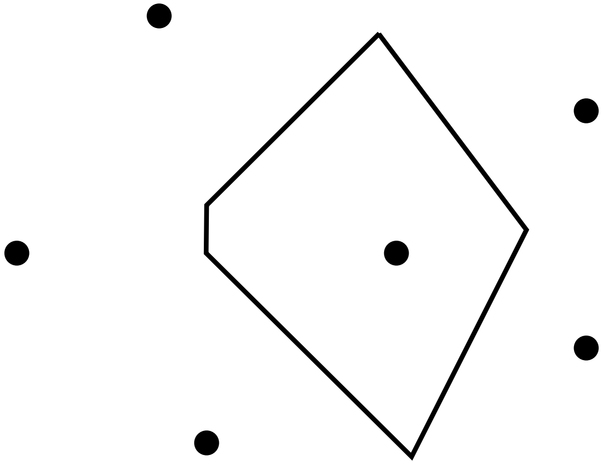
Some perpendicular bisectors



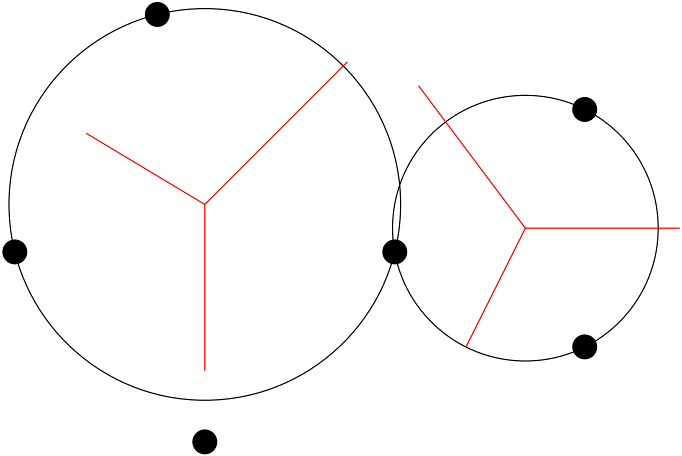
The edges of Voronoi polyhedron



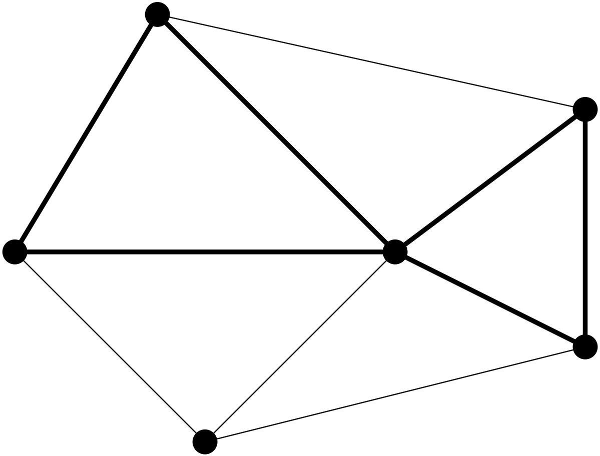
Voronoi polytope



Empty sphere



Delaunay polytopes



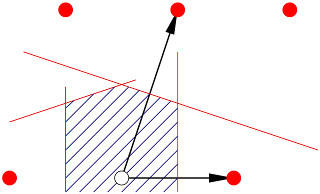
I. Delaunay polytopes in lattices

The Voronoi polytope of a lattice

- A lattice L is a rank n subgroup of $\mathbb{R}^n$, i.e. of the form

$$L = v_1\mathbb{Z} + \cdots + v_n\mathbb{Z}$$

- The Voronoi cell $DV(L)$ of L is defined by $\langle x, v\rangle \leq \frac{1}{2}||v||^2$ for $v \in L - \{0\}$.
- $DV(L)$ is a polytope, i.e. it has a finite number of vertices (of dimension 0), faces and facets (of dimension $n-1$)



- The translates $v + DV(L)$ with $v \in L$ tiles $\mathbb{R}^n$.
- Shortest vector in L define facets of the Voronoi polytope.

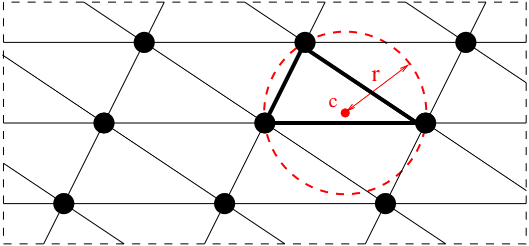
Empty sphere and Delaunay polytopes

A sphere $S(c, r)$ of radius r and center c in an n-dimensional lattice L is said to be an empty sphere if:

(i) $\|v - c\| \geq r$ for all $v \in L$,

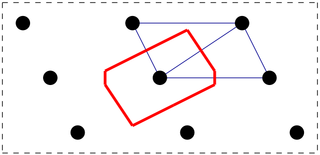
(ii) the set $S(c, r) \cap L$ contains $n + 1$ affinely independent points.

A Delaunay polytope P in a lattice L is a polytope, whose vertex-set is $L \cap S(c, r)$.



Voronoi and Delaunay in lattices

- Vertices of Voronoi polytope are center of empty spheres which defines Delaunay polytopes.
- Voronoi and Delaunay polytopes define dual tessellations of the space $\mathbb{R}^n$ by polytopes.
- Every k-dimensional face of a Delaunay polytope is orthogonal to a $(n-k)$-dimensional face of a Voronoi polytope.



- Given a lattice L, it has a finite number of orbits of Delaunay polytopes under translation.

Volume of Delaunay

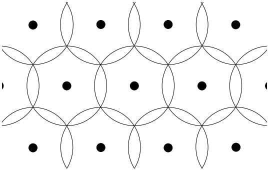
Take L an n-dimensional lattice.

- The number of vertices of a Delaunay polytope is at most 2^n and at least $n+1$.
- Given a Delaunay polytope P of a lattice L, define $L(P)$ the lattice generated by P. Denote by $\alpha(P)$ the index of $L(P)$ in L.
  - Voronoi: if $n \leq 4$, then $\alpha(P) = 1$.
  - Baranovski: if $n = 5$, then $\alpha(P) = 1$ or 2.
  - Ryshkov: if $n = 6$, then $\alpha(P) = 1$, 2 or 3.
  - Santos, Schürmann & Vallentin: $\max \alpha(P)$ grows exponentially with n.
  - Lovasz $\alpha(P) \leq \frac{2^n}{\binom{2n}{n}} n!$.
- The volume of a simplex is $\frac{\alpha(P)}{(n+1)!}$ so a lattice has at most $(n+1)!$ translation classes of Delaunay.
- Given a polytope P, is there an efficient method for finding all lattices containing P as a Delaunay?

II. Applications

Covering density of a lattice

- We consider covering of $\mathbb{R}^n$ by n-dimensional balls of the same radius, whose center belong to a lattice L.



- The covering density has the expression

$$\Theta(L) = \frac{\mu(L)^n \kappa_n}{det(L)} \geq 1$$

with $\mu(L)$ being the largest radius of Delaunay polytopes and κ_n the volume of the unit ball B^n.

- The fact that the covering radius of the Leech lattice is $\sqrt{2}$ has led to striking progress in hyperbolic Coxeter group theory.

Other applications

- The quantizing constant (in coding theory) of a lattice L is defined as

$$Q(L) = \int_{DV(L)} \|x\|^2 \mathtt{dx} \text{ and } quant(L) = \frac{Q(L)}{\det(L)^{1+\frac{2}{n}}}$$

- Delaunay/Voronoi polytopes gives an $\mathrm{Aut}(L)$-invariant cellular decomposition of the space $\mathbb{R}^n$ space.
  - This gives a method for computing the homology of $\mathbb{R}^n/\mathrm{Aut}(L)$.
  - This gives a method for computing the homology of $\mathrm{Aut}(L)$.

II. Examples

Root lattices

- Take $L = \mathbb{Z}^n$; Delaunay:

Name	Center	Nr. vertices	Radius
Cube	$(\frac{1}{2})^n$	2^n	$\frac{1}{2}\sqrt{n}$

- Take $\mathsf{D}_n = \{x \in \mathbb{Z}^n \mid \sum_{i=1}^n x_i \text{ is even}\}$; Delaunay:

Name	Center	Nr. vertices	Radius
Half-Cube	$(\frac{1}{2})^n$	$\frac{1}{2}2^n$	$\frac{1}{2}\sqrt{n}$
Cross-polytope	$(1, 0^{n-1})$	$2n$	1

- Take $\mathsf{E}_8 = \mathsf{D}_8 \cup (\frac{1}{2}^8) + \mathsf{D}_8$; Delaunay:

Name	Center	Nr. vertices	Radius
Simplex	$(\frac{5}{6}, \frac{1}{6}^7)$	9	$\sqrt{\frac{8}{9}}$
Cross-polytope	$(1, 0^7)$	16	1

- Take $\mathsf{A}_n = \{x \in \mathbb{Z}^{n+1} \text{ such that } \sum_{i=1}^{n+1} x_i = 0\}$.
  The Delaunay of A_n are obtained by section of the cube $[0, 1]^{n+1}$ by the hyperplanes $\sum_i x_i = k$.
  They are named $J(n+1, k)$, the number of vertices is $\binom{n+1}{k}$.

Root lattice E_6

- The Schlafli polytope *Sch*:
  - *Sch* has 27 vertices.
  - $skel(Sch)$ is a strongly regular graph.
  - Only 2 distances between distinct vertices of *Sch*.
  - $|\,\mathrm{Aut}(Sch)| = 51840$, the rotation subgroup is simple.
  - 2 orbits of facets, 3 orbits of flags.
  - Two interesting laminations:

levels	polytopes	polytopes
1	*vertex*	$J(6,1)$
0	$\frac{1}{2}H_5$	$J(6,2)$
-1	β_5	$J(6,1)$ (parallel)
	D_5 lamination	A_5 lamination

- The root lattice E_6:
  - Has $|\,\mathrm{Aut}(E_6)| = 2 \times 51840$
  - Has Delaunay polytopes *Sch*, $-Sch$ up to translation

Root lattice E_7

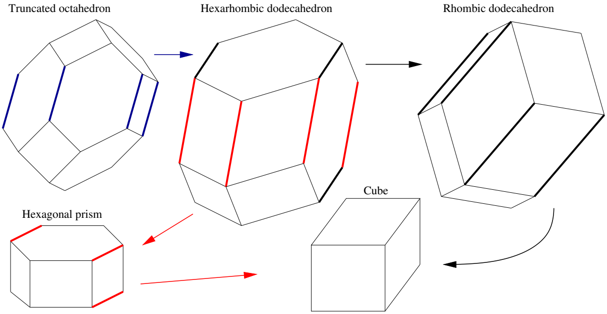
- The Gosset polytope *Gos*:
  - *Gos* has 56 vertices (centrally symmetric).
  - $skel(Gos)$ is a distance regular graph.
  - Only 3 distances between distinct vertices of *Sch*.
  - $|\mathrm{Aut}(Gos)| = 2903040$, the rotation subgroup is simple.
  - 2 orbits of facets, 3 orbits of flags.
  - Three interesting laminations:

levels	polytopes	polytopes	polytopes
2	*vertex*	$J(7,1)$	
1	*Sch*	$J(7,2)$	β_6
0	$-Sch$	$-J(7,2)$	$\frac{1}{2}H_6$
-1	*vertex*	$-J(7,1)$	$-\beta_6$
	E_6 lamination	A_6 lamination	D_6 lamination

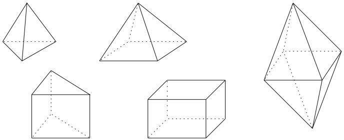
- The root lattice E_7:
  - Has $|\mathrm{Aut}(E_7)| = |\mathrm{Aut}(Gos)|$.
  - Has two orbits of Delaunay: Gosset (1 translation class) and regular simplex (72 translation classes).

3-dimensional lattices

- The 3-dimensional Voronoi polytopes:



- The 3-dimensional Delaunay polytopes:



II. Computational techniques

Closest Vector Problem

- Given a lattice L, a vector c, find all vectors $v \in L$ such that

$$||v - c|| \text{ is minimal}$$

  or in other term, if $M \in S^n_{>0}$ and $c \in \mathbb{R}^n$, find all $v \in \mathbb{Z}^n$ such that

$$^t(v - c)M(v - c) \text{ is minimal}$$

- CVP is conjecturally a NP problem.
- Only way is to do an exhaustive search in a set of possible solutions, two programs:
  - Lattice-CVP (Dutour) use a hypercube, performing well up to dimension 10.
  - Voro (Vallentin) use an ellipsoid, performing well up to dimension, say 40.

Finding an initial Delaunay polytope

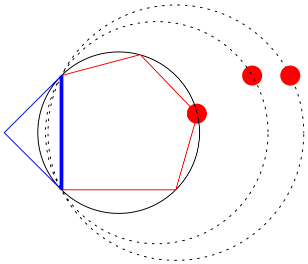
- Finding a Delaunay is equivalent to finding a vertex of the Voronoi polytope.
- The problem is that the Voronoi polytope is defined by an infinity of inequalities.
  - $g \leftarrow$ a random linear function.
  - $\mathcal{V} \leftarrow$ an initial set of non-zero elements of L.
  - Maximize $g(x)$ over the polytope defined by $\langle v, x \rangle \leq \frac{1}{2}\|v\|^2$ for $v \in \mathcal{V}$.

    Denote by x_0 the vertex realizing the maximum.
  - Find $\mathcal{C}$ the closest elements to x_0.
    - If $0 \in \mathcal{C}$ then return $\mathcal{C}$ as vertex-set of a Delaunay polytope.
    - Otherwise do $\mathcal{V} \leftarrow \mathcal{V} \cup \mathcal{C}$.

  This algorithm is implemented in the program finddel by Vallentin.

Finding adjacent Delaunays

- Given a Delaunay polytope and a facet of it, there exist a unique adjacent Delaunay polytope.
- We use an iterative procedure:
  - Select a point outside the facet.
  - Create the sphere around it.
  - If there is no interior point finish, otherwise rerun with this point.



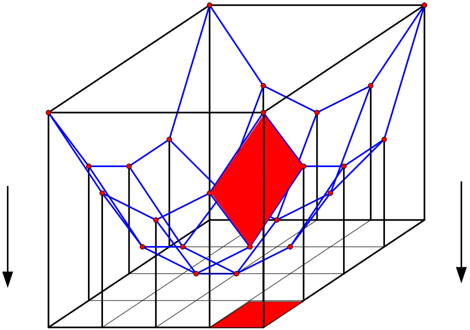
Finding Delaunay decomposition

- Find the isometry group of the lattice (program autom by Plesken & Souvignier).
- Find an initial Delaunay polytope and insert into list of orbits as undone.
- Iterate
  - Find the orbit of facets of undone Delaunay polytopes with the Recursive Adjacency Decomposition method.
  - For every facet, find the adjacent Delaunay polytope.
  - For every Delaunay test if they are isomorphic to existing ones. If not insert them to the list as undone.
  - Finish when every orbit is done.

Lifted Delaunay decomposition

- The Delaunay polytopes of a lattice L correspond to the facets of the convex cone $\mathcal{C}(L)$ with vertex-set:

$$\{(x, ||x||^2) \text{ with } x \in L\} \subset \mathbb{R}^{d+1} \ .$$



II. The Isomorphism and automorphism problems (book of tricks)

Automorphism groups

- A Delaunay polytope P has two automorphism groups
  - The group $Isom(P)$ of isometries preserving the Delaunay.
  - The group $\text{Aut}(P)$ of lattice automorphism preserving the Delaunay.
- $\text{Aut}(P) \subset Isom(P)$.
- If $L(P) \neq L$ then a priori $Isom(P) \neq \text{Aut}(P)$.
- Method 1 We consider centers $c = (c_1, \dots, c_n) \in \mathbb{R}^n$ with $c_i \in [0, 1[$.

$$\text{Aut}(P) = \text{Stabilizer}(GRP, c, ActionMod1)$$

  The trouble is that matrix actions are not easy: the above operation generates the full orbit.
- $Isom(P)$ is easy to get, consider the edge colored graph on the vertex-set of P with edge colors $\|v_i - v_j\|$ and use `nauty`.

Method 2 Iterated stabilizer method

- Compute the center $c = (c_1, \ldots, c_n)$ and denote D the smallest integer such that $Dc \in \mathbb{Z}^n$.
- For every divisor D' of D, we can reduce the center modulo $\frac{1}{D'}$, the action is now modulo $\frac{1}{D'}$.
  Denote the stabilizer $Stab_{D'}$ of this action. Then $Stab(c)$ is a subgroup of $Stab_{D'}(c)$.
- The strategy is now to consider a series of divisors

$$D = D_1 > D_2 > \cdots > D_p = 1$$

and an associated series of stabilizers

$$Stab_{D_1}(c) \supseteq Stab_{D_2}(c) \supseteq \cdots \supseteq Stab_{D_p}(c)$$

$Stab_{D_i}$ is computed from $Stab_{D_{i-1}}$; orbit size is $|Stab_{D_{i-1}}|/|Stab_{D_i}|$.

Some strategies

The computation of $\mathit{Isom}(P)$ is almost always relatively easy, then we can:

- Method 3 Compute the intersection

$$\mathrm{Aut}(P) = \mathit{Isom}(P) \cap \mathrm{Aut}(L)$$

  Well suited if $\mathrm{Aut}(P)$ is a group of small index in $\mathit{Isom}(P)$.
- Method 4 Iterate over all elements of $\mathit{Isom}(P)$, and select the ones which correspond to a matrix with integral coefficients. This yields $\mathrm{Aut}(P)$.
  This strategy is well suited if $\mathit{Isom}(P)$ is small (say, 10000 elements)

Method 6 Autom/Isom method

- The program autom by Plesken & Souvignier can compute the group of matrices $P \in GL_n(\mathbb{Z})$ satisfying

$$PM_i{}^tP = M_i$$

with M_i some symmetric positive definite matrices.

- Given a Gram matrix $M \in S^n_{>0}$ of the lattice and a center c of a Delaunay, form the matrix

$$A(c) = \begin{pmatrix} cMc^t + 1 & -cM \\ -Mc^t & M \end{pmatrix} \text{ and } B = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

- The group $\mathrm{Aut}(P)$ is the automorphism group of the family $(A(c), B)$ with $A(c) \in S^{n+1}_{>0}$ and $B \in S^{n+1}$.

The Λ_{23}^* method

- The shells of Λ_{23}^* are:
  - 4600 vectors of norm 3 (1 orbit) defining a sublattice O_{23} of index 2
  - 94208 vectors of norm 15/4 (1 orbit) spanning Λ_{23}^*
  - 93150 vectors of norm 4 (1 orbit) spanning Λ_{23}^*

  So Method 6 cannot be used due to the too large size of invariant base.
- O_{23} has a manageable invariant base; the automorphism/isomorphism problem is manageable for it. Also it has the property

$$\text{Aut}(O_{23}) = \text{Aut}(\Lambda_{23}^*)$$

- Strategy for computing stabilizer of a Delaunay D under $\text{Aut}(\Lambda_{23}^*)$ is:
  - Compute the stabilizer under $\text{Aut}(O_{23})$
  - If $t \in \Lambda_{23}^* - O_{23}$ then test isomorphism of D and $D + t$.

Crystallographic group case

Suppose now that the point set is no longer a lattice and that the symmetry group is crystallographic.

- All the polyhedral methods explained above applies unchanged.
- The problem is with the isomorphism tests
  - Method 1 is no longer usable.
  - Method 2 goes just as well
  - Method 3 is still usable but less powerful because less control over the occurring fractions.
  - Method 4 is just as well usable.
  - Method 6 does not work now.

II. Large scale examples

The O_{23}/Λ_{23}^* lattices

- We use Method 6 for isomorphism/Automorphism in O_{23}
- We respawn Delaunay computation every time we have more than 80 vertices.

Nr.	$\vert V\vert$	Aut
1	94208	84610842624000
2	24	1320
3	24	1320
4	32	1344
5	24	10200960

- (work in progress) Λ_{23}^* has the following features:
  - An incredible variety of Delaunay polytopes, 485000 in earliest account with 19000 orbits treated.
  - Most Delaunays have low number of vertices, their dual description is easy.
  - Most Delaunay have trivial or small stabilizer, Method 4 is perfect. Otherwise, use O_{23} for such decisions.
  - Only the MD5 invariants are stored in memory, all the rest is on disk.

Cut lattices

- The cut polytope CUT_n is a famous polytope appearing in combinatorial optimization.
- It has 2^{n-1} vertices, dimension $\frac{n(n-1)}{2}$ and $|\mathrm{Aut}(\mathrm{CUT}_n)| = 2^{n-1}n!$.
- The $\mathbb{Z}$-span of CUT_n is a lattice $L(\mathrm{CUT}_n)$ for which CUT_n is one of its Delone polytopes.
- Delaunay of CUT_n:

lattice	dimension	# orbit	covering density
$L(\mathrm{CUT}_3)$	3	2	2.09439
$L(\mathrm{CUT}_4)$	6	4	5.16771
$L(\mathrm{CUT}_5)$	10	12	40.80262
$L(\mathrm{CUT}_6)$	15	112	255.4255

Laminated lattices

- A n-dimensional lamination over a $(n-1)$-dimensional lattice L is one obtained by staking layers of lattice L.
- A laminated lattice is the one of highest density stacked over lower dimensional laminated lattices.

lattice	# orbits		# orbits
Λ_9	5	Λ_9^*	9
Λ_{10}	7	Λ_{10}^*	21
Λ_{11}^{max}	11	Λ_{11}^{max*}	18
Λ_{11}^{min}	18	Λ_{11}^{min*}	153
Λ_{12}^{max}	5	Λ_{12}^{max*}	8
Λ_{12}^{mid}	23	Λ_{12}^{mid*}	52
Λ_{12}^{min}	13	Λ_{12}^{min*}	78
Λ_{13}^{max}	18	Λ_{13}^{max*}	57
Λ_{13}^{mid}	46	Λ_{13}^{mid*}	125
Λ_{13}^{min}	129	Λ_{13}^{min*}	5683
Λ_{14}	65	Λ_{14}^*	1392
Λ_{15}	27	Λ_{15}^*	108
Λ_{16}	4	Λ_{16}^*	
Λ_{17}	28	Λ_{17}^*	720

The Coxeter lattices $A_{n,r}$

- Context: The best way to determine the covering density of a lattice is to compute its Delaunay polytopes. The Coxeter lattices are good candidates.
- The lattice A_n is defined as

$$A_n = \{x \in \mathbb{Z}^{n+1} \text{ such that } \sum x_i = 0\}$$

- If r divides $n+1$, then writes $q = \frac{n+1}{r}$ and define the lattice A_n^r by

$$A_n^r = A_n \cup v_{n,r} + A_n \cup \dots \cup (r-1)v_{n,r} + A_n$$

with

$$v_{n,r} = \frac{1}{r}\sum_{i=1}^{n+1} e_i - \sum_{i=1}^{q} e_i$$

- The dual of A_n^r is A_n^q. Also $A_8^3 = E_8$, $A_7^2 = E_7$.

Specificity of Coxeter lattices

- If $n \geq 9$, then the automorphism of A_n^r is $\mathbb{Z}_2 \times Sym(n+1)$ encoded on $n+3$ points.
- The lattice A_{21}^2 has 21 orbits of Delaunay polytopes, one orbit is formed of Delaunay polytopes with 40698 vertices.
- Every face of a Delaunay is encoded by its barycenter, thus we do not need permutation representations on huge number of vertices.
- The heuristic is to respawn the ADM whenever the number of vertices is greater than 70. This makes sometimes 16 levels of recursion.

lattice	# orbits		
A_{13}^2	10	A_{14}^3	17
A_{15}^2	10	A_{17}^3	26
A_{17}^2	15	A_{20}^3	40
A_{19}^2	15	A_{23}^3	55
A_{21}^2	21	A_{26}^3	75

VI. Second moment

Second moment of a lattice

- We want to compute

$$Q(L) = \int_{DV(L)} \|x\|^2 dx$$

This is called quantization error and is used in information theory.

- In fact the true integral we need is the symmetric $(n+1) \times (n+1)$ matrix

$$I_2(DV(L)) = \int_{DV(L)} (1, x)(1, x)^T dx$$

- If one is satisfied with approximate results, then Monte Carlo methods are to be preferred.

Decomposition method

- All methods for computing integrals over a polytope P rely on decomposing it into an union (signed or not) of simplices.
  - B. Büeler B., A. Enge and K. Fukuda, *Exact Volume Computation for Polytopes: a Practical Study*, Polytopes—combinatorics and computation (Oberwolfach, 1997), 131–154, DMV Sem., **29**, Birkhäuser, Basel, 2000.
- Two methods are used by us:
  - lrs can return a simplicial decomposition if one computes the facets from the vertices.
  - If one takes a random quadratic form and computes a Delaunay decomposition for it then "most" Delaunays are simplices. The remaining can be decomposed by further application of the method.

Lassere decomposition method

Suppose we have a n-dimensional polytope P and a group G acting on it by isometries.

- Compute the orbits of facets $F_1, \dots, F_s$ of size $n_1, \dots, n_s$
- Compute the isobarycenter $Iso(P)$ of the vertices of P.
- One has the formulas.

$$\begin{array}{rcl} vol(conv(F_i, Iso(P))) & = & \frac{1}{n} vol(F_i) \times d(F_i, Iso(P)) \\ vol(P) & = & \sum_{i=1}^{s} n_i vol(conv(F_i, Iso(P))) \end{array}$$

- We can express the integral $I_2(conv(F_i, Iso(P)))$ in terms of $I_2(F_i)$ the isobarycenter of F_i and its volume.
- The formula $I_2(P)$ is then

$$I_2(P) = \sum_{i=1}^{s} n_i \frac{1}{|G|} \sum_{g \in G} g I_2(conv(F_i, Iso(P))) g^T$$

Averaging operation

- If G is a group generated by $g_1, \dots, g_s$ acting on $\mathbb{R}^n$, x a vector, we want to compute the barycenter of the orbit Gx:

$$Iso(x) = \frac{1}{|G|} \sum_{g \in G} gx$$

  but we don't want to compute the orbit itself.
- Denote by $Mov(G)$ the smallest subspace of $\mathbb{R}^n$ invariant under G containing the vectors $g_i x - x$ for $1 \le i \le s$.
- Take a basis $v_1, \dots, v_m$ of $Mov(G)$ and write $g(x)$ as

$$g(x) = x + \sum_{i=1}^{m} \alpha_i v_i$$

  The system

$$g_i(Iso(x)) = Iso(x) \text{ for } 1 \le i \le s$$

  has a unique solution.

The recursive decomposition method for $I_2(DV(L))$

- We use Lassere's method recursively until the number of vertices is low enough.
- Faces of $DV(L)$ are encoded by their dual Delaunay and vertices generated only when needed.
- We have a banking system to keep computed integral.
- Some results:

Lattice L	$Q(L)$
Λ_9	$\frac{151301}{2099520} \simeq 0.07206$
Λ_9^*	$\frac{1371514291}{19110297600} \simeq 0.07176$
A_9^2	$\frac{2120743}{\sqrt[9]{5.2^8}13271040} \simeq 0.072166$
A_9^5	$\frac{8651427563}{\sqrt[9]{2.5^8}26578125000} \simeq 0.072079$
D_{10}^+	$\frac{4568341}{64512000} \simeq 0.07081$
D_{12}^+	$\frac{29183629}{412776000} \simeq 0.070700$
K_{12}	$\frac{797361941}{\sqrt{36567561000}} \simeq 0.070095$

THANK

YOU