Logarithmic Voronoi Cells

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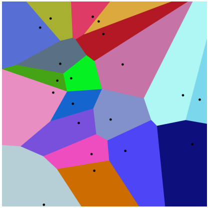
Voronoi cells in the Euclidean case

from Wikipedia:



Let X be a **finite** point configuration in $\mathbb{R}^n$.

- The *Voronoi cell* of $x \in X$ is the set of all points that are closer to x than any other $y \in X$, in the Euclidean metric.
- The subset of points that are equidistant from x and any other points in X is the *boundary* of the Voronoi cell of x.
- Voronoi cells partition $\mathbb{R}^n$ into convex polyhedra.

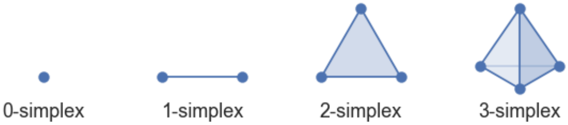
If X is a **variety**, each Voronoi cell is a convex semialgebraic set in the normal space of X at a point. The algebraic boundaries of these Voronoi cells were computed by Cifuentes, Ranestad, Sturmfels and Weinstein.

Log-Voronoi cells

We explore Voronoi cells in the context of algebraic statistics.

- A *probability simplex* is defined as

$$\Delta_{n-1} = \{(p_1, \ldots, p_n) \,:\, p_1 + \cdots + p_n = 1, p_i \geq 0 \text{ for } i \in [n]\}.$$



- A *statistical model* $\mathcal{M}$ is a subset of a probability simplex.
- An *algebraic statistical model* is a subset $\mathcal{M} = \mathcal{V}(f) \cap \Delta_{n-1}$ for some polynomial system of equations $f : \mathbb{C}^n \to \mathbb{C}^m$.
- For an empirical data point $u = (u_1, ..., u_n) \in \Delta_{n-1}$, the *log-likelihood function* defined by u assuming distribution $p = (p_1, ..., p_n) \in \mathcal{M}$ is

$$\ell_u(p) = u_1 \log p_1 + u_2 \log p_2 + \cdots + u_n \log p_n + \log(c).$$

Ice Cream! 

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(p_1, p_2, p_3)

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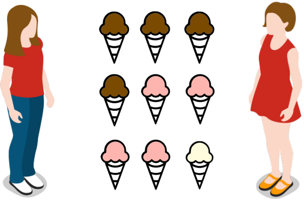

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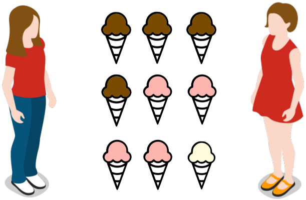

$$L = c \cdot p_1^{4/9} p_2^{4/9} p_3^{1/9}$$

$$\ell_u = 4/9 \cdot \log(p_1) + 4/9 \cdot \log(p_2) + 1/9 \cdot \log(p_3) + \log(c).$$

Log-Voronoi cells

There are two natural problems to consider:

1. The maximum likelihood estimation problem (MLE):

Given a sampled empirical distribution $u \in \Delta_{n-1}$, which point $p \in \mathcal{M}$ did it most likely come from? In other words, we wish to maximize $\ell_u(p)$ over all points $p \in \mathcal{M}$.

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2. Computing logarithmic Voronoi cells:

Given a point in the model $q \in \mathcal{M}$, what is the set of all points $u \in \Delta_{n-1}$ that have q as a global maximum when optimizing the function ℓ_u?

We call the set of all such elements $u \in \Delta_{n-1}$ above the *logarithmic Voronoi cell* of q.

Log-normal spaces and polytopes

Suppose our algebraic statistical model $\mathcal{M}$ is given by the vanishing set of the polynomial system $f = (f_1, \cdots, f_m)$. Let $u \in \Delta_{n-1}$ be fixed.

- The method of *Lagrange multipliers* can be used to find critical points of $\ell_u(x) = u_1 \log x_1 + u_2 \log x_2 + \cdots + u_n \log x_n$ given the constraints f.
- We form the *augmented Jacobian*:

$$A = \begin{bmatrix} \mathcal{J}_f \\ \nabla \ell_u \end{bmatrix} = \begin{bmatrix} \nabla f_1 \\ \vdots \\ \nabla f_m \\ \nabla \ell_u \end{bmatrix}$$

- All $(c+1) \times (c+1)$ minors of A must vanish, where c is the co-dimension of $\mathcal{M}$.

Log-normal spaces and polytopes

Fix some point $q \in \mathcal{M}$ and let u vary.

- Vanishing of $(c+1) \times (c+1)$ minors is a linear condition in u_i.
- The *log-normal space* of q is the *linear* space of possible data points u that have a chance of getting mapped to q via the MLE (all points at which all minors vanish).

$$\log \mathcal{N}_q(\mathcal{M}) = \{u_1 \boldsymbol{v}_1 + \cdots + u_n \boldsymbol{v}_n : u \in \mathbb{R}^n\} \text{ for some fixed } \boldsymbol{v}_i \in \mathbb{R}^n.$$

- Intersecting $\log \mathcal{N}_q$ with the simplex Δ_{n-1}, we obtain a polytope, which we call *log-normal polytope* of q.
- For log-normal polytope contains the logarithmic Voronoi cell of q.

The Hardy-Weinberg curve

Consider a model parametrized by

$$p \mapsto \left(p^2, 2p(1-p), (1-p)^2\right).$$

Performing implicitization, we find that the model $\mathcal{M} = \mathcal{V}(f)$ where $f : \mathbb{C}^3 \to \mathbb{C}^2$ is given by:

$$f = \begin{bmatrix} 4x_1x_3 - x_2^2 \\ x_1 + x_2 + x_3 - 1 \end{bmatrix}.$$

The augmented Jacobian is given by:

$$A = \begin{bmatrix} 4x_3 & -2x_2 & 4x_1 \\ 1 & 1 & 1 \\ u_1/x_1 & u_2/x_2 & u_3/x_3 \end{bmatrix}.$$

Fix a point $q \in \mathcal{M}$ and substitute x_i for q_i in A. All points $u \in \mathbb{R}^3$ at which the determinant vanishes define the log-normal space at q.

The Hardy-Weinberg curve

$\det A = 4u_1 - 4u_3 - 4u_2 \cdot \frac{x_1}{x_2} + 2u_1 \cdot \frac{x_2}{x_1} - 2u_3 \cdot \frac{x_2}{x_3} + 4u_2 \cdot \frac{x_3}{x_2}$

For example, at $p = 0.2$, we get a point $q = (0.04, 0.32, 0.64) \in \mathcal{M}$. The log-normal space at q is the plane

$$20u_1 + 7.5u_2 - 5u_3 = 0.$$

Sampling more points, we get the following pictures:

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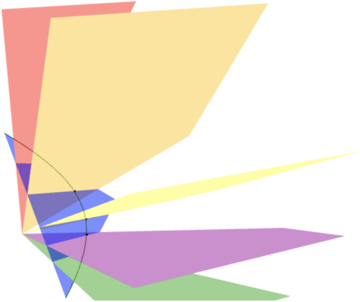

Log-normal spaces

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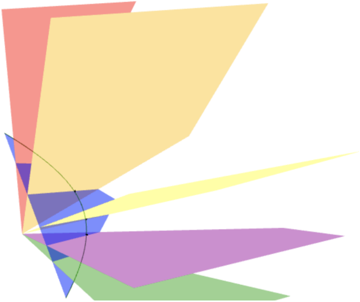

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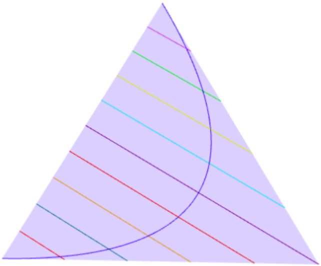

Log-normal polytopes = Log-Voronoi cells

Two-bits independence model

Consider a model parametrized by

$$(p_1, p_2) \mapsto \begin{bmatrix} p_1 p_2 \\ p_1(1-p_2) \\ (1-p_1)p_2 \\ (1-p_1)(1-p_2) \end{bmatrix}.$$

Computing the elimination ideal, we get $\mathcal{M} = \mathcal{V}(f)$ where

$$f = \begin{bmatrix} x_1x_4 - x_2x_3 \\ x_1 + x_2 + x_3 + x_4 - 1 \end{bmatrix}.$$

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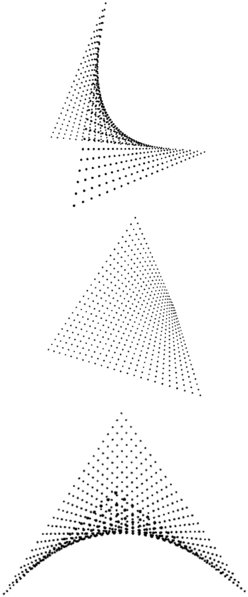

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$$A = \begin{bmatrix} x_4 & -x_3 & -x_2 & x_1 \\ 1 & 1 & 1 & 1 \\ u_1/x_1 & u_2/x_2 & u_3/x_3 & u_4/x_4 \end{bmatrix}.$$

For any point $q = (q_1, q_2, q_3, q_4) \in \mathcal{M}$. The four 3×3 minors at q are given by

$$\begin{array}{c} u_2 - u_3 - \frac{u_1 q_2}{q_1} + \frac{u_1 q_3}{q_1} + \frac{u_2 q_4}{q_2} - \frac{u_3 q_4}{q_3} \\ u_1 - u_4 - \frac{u_2 q_1}{q_2} + \frac{u_1 q_3}{q_1} - \frac{u_4 q_3}{q_4} + \frac{u_2 q_4}{q_2} \\ u_1 - u_4 + \frac{u_1 q_2}{q_1} - \frac{u_3 q_1}{q_3} - \frac{u_4 q_2}{q_4} + \frac{u_3 q_4}{q_3} \\ u_2 - u_3 + \frac{u_2 q_1}{q_2} - \frac{u_3 q_1}{q_3} - \frac{u_4 q_2}{q_4} + \frac{u_4 q_3}{q_4}. \end{array}$$

The log normal space at q is parametrized as

$$u_3 \begin{pmatrix} \frac{q_1^2 - q_1 q_4}{(q_1+q_2)q_3} \\ \frac{q_1 q_2 + q_2 q_3}{(q_1+q_2)q_3} \\ 1 \\ 0 \end{pmatrix} + u_4 \begin{pmatrix} \frac{q_1 q_2 + q_1 q_4}{(q_1+q_2)q_4} \\ \frac{q_2^2 - q_2 q_3}{(q_1+q_2)q_4} \\ 0 \\ 1 \end{pmatrix}.$$

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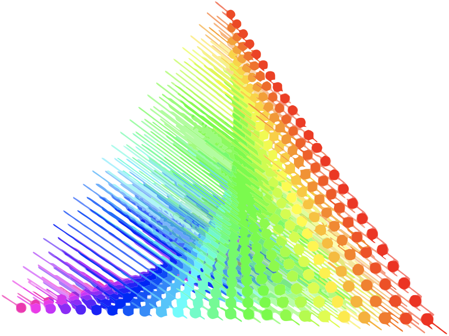

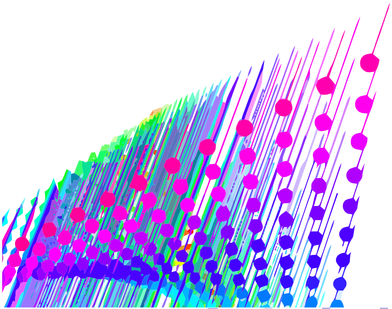

Twisted cubic

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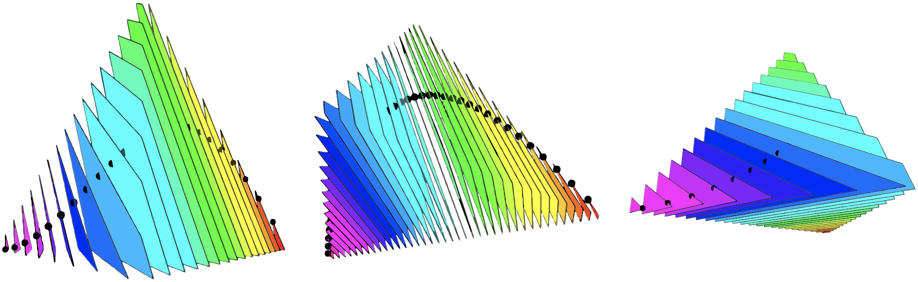

When are log-Voronoi cells polytopes?

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Let $\Theta \subseteq \mathbb{R}^d$ be a parameter space. Suppose $\mathcal{M}$ is given by

$$f : \Theta \to \Delta_{n-1} : (\theta_1, \cdots, \theta_d) \mapsto (f_1(\theta), \cdots, f_n(\theta)).$$

Then $\ell_u(p) = \sum_{i=1}^n u_i \log f_i(\theta)$. The *likelihood equations* are

$$\sum_{i=1}^n \frac{u_i}{f_i} \cdot \frac{\partial f_i}{\partial \theta_j} = 0 \text{ for } j \in [d].$$

The *maximum likelihood degree* (ML degree) of $\mathcal{M}$ is the number of complex solutions to the likelihood equations for generic data u.

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If $\mathcal{M}$ is a model of *ML degree 1*, then the logarithmic Voronoi cell at every $p \in \mathcal{M}$ equals its log-normal polytope.

When are log-Voronoi cells polytopes?

A discrete *linear model* is given parametrically by nonzero linear polynomials.

Theorem (A., Heaton)

Let $\mathcal{M}$ be a linear model. Then the logarithmic Voronoi cells are equal to their log-normal polytopes.

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For an $m \times n$ integer matrix A with $\mathbf{1} \in \text{rowspan}(A)$, the corresponding *toric model* $\mathcal{M}_A$ is defined to be the set of all points $p \in \Delta_{n-1}$ such that $\log(p) \in \text{rowspan}(A)$.

Theorem (A., Heaton)

Let A be an integer matrix with $\mathbf{1}$ in its row span and let $\mathcal{M}_A$ be the associated toric model. Then for any point $p \in \mathcal{M}$, the log-Voronoi cell of p is equal to the log-normal polytope at p.

Big example

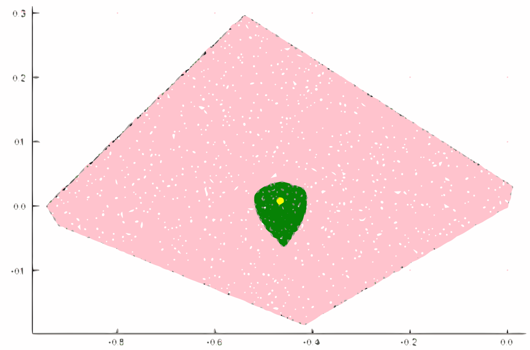
- $\mathcal{M}$ is a 3-dimensional model inside the 5-dimensional simplex given by:

$$
\begin{aligned}
f_0 &= x_0 + x_1 + x_2 + x_3 + x_4 + x_5 - 1 \\
f_1 &= 20x_0x_2x_4 - 10x_0x_3^2 - 8x_1^2x_4 + 4x_1x_2x_3 - x_2^3 \\
f_2 &= 100x_0x_2x_5 - 20x_0x_3x_4 - 40x_1^2x_5 + 4x_1x_2x_4 + 2x_1x_3^2 - x_2^2x_3 \\
f_3 &= 100x_0x_3x_5 - 40x_0x_4^2 - 20x_1x_2x_5 + 4x_1x_3x_4 + 2x_2^2x_4 - x_2x_3^2 \\
f_4 &= 20x_1x_3x_5 - 8x_1x_4^2 - 10x_2^2x_5 + 4x_2x_3x_4 - x_3^3
\end{aligned}
$$

- Pick point $p = \left(\frac{518}{9375}, \frac{124}{625}, \frac{192}{625}, \frac{168}{625}, \frac{86}{625}, \frac{307}{9375}\right) \in \mathcal{M}$.
- 225 4×4 minors of augmented Jacobian define the log-normal space.

Big example

- Log-normal space of p is 3-dimensional, and the log-normal polytope of p is a hexagon.
- Using the numerical Julia package HomotopyContinuation.jl, we may compute the logarithmic Voronoi cell of p:



(joint work with Alex Heaton and Sascha Timme)

Chaotic universe model

Consider running experiments with sample size d and choosing the model defined by

$$\mathcal{M} = \frac{\mathbb{Z}^n \cap d \cdot \Delta_{n-1}}{d}.$$

What are the logarithmic Voronoi cells of such model?

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For convenience we work with the scaled simplex $d \cdot \Delta_{n-1}$. Define $\mathcal{M}_{n,d}$ to be the set of all $N := \binom{n+d-1}{d}$ nonnegative integer vectors summing to d.

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Because $\mathcal{M}_{n,d}$ is a finite model, its logarithmic Voronoi cells are polytopes. What kinds of polytopes?

Chaotic universe model: Euclidean cells

Let $p \in \mathcal{M}_{n,d}$. What is its Euclidean Voronoi cell?

A *root polytope of type A_{n-1}* is the convex hull of $\{e_i - e_j : i \neq j\}$. This polytope is $(n-1)$-dimensional, denote it by $P_n \subseteq \mathbb{R}^n$. The Euclidean Voronoi cell of $p \in \mathcal{M}_{n,d}$ are the dual P_n^*.

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Theorem (S. Cho)

Every m-dimensional face of P_n is the convex hull of the vectors $\{e_i - e_j : i \in I, j \in J\}$ with $|I| + |J| = m + 2$, so there is a bijection between nontrivial faces of P_n and the set of ordered partitions of subsets of $[n]$ with two blocks.

Chaotic universe model: logarithmic cells

In the logarithmic setting, analogous polytopes $\log P_n(p)$ exist, playing the same role as the root polytopes in the Euclidean case. However, their details are more complicated.

The *logarithmic root polytope* for $p \in \mathcal{M}_{n,d}$ is defined as the convex hull of the $2\binom{n}{2}$ vertices v_{ij} for $i \neq j \in [n]$ given by the formulas

$$v_{ij} := \frac{1}{b_j p_j - a_i p_i}\left[a_i e_i - b_j e_j - \frac{(a_i - b_j)}{n}\mathbb{1}\right]$$

where

$$a_i := \log(\tfrac{p_i+1}{p_i}) \qquad b_j := \log(\tfrac{p_j}{p_j-1})$$

and where $\mathbb{1} := \sum_{k\in[n]} e_k$. Note that $a_i, b_j > 0$ are always positive real numbers and all vectors v_{ij} are orthogonal to $\mathbb{1}$. We denote the polytope by $\log P_n(p)$.

Chaotic universe model

Theorem (A., Heaton)

For $m \in \{0, 1, \ldots, n-2\}$, every m-dimensional face of the logarithmic root polytope for $p \in \mathcal{M}_{n,d}$ is given by the convex hull of the vertices v_{ij} for $i \in I, j \in J$, where I, J are disjoint nonempty subsets of $[n]$ such that $|I| + |J| = m + 2$. Thus there is a bijection between nontrivial faces of $\log P_n(p)$ and the set of ordered partitions of subsets of $[n]$ with two blocks, where the dimension of the face corresponding to (I, J) is $|I| + |J| - 2$.

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Define the linear functional $g = (g_1, \cdots, g_n)$. For each $\ell \in [n]$, let g_ℓ be

	P_n	$\log P_n$
If $\ell \in I$	1	$\sum_{i \in I \setminus \ell} a^{I \setminus \{\ell, i\}} b^J (a_i p_i - a_\ell p_\ell) + \sum_{j \in J} a^{I \setminus \ell} b^{J \setminus j} (b_j p_j - a_\ell p_\ell)$
If $\ell \in J$	-1	$\sum_{i \in I} a^{I \setminus i} b^{J \setminus \ell} (a_i p_i - b_\ell p_\ell) + \sum_{j \in J \setminus \ell} a^I b^{J \setminus \{\ell, j\}} (b_j p_j - b_\ell p_\ell)$
Else	0	$0,$

Chaotic universe model

Given a point $p \in \mathcal{M}_{n,d}$, the logarithmic Voronoi cell can be defined as the intersection of $d \cdot \Delta_{n-1}$ with all the halfspaces $H_q(u) \geq 0$ for all points $q \in \mathcal{M}_{n,d}$ with $p \neq q$ where

$$H_q(u) := \sum_{i \in [n]} u_i \log\left(\frac{p_i}{q_i}\right).$$

This system of inequalities is *sufficient* to define the logarithmic Voronoi cell. However, not all of these inequalities are *necessary*. Let $p \in \mathcal{M}_{n,d}$ with every entry $p_i > 1$. A *sufficient system of inequalities* defining the logarithmic Voronoi cell is given by the $2\binom{n}{2}$ halfspaces $u \in \mathbb{R}^n$ such that $H_\delta(u) \geq 0$ for $\delta \in R := \{e_i - e_j : i \neq j,\ i, j \in [n]\}$ and the affine plane $\sum u_i = d$, where

$$H_\delta(u) := \sum_{i \in [n]} u_i \log\left(\frac{p_i}{p_i + \delta_i}\right).$$

Chaotic universe model

Theorem (A., Heaton)

The logarithmic Voronoi cells for $p \in \mathcal{M}_{n,d}$ with all $p_i > 1$ are the dual polytopes $(\log P_n(p))^*$ of the logarithmic root polytopes $\log P_n(p)$.

What family of polytopes are these?

Chaotic universe model

Theorem (A., Heaton)

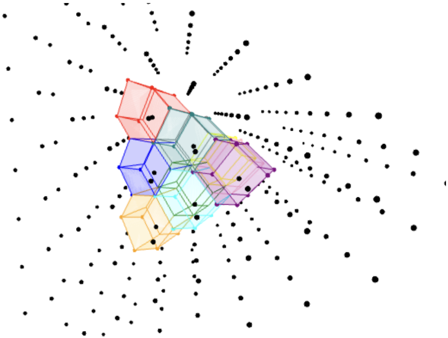
The logarithmic Voronoi cells for $p \in \mathcal{M}_{n,d}$ with all $p_i > 1$ are the dual polytopes $(\log P_n(p))^*$ of the logarithmic root polytopes $\log P_n(p)$.

What family of polytopes are these? For $n = 2, 3, 4, 5, 6, 7$ the f-vectors for the logarithmic Voronoi cells of any point $p \in \mathcal{M}_{n,d}$ with $p_i > 1$ in all coordinates are as follows:

$$\begin{array}{ll} n = 2 & (1, 2, 1) \\ n = 3 & (1, 6, 6, 1) \\ n = 4 & (1, 14, 24, 12, 1) \\ n = 5 & (1, 30, 70, 60, 20, 1) \\ n = 6 & (1, 62, 180, 210, 120, 30, 1) \\ n = 7 & (1, 126, 434, 630, 490, 210, 42, 1) \end{array}$$

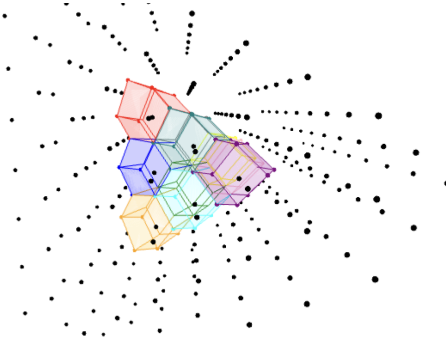
They are combinatorially isomorphic to the dual of the corresponding root polytope, as in the Euclidean case.

Examples

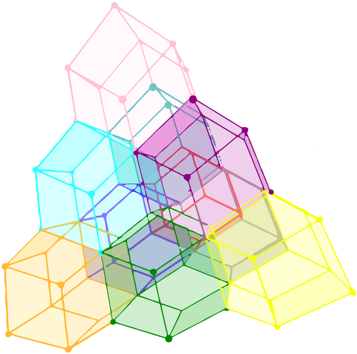


$\mathcal{M}_{4,10}$

Examples

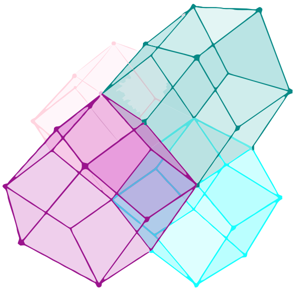


$\mathcal{M}_{4,10}$



$\mathcal{M}_{4,10}$

Voronoi



$\mathcal{M}_{4,9}$

"I noticed already long ago that the task of dividing the *n*-dimensional analytical space into convex congruent polyhedra is closely related to the arithmetic theory of positive quadratic forms" – G. Voronoi.

Voronoi was interested in studying cells of lattices in $\mathbb{Z}^n$ with the aim of applying them to the theory of quadratic forms.

Fun applications

Voronoi decomposition finds applications to the analysis of spatially distributed data in many fields of science, including mathematics, physics, biology, archaeology, and even cinematography.

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In this paper, the author uses Voronoi cells to optimize search paths in an attempt to improve the final 6-minute scene of Andrei Tarkovsky's *Offret* (the Sacrifice).

Cakes!

Voronoi diagrams in baking: Ukrainian pastry chef Dinara Kasko uses Voronoi diagrams to 3D-print silicone molds which she uses to make cakes!

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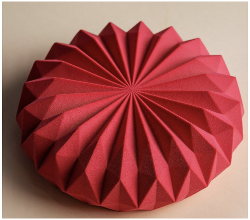

Thanks!