Logarithmic Voronoi Cells

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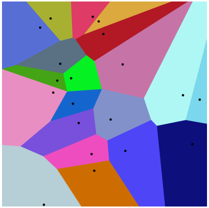
Table of Contents

Introduction

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

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

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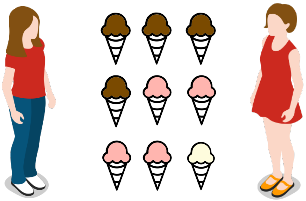
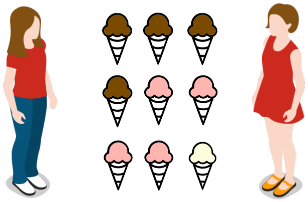


Ice Cream! 

(p_1, p_2, p_3)



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

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

Log-Voronoi cells

There are two natural problems to consider:

1. The maximum likelihood estimation problem (MLE):

Given a sampled empirical distribution $u \in \Delta$, 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 $p \in \mathcal{M}$.

Log-Voronoi cells

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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 $u \in \Delta$ that have q as a global maximum when optimizing the function ℓ_u?

We call the set of all such elements $u \in \Delta$ 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 $u \in \Delta$ 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).

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

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

Example 1: The Hardy-Weinberg curve

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:

The Hardy-Weinberg curve

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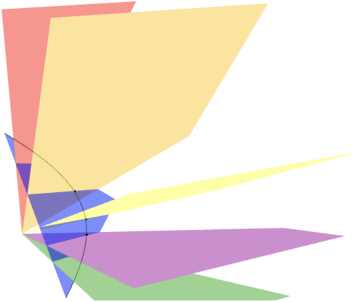

Log-normal spaces

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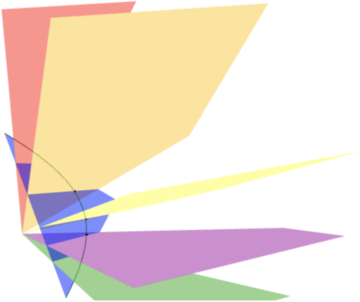
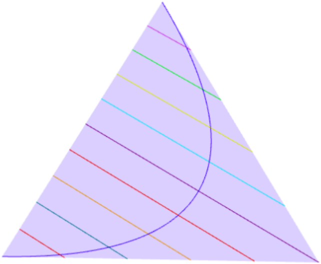


Log-normal spaces



Log-normal polytopes = Log-Voronoi cells

Example 2: Two-bits independence model

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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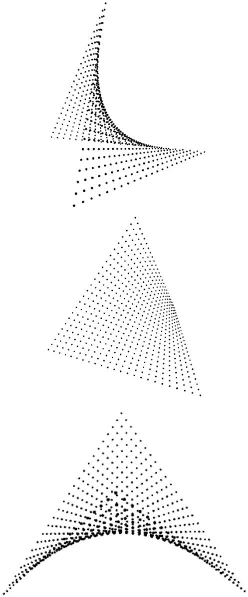

Two-bits independence model

The augmented Jacobian is given by

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

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

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

The log normal space at q is parametrized as

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

Intersecting with the simplex, we get that the log-normal polytope at each point is a line segment.

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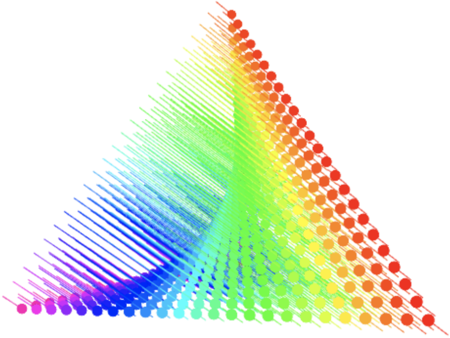
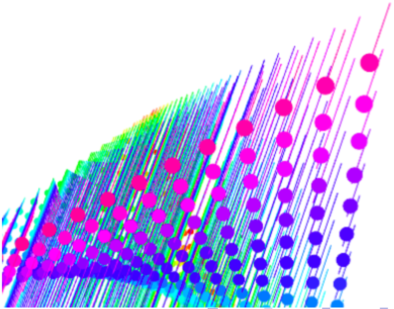


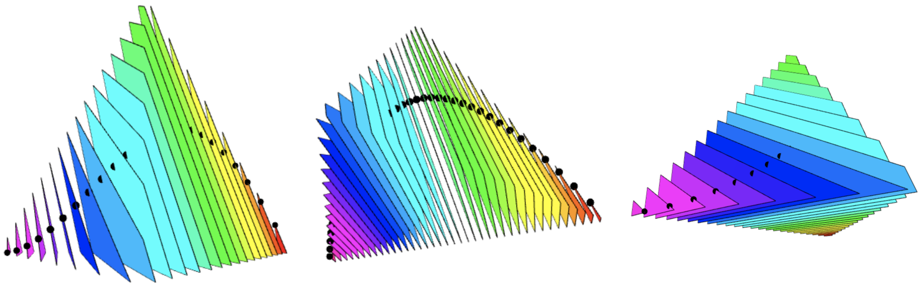


Example 3: Twisted cubic

Twisted cubic

$\mathcal{M}$ is parametrized by

$$p \mapsto \left(p^3, 3p^2(1-p), 3p(1-p)^2, (1-p)^3\right).$$



Example 4: Big example

Big example

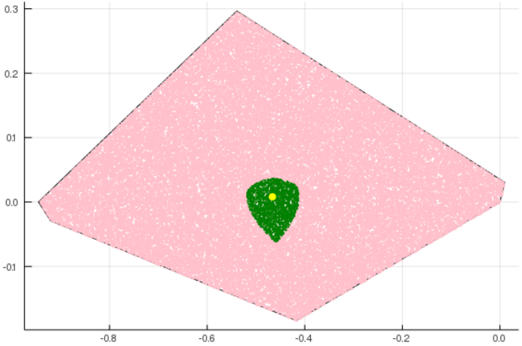
- $\mathcal{M}$ is a 3-dimensional model inside the 5-dimensional simplex given by:

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

- 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)