Logarithmic Voronoi polytopes

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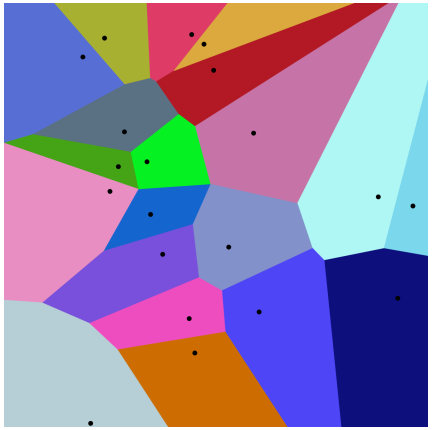
Voronoi cells in the Euclidean case

from Wikipedia:



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

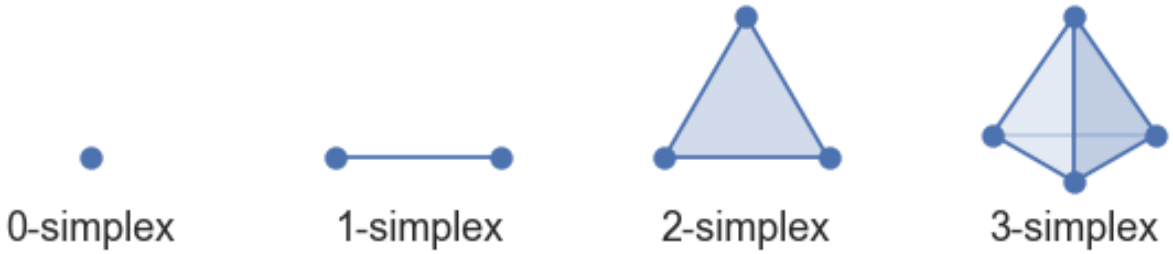
- The *Voronoi cell* of $x \in X$ is the set of all points that are closer to x than any other $y \in X$, in the Euclidean metric.
- The subset of points that are equidistant from x and any other points in X is the *boundary* of the Voronoi cell of x.
- Voronoi cells partition $\mathbb{R}^n$ into convex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

Basic definitions

- A *probability simplex* is defined as

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



- An *algebraic statistical model* is a subset $\mathcal{M} = \mathcal{V} \cap \Delta_{n-1}$ for some variety $\mathcal{V} \subseteq \mathbb{C}^n$.
- 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

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

Maximum likelihood estimation

Fix a model $\mathcal{M} \in \Delta_{n-1}$.

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 $\ell_u(x)$ over all points $p \in \mathcal{M}$.

The *maximum likelihood degree* (ML degree) of $\mathcal{M}$ is the number of complex solutions when optimizing the log-likelihood function $\ell_u(x)$ for generic data u. It measures complexity of MLE.

MLE is an optimization problem very important in algebraic statistics!

Logarithmic Voronoi cells

The "inverse" problem:

Fix a point $p \in \mathcal{M}$. What is the set of all points $u \in \Delta_{n-1}$ that have p as a global maximum when optimizing the function $\ell_u(x)$?

The set of all such elements $u \in \Delta_{n-1}$ the *logarithmic Voronoi cell* at p.

Logarithmic Voronoi cells

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Proposition (A., Heaton)

Logarithmic Voronoi cells are convex sets.

Proof: Exercise.

When are logarithmic Voronoi cells polytopes?

There are families of models on which the log-likelihood function is strictly concave. This guarantees that $\ell_u(x)$ has the unique critical point of on the model for every $u \in \Delta_{n-1}$, despite the ML degree possibly being large. Examples of such families include toric models and linear models.

Theorem (A., Heaton)

If $\mathcal{M}$ is a toric model or a linear model, the logarithmic Voronoi cell at any point $p \in \mathcal{M}$ is a polytope.

How to compute logarithmic Voronoi polytopes?

Let $\mathcal{M}$ be a toric model or a linear model. given by the vanishing set of the polynomial system $f = \{f_1, \ldots, f_m\}$. **Fix $u \in \Delta_{n-1}$ (for now).**

- 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.
- Form the *augmented Jacobian*:

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

- Critical points are found by requiring that the gradient of ℓ_u lies in the rowspace of $\mathcal{J}_f$.
- All $(c+1) \times (c+1)$ minors of A must vanish, where c is the co-dimension of $\mathcal{M}$.

How to compute logarithmic Voronoi polytopes?

Let $\mathcal{M}$ be a toric model or a linear model. given by the vanishing set of the polynomial system $f = \{f_1, \ldots, f_m\}$. **Now fix a point $p \in \mathcal{M}$.**

- Vanishing of $(c+1) \times (c+1)$ minors is a linear condition in u.
- The linear space of all $u \in \mathbb{R}^n$ for which the minors vanish is the *log-normal space* at p.
- Intersecting the log-normal space at p with Δ_{n-1}, we get a polytope.
- This polytope is the set of all data points $u \in \Delta_{n-1}$ that have p as a critical point of $\ell_u(x)$.
- This polytope is the logarithmic Voronoi polytope at p.

The Hardy-Weinberg curve

Consider a model parametrized by

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

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

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 $\theta = 0.2$, we get a point $p = (0.04, 0.32, 0.64) \in \mathcal{M}$. 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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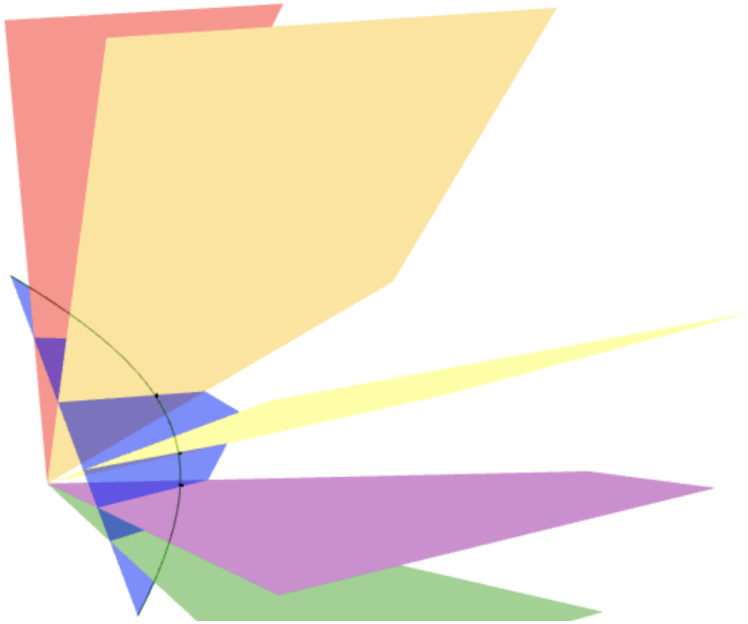

Log-normal spaces

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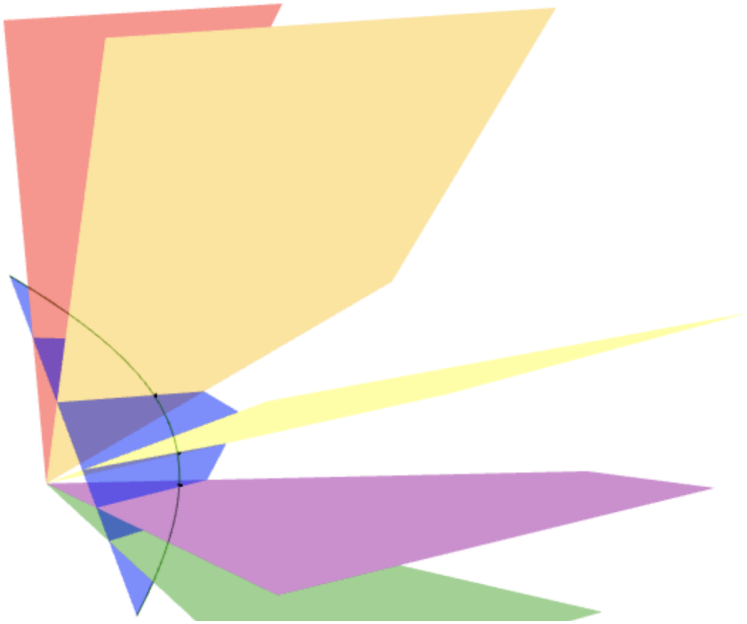
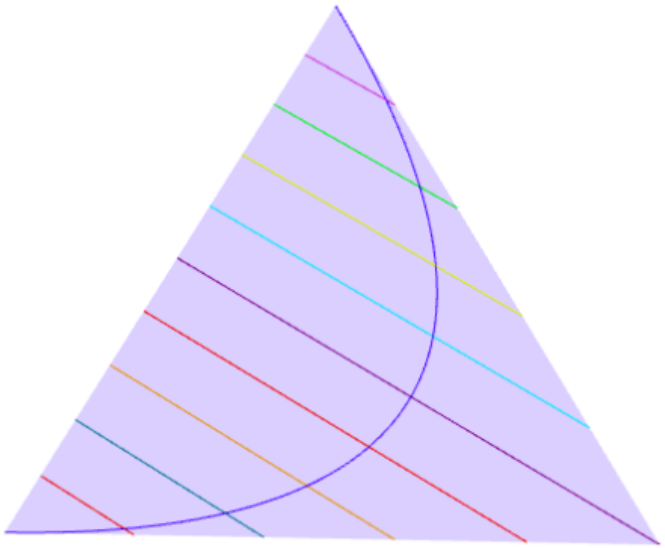


Log-normal spaces

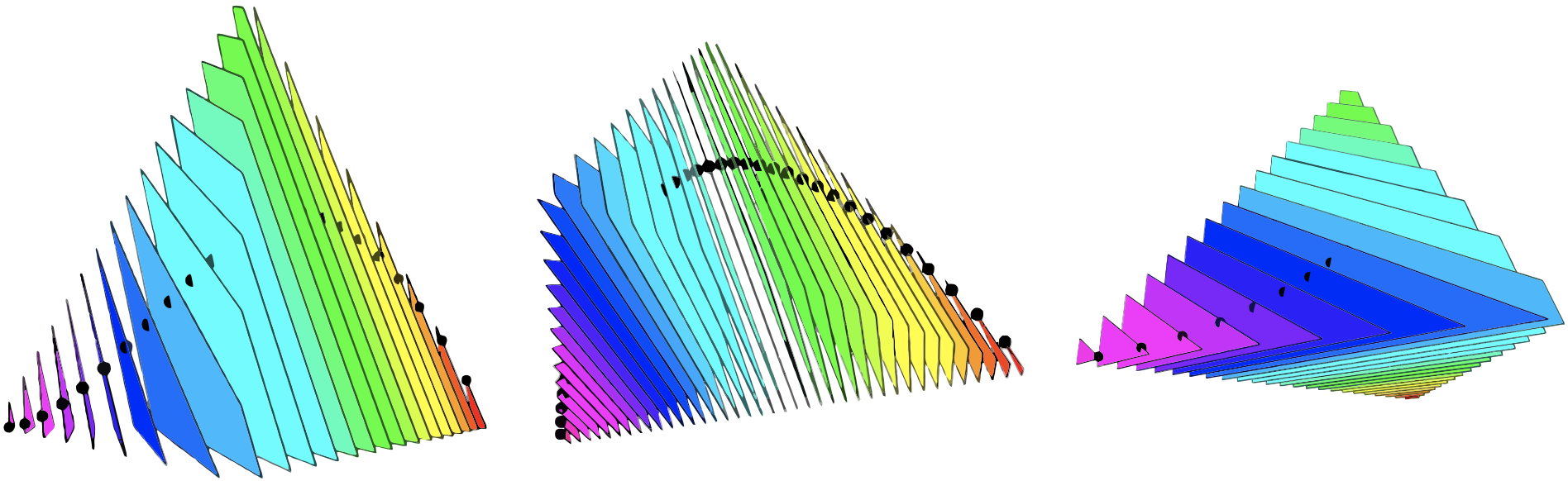


Logarithmic Voronoi polytopes

The twisted cubic curve

$\mathcal{M}$ is parametrized by

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



Linear models

Definition

A *discrete linear model* is an algebraic statistical model given parametrically by linear polynomials inside the probability simplex. It is a polytope!

Let $\mathcal{M}$ be a d-dimensional linear model given as the image of

$$\Theta \to \Delta_{n-1} : \theta \mapsto (f_1(\theta), \ldots, f_n(\theta))$$

where $\sum f_i(\theta) = 1$ and $f_i(\theta) > 0$. Every such model can be re-written as

$$\mathcal{M} = \{c - Bx : x \in \Theta\}$$

where B is a $n \times d$ matrix, whose columns sum to 0, and $c \in \mathbb{R}^n$ is a vector, whose coordinates sum to 1.

Vertices of logarithmic Voronoi polytopes

A *co-circuit* of B is a vector $v \in \mathbb{R}^n$ of minimal support such that $vB = 0$. A co-circuit is *positive* if all its coordinates are positive. We call a point $p = (p_1, \ldots, p_n) \in \mathcal{M}$ is *interior* if $p_i > 0$ for all $i \in [n]$.

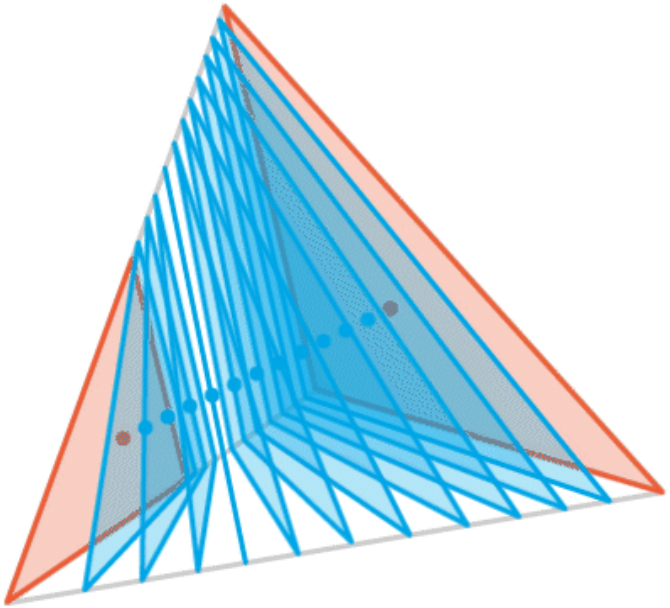
For an interior point $p \in \mathcal{M}$, the logarithmic Voronoi polytope at p is

$$\log \mathrm{Vor}_{\mathcal{M}}(p) = \left\{ r \cdot \mathrm{diag}(p) \in \mathbb{R}^n : rB = 0,\ r \geq 0,\ \sum_{i=1}^{n} r_i p_i = 1 \right\}.$$

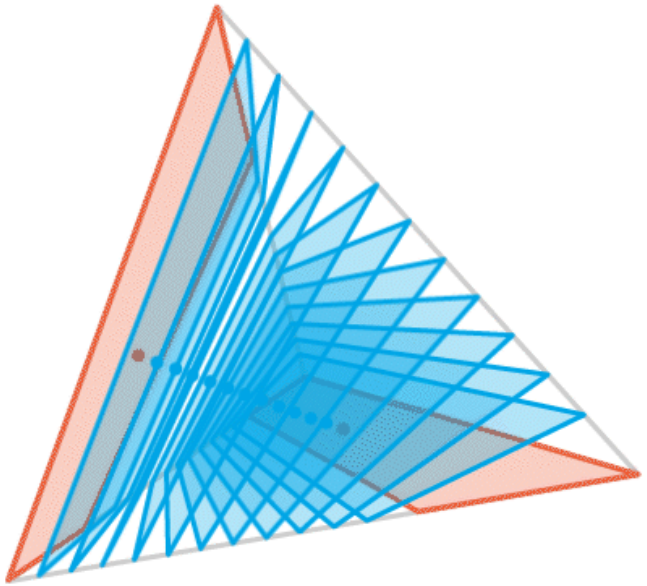
Proposition (A.)

For any interior point $p \in \mathcal{M}$, the vertices of $\log \mathrm{Vor}_{\mathcal{M}}(p)$ are of the form $v \cdot \mathrm{diag}(p)$ where v are unique representatives of the positive co-circuits of B such that $\sum_{i=1}^{n} v_i p_i = 1$.

Examples: $d = 1$



$B = [1, -5, 3, 1]^T$
$c = (1/4, 1/4, 1/4, 1/4)$



$B = [-2, -1, 1, 2]^T$
$c = (1/4, 1/4, 1/4, 1/4)$

Theorem (A.)

Every $(n-d-1)$-dimensional polytope with at most n facets appears as a logarithmic Voronoi cell of a d-dimensional linear model inside Δ_{n-1}.

Combinatorial type doesn't change

Theorem (A.)

Logarithmic Voronoi cells of all interior points in a linear model have the same combinatorial type.

So, it suffices to compute the combinatorial type for **any** interior point on a linear model.

Example

Consider the linear model $\mathcal{M}$ given as the image of the map

$$(x, y) \mapsto 1/4 \cdot (3x,\ y,\ y - x,\ 2 - 2x,\ 2 - 2y)\,.$$

What are the vertices of $\mathcal{M}$?

```
#get vertices of the model:
vars=var('x,y')
def model(x,y):
    return vector((3/4*x, 1/4*y, 1/4*(y-x), 1/2*(1-x), 1/2*(1-y)))

m=model(x,y)
P=Polyhedron(ieqs=[(0,QQ(m[i].coefficient(x)),QQ(m[i].coefficient(y))) for i in range(3)]
                 +[(1/2,QQ(m[i].coefficient(x)),QQ(m[i].coefficient(y))) for i in range(3,5)])

P.vertices_list()
P.f_vector()
```

```
[[0, 0], [1, 1], [0, 1]]
(1, 3, 3, 1)
```

```
for vert in P.vertices_list():
    model(x,y).subs({x:vert[0],y:vert[1]})
```

```
(0, 0, 0, 1/2, 1/2)
(3/4, 1/4, 0, 0, 0)
(0, 1/4, 1/4, 1/2, 0)
```

Example

Logarithmic Voronoi polytopes are triangles!

```
#get the vertices of a logarithmic Voronoi cell
vars=var('u1,u2,u3,u4,u5')
ll(x,y) = u1*log(m[0])+u2*log(m[1])+u3*log(m[2])+u4*log(m[3])+u5*log(m[4])
grad=vector((ll(x,y).derivative(x), ll(x,y).derivative(y)))

a=1/5; b=1/2
ev=grad.subs(x=a, y=b)

Q=Polyhedron(ieqs=[(0,1,0,0,0,0), (0,0,1,0,0,0), (0,0,0,1,0,0),(0,0,0,0,1,0),(0,0,0,0,0,1)],
             eqns=[(0,ev[i].coefficient(u1),ev[i].coefficient(u2),ev[i].coefficient(u3),
                      ev[i].coefficient(u4),ev[i].coefficient(u5)) for i in range(2)]
                  +[(-1,1,1,1,1,1)], backend='normaliz');
```

```
Q=Q.change_ring(QQ)
Q.vertices_list()
Q.f_vector()
```

```
[[0, 1/2, 0, 0, 1/2], [1/5, 0, 0, 4/5, 0], [1/5, 0, 3/10, 0, 1/2]]
(1, 3, 3, 1)
```

Big example

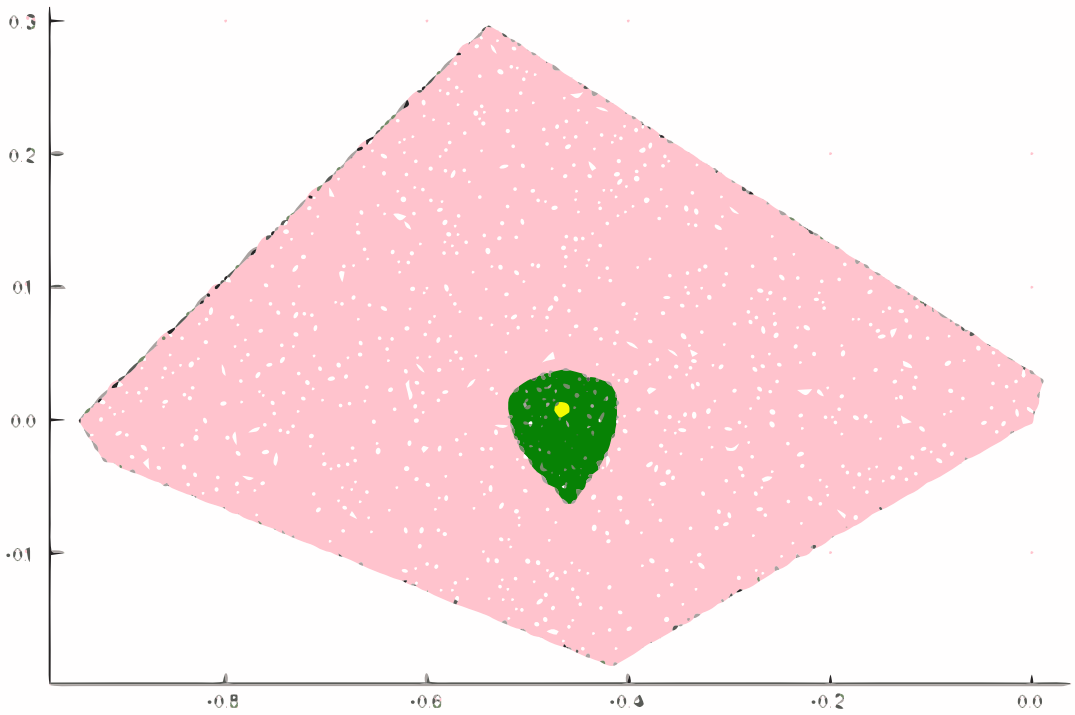
- $\mathcal{M}$ is a 3-dimensional model inside the 5-dimensional simplex given by:

$$
\begin{aligned}
f_1 &= x_0 + x_1 + x_2 + x_3 + x_4 + x_5 - 1 \\
f_2 &= 20x_0x_2x_4 - 10x_0x_3^2 - 8x_1^2x_4 + 4x_1x_2x_3 - x_2^3 \\
f_3 &= 100x_0x_2x_5 - 20x_0x_3x_4 - 40x_1^2x_5 + 4x_1x_2x_4 + 2x_1x_3^2 - x_2^2x_3 \\
f_4 &= 100x_0x_3x_5 - 40x_0x_4^2 - 20x_1x_2x_5 + 4x_1x_3x_4 + 2x_2^2x_4 - x_2x_3^2 \\
f_5 &= 20x_1x_3x_5 - 8x_1x_4^2 - 10x_2^2x_5 + 4x_2x_3x_4 - x_3^3
\end{aligned}
$$

- 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.

Non-polytopal cells

- 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.



Thanks!