Logarithmic Voronoi cells for Gaussian models

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Gaussian models

Let X be an m-dimensional random vector, which has the density function

$$p_{\mu,\Sigma}(x) = \frac{1}{(2\pi)^{m/2}(\det \Sigma)^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right\}, \quad x \in \mathbb{R}^m$$

with respect to the parameters $\mu \in \mathbb{R}^m$ and $\Sigma \in \mathrm{PD}_m$.

Such X is distributed according to the *multivariate normal distribution*, also called the *Gaussian distribution* $\mathcal{N}(\mu, \Sigma)$.

For $\Theta \subseteq \mathbb{R}^m \times \mathrm{PD}_m$, the statistical model

$$\mathcal{P}_\Theta = \{\mathcal{N}(\mu,\Sigma) : \theta = (\mu,\Sigma) \in \Theta\}$$

is called a *Gaussian model*. We identify the Gaussian model $\mathcal{P}_\Theta$ with its parameter space Θ.

Gaussian models

For a sampled data consisting of n vectors $X^{(1)}, \cdots, X^{(n)} \in \mathbb{R}^m$, we define the *sample mean* and *sample covariance* as

$$\bar{X} = \frac{1}{n}\sum_{i=1}^{n} X^{(i)} \qquad \text{and} \qquad S = \frac{1}{n}\sum_{i=1}^{n}(X^{(i)} - \bar{X})(X^{(i)} - \bar{X})^T,$$

respectively. The *log-likelihood function* is defined as

$$\ell_n(\mu, \Sigma) = -\frac{n}{2}\log\det\Sigma - \frac{1}{2}\operatorname{tr}\left(S\Sigma^{-1}\right) - \frac{n}{2}(\bar{X} - \mu)^T\Sigma^{-1}(\bar{X} - \mu).$$

In practice, we will only consider models given by parameter spaces of the form $\Theta = \mathbb{R}^m \times \Theta_2$ where $\Theta_2 \subseteq \mathrm{PD}_m$. **Thus, a Gaussian model is a subset of** PD_m. The log-likelihood function is then

$$\ell_n(\Sigma, S) = -\frac{n}{2}\log\det\Sigma - \frac{n}{2}\operatorname{tr}(S\Sigma^{-1}).$$

Algebraic models

All Gaussian models discussed in this talk are **algebraic**. In other words,

$$\Theta = \mathcal{V} \cap \mathrm{PD}_m,$$

where $\mathcal{V} \subseteq \mathbb{C}^m$ is a variety given by polynomials in the entries of $\Sigma = (\sigma_{ij})$.

Natural questions

Fix a Gaussian model $\Theta \subseteq \mathrm{PD}_m$.

1. The maximum likelihood estimation problem (MLE):

Given a sample covariance matrix $S \in \mathrm{PD}_m$, which matrix $\Sigma \in \Theta$ did it most likely come from? In other words, we wish to maximize $\ell_n(\Sigma, S)$ over all points $\Sigma \in \Theta$.

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2. Computing logarithmic Voronoi cells:

> Given a matrix $\Sigma \in \Theta$, what is the set of all $S \in \mathrm{PD}_m$ that have Σ as a global maximum when optimizing the function $\ell_n(\Sigma, S)$ over Θ?

The set of all such matrices $S \in \mathrm{PD}_m$ is the *logarithmic Voronoi cell* at Σ.

Logarithmic Voronoi cells

Proposition (A., Heaton & A., Hoșten)

Logarithmic Voronoi cells are covex sets.

The *maximum likelihood degree* (ML degree) of Θ is the number of complex critical points in $\mathrm{Sym}_m(\mathbb{C})$ when optimizing $\ell_n(\Sigma, S)$ over Θ for a generic matrix S.

For $\Sigma \in \Theta$, the *log-normal matrix space* at Σ is the set of $S \in \mathrm{Sym}_m(\mathbb{R})$ such that Σ appears as a critical point of $\ell_n(\Sigma, S)$. The intersection of this space with PD_m is the *log-normal spectrahedron* $\mathcal{K}_\Theta\Sigma$ at Σ.

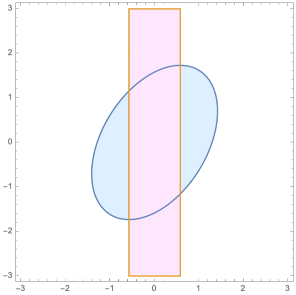
The logarithmic Voronoi cell at Σ is always contained in the log-normal spectrahedron at Σ.

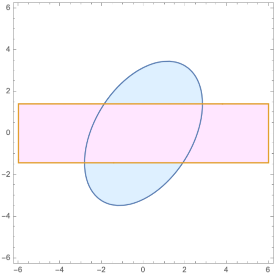
Example

Consider the model Θ given parametrically as

$$\Theta = \{\Sigma = (\sigma_{ij}) \in \mathrm{PD}_3 : \sigma_{13} = 0 \text{ and } \sigma_{12}\sigma_{23} - \sigma_{22}\sigma_{13} = 0\}.$$

This model is the union of two linear four-dimensional planes. It has ML degree 2. The log-normal spectrahedron of each point $\Sigma \in \Theta$ is an ellipse. Each log-Voronoi cell is given as:





Spectrahedral cells

When are logarithmic Voronoi cells equal to the log-normal spectrahedra?

Theorem (A., Hoșten)

If Θ is a linear concentration model or a model of ML degree one, the logarithmic Voronoi cell at any $\Sigma \in \Theta$ equals the log-normal spectrahedron at Σ. In particular, this includes both undirected and directed graphical models.

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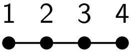
Let $G = (V, E)$ be a simple undirected graph with $|V(G)| = m$. A *concentration model* of G is the model

$$\Theta = \{\Sigma \in \mathrm{PD}_m : (\Sigma)^{-1}_{ij} = 0 \text{ if } ij \notin E(G) \text{ and } i \neq j\}.$$

The logarithmic Voronoi cell at Σ is:

$$\log \mathrm{Vor}_{\Theta}(\Sigma) = \{S \in \mathrm{PD}_m : \Sigma_{ij} = S_{ij} \text{ for all } ij \in E(G) \text{ and } i = j\}.$$

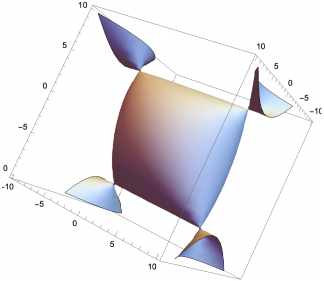
Example

The concentration model of 

is defined by

$$\Theta = \{\Sigma = (\sigma_{ij}) \in \mathrm{PD}_4 : (\Sigma^{-1})_{13} = (\Sigma^{-1})_{14} = (\Sigma^{-1})_{24} = 0\}.$$

Let $\Sigma = \begin{pmatrix} 6 & 1 & \frac{1}{7} & \frac{1}{28} \\ 1 & 7 & 1 & \frac{1}{4} \\ \frac{1}{7} & 1 & 8 & 2 \\ \frac{1}{28} & \frac{1}{4} & 2 & 9 \end{pmatrix}$.



Then $\log \mathrm{Vor}_\Theta(\Sigma) = \left\{ (x, y, z) : \begin{pmatrix} 6 & 1 & x & y \\ 1 & 7 & 1 & z \\ x & 1 & 8 & 2 \\ y & z & 2 & 9 \end{pmatrix} \succ 0 \right\}.$

Covariance models and the bivariate correlation model

Let $A \in \mathrm{PD}_m$ and let $\mathcal{L}$ be a linear subspace of $\mathrm{Sym}_m(\mathbb{R})$. Then $A + \mathcal{L}$ is an affine subspace of $\mathrm{Sym}(\mathbb{R}^m)$. Models defined by $\Theta = (A + \mathcal{L}) \cap \mathrm{PD}_m$ are called *covariance models*.

The *bivariate correlation model* is the covariance model

$$\Theta = \left\{ \Sigma_x = \begin{pmatrix} 1 & x \\ x & 1 \end{pmatrix} : x \in (-1, 1) \right\}.$$

This model has ML degree 3. For a general matrix $S = (S_{ij}) \in \mathrm{PD}_2$, the critical points are given by the roots of the polynomial

$$f(x) = x^3 - bx^2 - x(1 - 2a) - b,$$

where $b = S_{12}$ and $a = (S_{11} + S_{22})/2$ [Améndola and Zwiernik].

The bivariate correlation model

Fix $c \in (-1, 1)$ so $\Sigma_c \in \Theta$. The log-normal spectrahedron of Σ_c is

$$\begin{aligned}\mathcal{K}_\Theta(\Sigma_c) &= \{S \in \mathrm{PD}_2 : f(c) = 0\} \\ &= \{S \in \mathrm{PD}_2 : a = (bc^2 - c^3 + b + c)/2c\} \\ &= \left\{ S_{b,k} = \begin{pmatrix} k & b \\ b & 2a - k \end{pmatrix} \succ 0 : \substack{0 \le k \le 2a, \\ a = (bc^2 - c^3 + b + c)/2c} \right\}.\end{aligned}$$

Theorem (A., Hoșten)

Let Θ be the bivariate correlation model and let $\Sigma_c \in \Theta$. If $c > 0$, then

$$\log \mathrm{Vor}_\Theta(\Sigma_c) = \{S_{b,k} \in \mathcal{K}_\Theta(\Sigma_c) : b \ge 0\}.$$

If $c < 0$, then

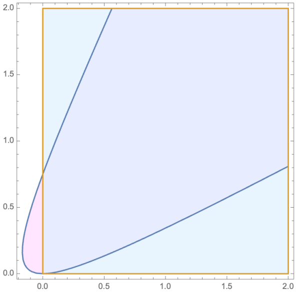
$$\log \mathrm{Vor}_\Theta(\Sigma_c) = \{S_{b,k} \in \mathcal{K}_\Theta(\Sigma_c) : b \le 0\}.$$

The bivariate correlation model

Important things to note:

- The log-Voronoi cell of Σ_c is strictly contained in the log-normal spectrahedron of Σ_c.
- Logarithmic Voronoi cells of Θ are semi-algebraic sets! **This is extremely surprising!**

The logarithmic Voronoi cell and the log-normal spectrahedron at $c = 1/2$:



The boundary: transcendental?

Given a Gaussian model Θ and $\Sigma \in \Theta$, the matrix $S \in \mathrm{PD}_m$ is on the *boundary* of $\log \mathrm{Vor}_\Theta(\Sigma)$ if $S \in \log \mathrm{Vor}_\Theta(\Sigma)$ and there is some $\Sigma' \in \Theta$ such that $\ell(\Sigma, S) = \ell(\Sigma', S)$.

The bivariate correlation models fit into a larger class of models known as *unrestricted correlation models*

$$\Theta = \{\Sigma \in \mathrm{Sym}(\mathbb{R}^m) : \Sigma_{ii} = 1,\ i \in [m]\} \cap \mathrm{PD}_m\,.$$

When $m = 3$, the model is the elliptope. Its ML degree is 15.

Theorem (A., Hoșten)

The boundaries of logarithmic Voronoi cells for general points on the elliptope cannot be described by polynomials over $\overline{\mathbb{Q}}$.

Conjecture

The logarithmic Voronoi cells for general points on the elliptope are not semi-algebraic.

Thanks!