

# 1. Introduction

## Basic notions

Statistics: probability density

Algebra: ring, field.

## Outline

Discrete and Gaussian statistical models

Maximum likelihood estimation

Algebraic geometry basics

Algebraic models

## Statistical models

**Definition.** Let  $\Omega$  be a measurable space ('sample space'),  $\text{Prob}(\Omega)$  the set of all probability densities on  $\Omega$ . A *statistical model* is a subset  $\mathcal{M} \subseteq \text{Prob} \Omega$ . A *parametric* statistical model is a statistical model  $\mathcal{M}$  together with a set  $\Theta \subseteq \mathbb{R}^d$  and a surjection  $\Theta \rightarrow \mathcal{M}$ .

**Maximum likelihood estimation problem:** given  $e = (e_1, \dots, e_N) \in \Omega^N$  independent and identically distributed (i.i.d.) samples, find  $x \in \mathcal{M}$  such that its density  $f_x \in \text{Prob} \Omega$  maximises (since i.i.d.)

$$f_x^N(e) = \prod_{i=1}^n f_x(e_i)$$

This is equivalent to the problem ( $\star$ )

$$\max_{x \in \mathcal{M}} \sum_{i=1}^n \log f_x(e_i)$$

### Example 1

$\Omega = (0, 1, 2, 3)$

$\Delta_3 = \{(p_0, p_1, p_2, p_3) \in \mathbb{R}^4 \mid p_j \geq 0 \text{ for all } j, \sum_j p_j = 1\}$

*Independence model* (see Fig. 1):

$\Theta = \{(\theta, \eta) \in (0, 1) \times (0, 1)\}$

$p : \Theta \rightarrow \Delta_3, (\theta, \eta) \mapsto (\theta\eta, (1-\theta)\eta, (1-\theta)\eta, (1-\theta)(1-\eta))$

$\mathcal{M} = \text{im } p = \{p \in \Delta_3 \mid p_0 p_3 - p_1 p_2 = 0\}$ .

If  $e = (0, 0, 1, 3, 3)$  then

$$(\star) \Leftrightarrow \max_{p \in \mathcal{M}} 2 \log p_0 + \log p_1 + 2 \log p_3.$$

Data vector:  $e \rightarrow u = (2, 1, 0, 2) \in \mathbb{N}^4$ .

**Definition.** A discrete statistical model on  $n + 1$  outcomes is a subset  $\mathcal{M} \subseteq \Delta_n$ , where

$$\Delta_n = \{p \in \mathbb{R}^{n+1} \mid p_j \geq 0 \text{ for all } j, \sum_j p_j = 1\}.$$

A data vector is  $u \in \mathbb{N}^{n+1}$ .

An empirical distribution is  $q = u/|u|$  where  $|u| = \sum_j u_j$  or just any  $q \in \Delta_n$ .

The log-likelihood function given  $q \in \Delta_n$  is

$$\ell : \mathcal{M} \times \Delta_n \rightarrow \mathbb{R}, \quad \ell(p, q) = \sum_{j=0}^n q_j \log p_j$$

The ML estimation problem given  $q$  is

$$\max_{p \in \mathcal{M}} \sum_{j=0}^n q_j \log p_j.$$

## Example 2

Let  $\Omega = \mathbb{R}^n$ . The Gaussian probability densities on  $\Omega$  with mean zero correspond 1:1 with the positive definite  $n \times n$  symmetric matrices. These are interpreted either as covariance matrices  $\Sigma$  or concentration matrices  $K = \Sigma^{-1}$ .

$$\Sigma = \begin{pmatrix} \text{Var}(X) & \text{Cov}(X, Y) & \text{Cov}(X, Z) \\ \dots & \text{Var}(Y) & \text{Cov}(Y, Z) \\ \dots & \dots & \text{Var}(Z) \end{pmatrix}$$

$\Sigma$  covariance matrix  $\rightsquigarrow$

$$f_{\Sigma}(x) = (2\pi)^{-n/2} \det(\Sigma)^{-1/2} \exp\left(-\frac{1}{2} x^T \Sigma^{-1} x\right).$$

$n = 3 \rightsquigarrow$  Gaussian random variables  $X, Y, Z$ .

$$\text{PD}_3 = \{M \in \text{Sym}_2(n \times n, \mathbb{R})\}$$

$$X \perp\!\!\!\perp Y \Leftrightarrow \text{Cov}(X, Y) = 0 \quad (\text{since Gaussian})$$

$$\text{Independence covariance model: } \mathcal{M} = \{\Sigma = (\sigma_{ij}) \in \text{PD}_3 \mid \sigma_{12} = 0\}$$

Independence concentration model:

$$\mathcal{M} = \{K \in \text{PD}_3 \mid K^{-1} \in \mathcal{M}\} = \{K = (k_{ij}) \in \text{PD}_3 \mid k_{12}k_{23} - k_{13}k_{33} = 0\}.$$

If  $e = (e_1, e_2, e_3) \in (\mathbb{R}^3)^3$ , then by [Sullivant] Prop. 5.3.7:

$$(\star) \Leftrightarrow \max_{\Sigma \in \mathcal{M}} -\log \det(\Sigma) - \text{tr}(S\Sigma^{-1}),$$

with  $S = (1/3) \sum_{j=1}^3 e_j e_j^T$  ("sample covariance").

**Definition.** A Gaussian statistical model on  $n$  random variables is a subset  $\mathcal{M} \subseteq \text{PD}_n$ , where

$$\text{PD}_n = \{\Sigma \in \text{Mat}(n \times n, \mathbb{R}) \mid \Sigma \text{ symmetric pos. def.}\}$$

A data vector is  $e \in (\mathbb{R}^n)^N$ .

An empirical distribution is  $S = (1/n) \sum_{j=1}^n e_j e_j^T$  or just any  $S \in \text{PD}_n$ .

The negated log-likelihood function is

$$\ell : \mathcal{M} \times \text{PD}_n \rightarrow \mathbb{R}$$

given by

$$\ell_{\text{cov}}(\Sigma, S) = \log \det(\Sigma) + \text{tr}(S\Sigma^{-1}) \quad (\text{covariance version})$$

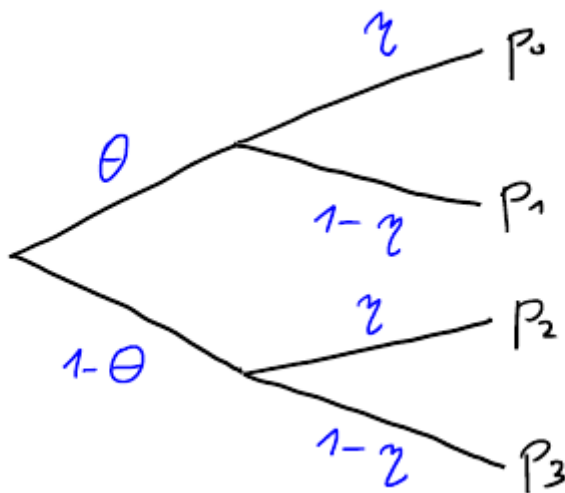
$$\ell_{\text{con}}(K, S) = \log \det(K) - \text{tr}(SK) \quad (\text{concentration version}).$$

The ML estimation problem given  $S$  is then

$$\min_{x \in \mathcal{M}_{\text{cov}}} \ell_{\text{cov}}(\Sigma, S) \quad (\text{covariance version})$$

$$\max_{x \in \mathcal{M}_{\text{con}}} \ell_{\text{con}}(\Sigma, S) \quad (\text{concentration version}).$$

**Fig. 1**



## Algebraic geometry basics

### Definitions.

$K$  a field  $\rightsquigarrow$

$K[x_1, \dots, x_n] = \{\text{polynomials in the variables } x_1, \dots, x_n \text{ with coefficients in } K\}$  *polynomial*

$K^n = \{(x_1, \dots, x_n) \mid x_i \in K\}$  *affine space*

$K(x_1, \dots, x_n) = \{f/g \mid f, g \in K[x_1, \dots, x_n], g \neq 0\}$  *field of rational functions*

$f_1, \dots, f_k$  polynomials  $\rightsquigarrow$

$I = \langle f_1, \dots, f_k \rangle = \left\{ \sum_{j=1}^k g_j f_j \mid g_j \in K[x_1, \dots, x_n] \right\}$  the *ideal* generated by  $f_1, \dots, f_k$

$V(I) = \{x \in K^n \mid f_1(x) = \dots = f_k(x) = 0\} = \{x \mid g(x) = 0 \text{ for all } g \in I\}$  the *algebraic variety*

An *ideal*: any such  $I = \langle f_1, \dots, f_k \rangle$ .

A *variety*: any such  $V = V(I)$ .

$S \subseteq K^n$  a subset  $\rightsquigarrow$

$$\bar{S} = \bigcap_{V \supseteq S \text{ variety}} V \quad \text{the closure of } S$$

$I(S) = \{f \in K[x_1, \dots, x_n] \mid f(x) = 0 \text{ for all } x \in S\}$  the *ideal of } S*

$I \subseteq K[x_1, \dots, x_n]$  an ideal  $\rightsquigarrow$

$\sqrt{I}$  or  $\text{rad}(I) = \{g \in K[x_1, \dots, x_n] \mid \exists k \in \mathbb{N} : g^k \in I\}$  the *radical of } I*

**Hilbert's Nullstellensatz:** if  $K = \mathbb{C}$  then for all ideals  $I$  and sets  $S \subseteq K^n$ :

$$I(V(I)) = \text{rad}(I),$$

$$V(I(S)) = \bar{S}.$$

### Examples.

1. Let  $I = \langle x^2 \rangle \subseteq K[x]$ . Then  $\text{rad}(I) = \langle x \rangle$  and  $V(I) = V(\langle x \rangle) = \{0\}$ .
2. From the Nullstellensatz it follows that  $V(I_1) = V(I_2) \Leftrightarrow \text{rad}(I_1) = \text{rad}(I_2)$ .
3. The Nullstellensatz does not work over  $\mathbb{R}$ : take  $I_1 = \langle x^2 + 1 \rangle \subset \mathbb{R}[x]$ . Then  $V(I_1) = \emptyset = V(\mathbb{R}[x])$  but  $\text{rad}(I_1) \neq \mathbb{R}[x]$ .

**Definition.** Let  $K = \mathbb{R}$  and  $f_1, \dots, f_k, g_1, \dots, g_\ell \in \mathbb{R}[x_1, \dots, x_n]$ . Then

$$\text{semialg}(f_1, \dots, f_k \mid g_1, \dots, g_\ell) = \{x \in \mathbb{R}^n \mid f_i(x) = 0, g_j(x) > 0 \text{ for all } i, j\}$$

is the *semialgebraic set* defined by the  $f_i, g_j$ .

A *semialgebraic set*: any such  $\mathcal{M} = \text{semialg}(f_i \mid g_j)$ .

Its *complexification* is  $\mathcal{M}_{\mathbb{C}} = V(f_1^{\mathbb{C}}, \dots, f_k^{\mathbb{C}}) \subseteq \mathbb{C}^n$ , where  $f_i^{\mathbb{C}}$  is the image of  $f_i$  in  $\mathbb{C}[x_1, \dots, x_n]$ .

## Algebraic models

**Definition.** An *algebraic model*  $\mathcal{M} \subseteq \mathcal{N}$  is a semialgebraic subset  $\mathcal{M}$  of a semialgebraic set  $\mathcal{N}$  of probability densities on some space  $\Omega$ .

$\mathcal{N}$  is the space of *empirical distributions*.

Its *complexification* is  $\mathcal{M}_{\mathbb{C}} \subseteq \mathcal{N}_{\mathbb{C}}$

**Examples:** [Example 1](#), [Example 2](#).

