Maximum likelihood estimators for discrete exponential families and random graphs

Tomasz Skalski

Wrocław University of Science and Technology

Université d'Angers

(joint research with K. Bogdan and M. Bosy)

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Discrete exponential families – Notation

- $\mathcal{X} = \{x_1, \ldots, x_K\}$ – finite state space, $K = |\mathcal{X}|$
- $\mu : \mathcal{X} \to (0, \infty)$ – weight function
- $\mathcal{B} \subset \mathbb{R}^{\mathcal{X}}$ – linear space of functions ($\phi = \mathbb{1} \in \mathcal{B}$)
- $\mathcal{B}_+ = \{\phi \in \mathcal{B} : \phi \geq 0\}$ – subclass (cone) of non-negative functions
- $Z(\phi) = \sum_{x \in \mathcal{X}} e^{\phi(x)} \mu(x)$ – normalising constant (partition function)
- $p = e(\phi) = \frac{e^{\phi}}{Z(\phi)}$ – exponential density
- $e(\mathcal{B}) = \{p = e(\phi) : \phi \in \mathcal{B}\}$ – exponential family

MLE

Definition

Let $x_1, \ldots, x_n$ *be a sample from the finite set* $\mathcal{X}$ *and let* $\phi \in \mathcal{B}$. *The likelihood function of* $p = e(\phi)$ *is defined as:*

$$L_p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i).$$

log-likelihood function: $\ell_p(x_1, \ldots, x_n) = \log L_p(x_1, \ldots, x_n)$.

Definition

The $\hat{p} \in e(\mathcal{B})$ *is called the maximum likelihood estimator (MLE), if*

$$L_{\hat{p}}(x_1, \ldots, x_n) = \sup_{p \in e(\mathcal{B})} L_p(x_1, \ldots, x_n).$$

Existence of MLE

History

- *O. Barndorff-Nielsen (1978) – criterion of existence of MLE for the exponential families in terms of convex geometry*
- *S. J. Haberman (1974) – criterion of existence of MLE in hierarchical log-linear models*
- *K. Bogdan, M. Bogdan (2000) – criterion of existence of for exponential families of continuous functions on* $[0, 1]$ *in terms of sets of uniqueness.*
- *N. Eriksson, S. E. Fienberg, A. Rinaldo, S. Sullivant (2006) – interpretation of the criterion in terms of polyhedral geometry*
- *A. Rinaldo, S. E. Fienberg, Y. Zhou (2009) – application to exponential models of random graphs (ERGM).*
- *K. Bogdan, M. Bosy, TS (2019+, this talk) – criterion of existence of MLE in discrete exponential families in terms of sets of uniqueness.*

Existence of MLE

Maximization of likelihood is fundamental in estimation, model selection and testing. In many procedures it is important to know if MLE actually exists for given data $x_1 \ldots, x_n$ and the linear space of exponents.

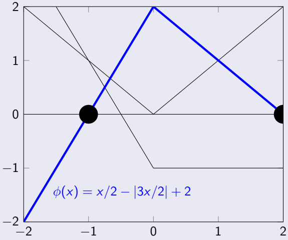
Sets of uniqueness

Definition

We say that $U \subset \mathcal{X}$ *is a set of uniqueness for* $\mathcal{B}$*, if* $\phi \equiv 0$ *is the only function in* $\mathcal{B}$ *such that* $\phi(U) = 0$*.*

Example

Let $\mathcal{X} = \{-2, -1, 0, 1, 2\}$*. Let* $\mathcal{B}$ *denote the class of all the real functions on* $\mathcal{X}$ *that are linear (affine) both on* $\{-2, -1, 0\}$ *and on* $\{0, 1, 2\}$*.*



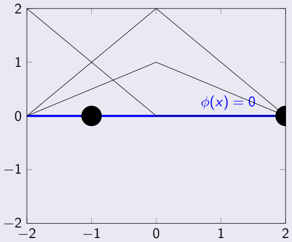
Then the set $\{-1, 1, 2\}$ *is of uniqueness for* $\mathcal{B}$*, but the set* $\{-1, 2\}$ *is not.*

Definition

U is a set of uniqueness for $\mathcal{B}_+$, if $[\phi \in \mathcal{B}_+,\ \phi(U) = 0\,] \Rightarrow [\,\phi \equiv 0\,]$.

Example

Again, let $\mathcal{X} = \{-2, -1, 0, 1, 2\}$ and let $\mathcal{B}$ be the class of all the real functions on $\mathcal{X}$ that are linear (affine) on $\{-2, -1, 0\}$ and on $\{0, 1, 2\}$.



Then the set $\{-1, 2\}$ is of uniqueness for $\mathcal{B}_+$.

Existence of MLE – main criterion

Theorem (K. Bogdan, M. Bosy, TS (2019+))

The maximum likelihood estimator for $e(\mathcal{B})$ and $x_1, \ldots, x_n \in \mathcal{X}$ exists if and only if $\{x_1, \ldots, x_n\}$ is a set of uniqueness for $\mathcal{B}_+$.

Proof.

($\Rightarrow$) If $\{x_1, \ldots, x_n\}$ is not of uniqueness for $\mathcal{B}_+$, we may subtract from every candidate for MLE ϕ a non-negative function ψ vanishing on $\{x_1, \ldots, x_n\}$, so $\psi - \phi = \psi$ on $\{x_1, \ldots, x_n\}$. Thus $Z(\psi - \phi) < Z(\psi)$ and the resulting likelihood is increased. □

Existence of MLE – main criterion

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Proof.

($\Leftarrow$) We introduce a special seminorm related to given set of uniqueness on $\mathcal{B}$ and compare it with an oscillation seminorm. □

Applications

There are two types of application we propose:

- Conditions for the existence of MLE for specific exponential families
- Probability bounds for MLE for i.i.d. samples

For the i.i.d. random variables $X_1, X_2, \ldots$ valued in $\mathcal{X}$ it will be useful to define the following (random) time:

$$\nu_{uniq} = \inf\{n \geq 1 : \{X_1, \ldots, X_n\} \text{ is a set of uniqueness for } \mathcal{B}_+\}$$

Threshold functions

Definition (Threshold)

A function $n^* = n^*(K)$ *is a threshold of the size of the sample* $\mathbb{X} = (X_1, \ldots, X_n)$ *for a given (monotone) property* $\mathscr{P}$ *if*

$$\lim_{K\to\infty} \mathbb{P}(\mathbb{X} \in \mathscr{P}) = \begin{cases} 0 & \text{if } n(K)/n^*(K) \to 0, \qquad K \to \infty, \\ 1 & \text{if } n(K)/n^*(K) \to \infty, \qquad K \to \infty. \end{cases}$$

Definition (Sharp threshold)

A function $n^* = n^*(K)$ *is a sharp threshold of the size of the sample* $\mathbb{X} = (X_1, \ldots, X_n)$ *for a given (monotone) property* $\mathscr{P}$ *if for every* $\varepsilon > 0$

$$\lim_{K\to\infty} \mathbb{P}(\mathbb{X} \in \mathscr{P}) = \begin{cases} 0 & \text{if } n(K)/n^*(K) < 1 - \varepsilon, \\ 1 & \text{if } n(K)/n^*(K) > 1 + \varepsilon. \end{cases}$$

Threshold functions

Example

Examples of monotone properties:

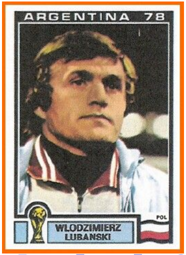
- $\mathbb{X} = (X_1, \ldots, X_n) \supset \mathcal{X}$,
- $|\{X_1, \ldots, X_n\}| \geq 3$,
- $\exists \;\; 1 \leq i, j \leq n : \quad X_i + X_j = K + 1$,
- $\ldots$

Let $\mathcal{B} = \mathbb{R}^{\mathcal{X}}$. As $\mathcal{X}$ is the only set of uniqueness for $\mathcal{B}_+$, we observe that

Lemma

MLE for $e(\mathbb{R}^{\mathcal{X}})$ and $x_1, \ldots, x_n$ exists if and only if $\{x_1, \ldots, x_n\} = \mathcal{X}$.

Then the existence of MLE for $\{x_1, \ldots, x_n\}$ is a reformulation of the Coupon Collector Problem.



Applications – $\mathbb{R}^{\mathcal{X}}$

Corollary

Let $\mathcal{B} = \mathbb{R}^{\mathcal{X}}$ *and* $K = |\mathcal{X}|$. *Let* $X_1, X_2, \ldots$ *be independent random variables, each with uniform distribution on* $\mathcal{X}$. *Then, for every* $c \in \mathbb{R}$,

$$\lim_{K \to \infty} (\nu_{uniq} < K \log K + Kc) = e^{-e^{-c}}.$$

In particular, $n^*(K) = K \log K$ *is a sharp threshold of the sample size for the existence of MLE for* $e(\mathcal{X})$.

Applications – Rademacher functions

For $k \in \mathbb{N}$ consider the discrete hypercube $\mathcal{X} = Q_k = \{-1, 1\}^k$. Let $K = |\mathcal{X}| = 2^k$.
For $j = 1, \ldots, k$ we define Rademacher functions:

$$r_j(\chi) = \chi_j, \quad \chi = (\chi_1, \ldots, \chi_k) \in Q_k.$$

Denote $r_0(\chi) = 1$.

Applications – Rademacher functions

Theorem (K. Bogdan, M. Bosy, TS (2019+))

Let $\mathcal{B}^k = Lin\{r_0, r_1, \ldots, r_k\}$. MLE for $e(\mathcal{B}^k)$ and $x_1, \ldots, x_n \in Q_k$ exists if and only if for all $j = 1, \ldots, k$ we have $\{r_j(x_1), \ldots, r_j(x_n)\} = \{-1, 1\}$.

In other words, the condition above is satisfied if and only if $\{x_1, \ldots, x_n\}$ intersects with every half-cube of Q_k,
e.g. $\{x_1 = (-1, -1, \ldots, -1), x_2 = (1, 1, \ldots, 1)\}$.

Theorem (K. Bogdan, M. Bosy, TS (2019+))

Let $k \in \mathbb{N}$, $n(k) = \log_2 k + b + o(1)$. Let $X_1, \ldots, X_{n(k)}$ be independent random variables, each with uniform distribution on Q_k. Then

$$\lim_{k\to\infty} \mathbb{P}(\{X_1, \ldots, X_{n(k)}\} \textit{ is a set of uniqueness for } \mathcal{B}_+) = \\ = \exp\{-2^{1-b}\}.$$

and $n^*(K) = \log_2 k = \log_2 \log_2 K$ is a sharp threshold of the sample size for the existence of MLE for $e(\mathcal{B}^k)$ and i.i.d. uniform samples on Q_k.

We consider simple undirected graphs containing no loops or multiple edges. Let N and m denote the number of vertices and edges of the graph. Let $\mathcal{G}_N$ denote the family of all the graphs with N vertices.
For graphs $G = (V, E_1)$, $H = (V, E_2)$ we let, as usual,

$$G \cup H := (V, E_1 \cup E_2), \qquad G \cap H := (V, E_1 \cap E_2).$$

Also, by $G \subset H$ we mean $E_1 \subset E_2$.
We define $\chi_{r,s}(G) = 1 - 2\mathbb{1}_G(r, s)$ and consider the following linear space

$$\mathcal{B}^{\mathcal{G}_N} = \mathrm{Lin}\left\{ 1, \chi_{r,s}(G) : 1 \leq r < s \leq N \right\}.$$

Consider coefficients $c \in \mathbb{R}^{\binom{V}{2}}$, indexed by the edges of the complete graph K_N, and the following exponential family:

$$e(\mathcal{B}^{\mathcal{G}_N}) = \left\{ p_c := e^{\phi_c - \psi(\phi_c)} : c \in \mathbb{R}^{\binom{V}{2}} \right\},$$

where

$$\phi_c(G) = \sum_{(r,s)\in\binom{V}{2}} c_{r,s}\chi_{r,s}(G), \qquad \psi(\phi_c) = \log \sum_{G\in\mathcal{G}_N} e^{\phi_c(G)},$$

and $G \in \mathcal{G}_N$.

Observation

Fix $c \in \mathbb{R}^{\binom{V}{2}}$. In the random graph $\mathbb{G}$ sampled from $p_c \in e(\mathcal{B}^{\mathcal{G}_N})$, each edge (r, s) appears independently with probability

$$p_{r,s} = \frac{e^{c_{r,s}}}{1 + e^{c_{r,s}}}.$$

Applications – ERGM

Theorem (K. Bogdan, M. Bosy, TS (2019+))

MLE for $e(\mathcal{B}^{\mathcal{G}_N})$ *and* $G_1, \ldots, G_n \in \mathcal{G}_N$ *exists if and only if*

$$\bigcup_{i=1}^{n} G_i = K_N \qquad \text{and} \qquad \bigcap_{i=1}^{n} G_i = \overline{K_N}.$$

Lemma (K. Bogdan, M. Bosy, TS (2019+))

Let $\{\mathbb{G}_1, \ldots, \mathbb{G}_n\}$ *be independent random graphs from* $p_c \in e(\mathcal{B}^{\mathcal{G}_N})$*. Then the probability of the existence of MLE for* $e(\mathcal{B}^{\mathcal{G}_N})$ *equals*

$$\prod_{1 \le r < s \le N} \left(1 - p_{r,s}^n - (1 - p_{r,s})^n\right).$$

In particular, $n^*(N) = \log N$ *is a threshold of the sample size* n *for the existence of MLE for* $e(\mathcal{B}^{\mathcal{G}_N})$*.*

Let $k \in \mathbb{N}, 1 \leq q \leq k$, and $\mathcal{B}_q^k = \mathrm{Lin}\{w_S : S \subset \{1, \ldots, k\} \text{ and } |S| \leq q\}$, where $w_S(x) = \prod_{i \in S} r_i(x), x \in Q_k, S \subset \{1, \ldots, k\}$, are the Walsh functions.

Observation

$\mathcal{B}_q^k$ is the linear space spanned by indicator functions of the sub-cubes of Q_k, obtained by fixing q out of k coordinates.

- $q = 1$: Rademacher functions (already discussed)
- $q = 2$: The Ising model

$\mathcal{B}^k_{k-1}$ corresponds to indicators of edges of Q_k. Consider the following partition: $Q_k = \mathcal{E} \cup \mathcal{O}$:

Definition

- $\mathcal{E} := \{\chi \in Q_k : \chi \textit{ has even number of positive coordinates}\}$
- $\mathcal{O} := \{\chi \in Q_k : \chi \textit{ has odd number of positive coordinates}\}$

Theorem (K. Bogdan, M. Bosy, TS (2019+))

MLE exists for $e(\mathcal{B}^k_{k-1})$ *and* $x_1, \ldots, x_n \in Q_k$ *if and only if* $\mathcal{E} \subset \{x_1, \ldots, x_n\}$ *or* $\mathcal{O} \subset \{x_1, \ldots, x_n\}$.

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Tack för att ni kom idag!