Maximum likelihood estimators for discrete exponential families and random graphs

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Discrete exponential families – Notation

- $\mathcal{X} = \{x_1, \ldots, x_K\}$ – finite state space
- $\mathcal{B} \subset \mathbb{R}^{\mathcal{X}}$ – linear space of functions ($\phi \equiv \mathbb{1} \in \mathcal{B}$)
- $\mathcal{B}_+ = \{\phi \in \mathcal{B} : \phi \geq 0\}$ – subclass (cone) of non-negative functions
- $e(\phi) = exp\{\phi\}/Z(\phi)$ – exponential density
- $Z(\phi)$ – normalising constant (partition function)
- $e(\mathcal{B}) = \{p = e(\phi) : \phi \in \mathcal{B}\}$ – exponential family
- $L_p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i)$, $x_i \in \mathcal{X}$ – likelihood function

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:

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

To facilitate the calculations the log-likelihood function is being often used: $\ell_p(x_1, \ldots, x_n) = \log L_p(x_1, \ldots, x_n)$.

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 of a parameter (from the exponential family) for a given sample* $x_1, \ldots, x_n$.
  - *Beautiful, but cumbersome to apply*
- *S. J. Haberman (1974) – criterion of MLE existence in hierarchical log-linear models*
- *N. Eriksson, S. E. Fienberg, A. Rinaldo, S. Sullivant (2006) – interpreting the above criterion in terms of polyhedral geometry*
- *K. Bogdan, M. Bogdan (2000) – criterion of MLE existence for exponential families of continuous functions on* $[0,1]$.
- *A. Rinaldo, S. E. Fienberg, Y. Zhou (2009) – application of MLE existence in exponential random graph models (ERGM).*
- *K. Bogdan, M. Bosy, TS (2020+) – criterion of MLE existence in discrete exponential families.*

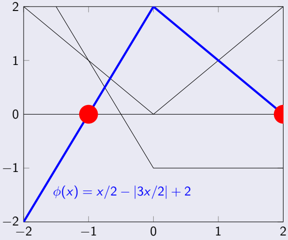
Sets of uniqueness

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) on $\{-2, -1, 0\}$ and on $\{0, 1, 2\}$.



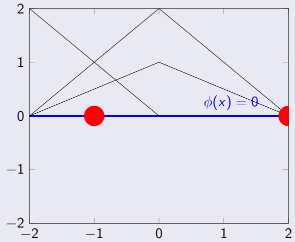
Then the set $\{-2, 2\}$ is of uniqueness for $\mathcal{B}$, but the set $\{-1, 2\}$ is not.

Remark

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

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 $\mathcal{B}_+$.

MLE existence – main criterion

Theorem (K. Bogdan, M. Bosy, TS (2020+))

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* $\mathcal{B}_+$*.*

Applications

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.
There are two types of results obtained with sets of uniqueness we propose below:

- Conditions for existence of MLE
- Probability bounds for MLE for an i.i.d. sample

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

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

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

Let $\mathcal{B} = \mathbb{R}^{\mathcal{X}}$. As $\mathcal{X}$ is the only one set of uniqueness in this setting, one may observe that

Lemma

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

Thus, the problem of obtaining the existence of MLE for $\{x_1, \ldots, x_n\}$ resembles the Coupon Collector Problem. Therefore

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

Applications – Rademacher functions

For $k \in \mathbb{N}$ consider the hypercube $\mathcal{X} = Q_k = \{-1, 1\}^k$. Let $K = |\mathcal{X}| = 2^k$.
For $j = 1, \ldots, k$ and $\chi = (\chi_1, \ldots, \chi_k) \in Q_k$ we define Rademacher functions:

$$r_j(\chi) = \chi_j,$$

and we denote $r_0(\chi) = 1$. In other words, the Rademacher functions may be seen as affine transforms of the indicators of half-cubes.

Observation

Moreover, the linear space of products of q Rademacher functions corresponds to the linear space of indicators of sub-cubes of Q_k created by fixing q of k coordinates.

Applications – Rademacher functions

Theorem (K. Bogdan, M. Bosy, TS (2020+))

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.

Theorem (K. Bogdan, M. Bosy, TS (2020+))

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 $\log_2 k = \log_2 \log_2 K$ 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.

Applications – ERGM

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

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

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

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

We also consider coefficients $c \in \mathbb{R}^{\binom{V}{2}}$ corresponding to all edges of a complete graph K_N and the following exponential family:

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

where

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

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

Observation

Fix $c \in \mathbb{R}^{\binom{V}{2}}$. Then in the random graph $\mathbb{G}$ sampled from $\mathcal{G}_{N,c}$ 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 (2020+))

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 (2020+))

Let $\{\mathbb{G}_1, \ldots, \mathbb{G}_n\}$ *be independently distributed random graphs from* $\mathcal{G}_{N,c}$*. 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, $\log N$ *is a threshold of the sample size* n *for the existence of MLE for* $e(\mathcal{B}^{\mathcal{G}_N})$.

Applications – Products of Rademacher functions

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

Recall the previously mentioned observation:

Observation

The linear space of products of q Rademacher functions corresponds to the linear space of indicators of sub-cubes of Q_k created by fixing q of k coordinates.

- $q = 1$: Rademacher functions (already considered)
- $q = 2$: connections with the Ising model

Applications – Products of $(k-1)$ Rademacher functions

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

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 (2020+))

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 $\mathcal{O} \subset \{x_1, \ldots, x_n\}$.

Dynkin system

Definition

Let $\mathcal{X}$ be a non-empty set, and let $\mathcal{D}$ be a collection of subsets of $\mathcal{X}$. $\mathcal{D}$ is called a Dynkin system if the following conditions hold:

- $\mathcal{X} \in \mathcal{D}$;
- if $A, B \in \mathcal{D}$ and $A \subset B$, then $B \setminus A \in \mathcal{D}$;
- if $A_1, A_2, A_3, \dots \in \mathcal{D}$ and $A_j \subset A_{j+1}$ for $j \in \mathbb{N}$, then $\bigcup_{j=1}^{\infty} A_j \in \mathcal{D}$.

Let $\mathcal{Y}$ be a collection of subsets of $\mathcal{X}$. The smallest Dynkin system containing $\mathcal{Y}$ is called the Dynkin system generated by $\mathcal{Y}$, denoted $\mathcal{D}(\mathcal{Y})$.

Let $1 \leq q \leq k$. Define S_q^k as set of all $(k-q)$-dimensional subcubes of Q_k.

Lemma

If U is a set of uniqueness for $\mathcal{B}_{q+}^k$, then U intersects with every non-empty element of $\mathcal{D}(S_q^k)$.

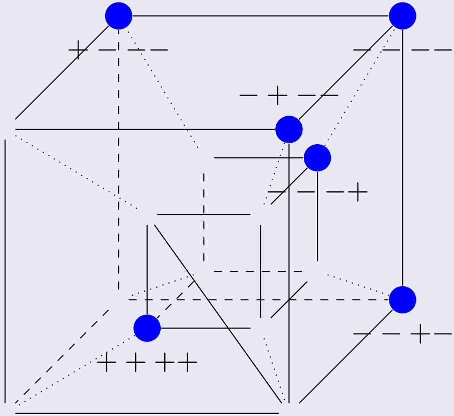
Lemma

If U is a set of uniqueness for $\mathcal{B}^k_{q_+}$, then U intersects with every non-empty element of $\mathcal{D}(S^k_q)$.

For $q = 1$ and $q = k - 1$ the above implication can be replaced with an equivalence. For general q the converse implication is false:

Counterexample ($k = 4, q = 2$)

Let $k = 4$ and $q = 2$. The following set (which consists of all points with exactly $0, 1$ or 4 positive coordinates) intersects with every non-empty element of $\mathcal{D}(S_2^4)$, but its not of uniqueness for $\left(\mathcal{B}_2^4\right)_+$.



Dynkin multi-system

Definition

Let $\mathcal{X}$ be a non-empty set, and let $\mathcal{D}$ be a collection of subsets of $\mathcal{X}$. $\mathcal{D}$ is called a multi-Dynkin system if the following conditions hold:

- $\mathcal{X} \in \mathcal{D}$;
- if $A, B \in \mathcal{D}$ and $A \subset B$, then $B - A \in \mathcal{D}$;
- if $A_1, A_2, A_3, \cdots \in \mathcal{D}$, then $\sum_{j=1}^{\infty} A_j \in \mathcal{D}$.

Analogously, let $\mathcal{Y}$ be a collection of multi-sets in $\mathcal{X}$. The smallest multi-Dynkin system containing $\mathcal{Y}$ is called the multi-Dynkin system generated by $\mathcal{Y}$, denoted $\mathcal{MD}(\mathcal{Y})$.

Observation

For each family $\mathcal{F}$ of sets we have

$$\mathcal{D}(\mathcal{F}) \subset \mathcal{MD}(\mathcal{F}).$$

Theorem (K. Bogdan, TS, T. Stroiński (in preparation))

Let $\mathcal{X}$ be a finite set and let $\mathcal{S} \subset 2^{\mathcal{X}}$. Then the set $U \subset \mathcal{X}$ is of uniqueness for $(\mathcal{B}_{\mathcal{S}})_+$ if and only if U has a non-empty intersection with each non-empty member of a multi-Dynkin system $\mathcal{MD}(\mathcal{S})$ generated by $\mathcal{S}$.

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