Parametric Models and Maximum Likelihood Estimation

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Outline

Density Estimation Problem

- Let P be an unknown probability distribution on a measurable set $\mathcal{X} \subset \mathbb{R}^d$.

- Assume that P has a probability density function $p : \mathcal{X} \to \mathbb{R}$.

- Given i.i.d. data $X_1, \ldots, X_n$ from the unknown P, we are interested in estimating the density function p.

- This is the task of density estimation.

Notation

We may write $X_1, \ldots, X_n \sim p$ (i.i.d.) with the density function p.

Density Estimation Problem

- There are mainly two approaches to this problem: parametric and nonparametric.

Parametric approach

- Define a model of a finite degree of freedom for the unknown density p.
- This is called a parametric model, and indexed by a finite number of parameters.
- Assumptions of the model are often made on the shape of the unknown density p.
- Density estimation is done by estimating the parameters from the data $X_1, \ldots, X_n \sim p$.

Density Estimation Problem

Nonparametric approach

- Define a model with infinite degree of freedom.
- Increase the complexity of the model as more data become available.
- Assumptions of the model are often made on the smoothness of the unknown density p.
- e.g., kernel density estimation [Silverman, 1986].

- In this course we'll only focus on the parametric approach (while the nonparametric approach is also important).

Parameter Approach to Density Estimation

- In the parametric approach, we define a parametric model for the unknown density function p generating data $X_1, \ldots, X_n$.

Parametric Model

- Let Θ be a set of parameter vectors (e.g., $\Theta \subset \mathbb{R}^q$).
- For each $\theta \in \Theta$, define a probability density function $p_\theta : \mathcal{X} \to [0, \infty)$.
- A parametric model is defined as the set of such density functions:

$$\mathcal{P}_\Theta := \{p_\theta \mid \theta \in \Theta\}.$$

Parametric Approach to Density Estimation

Remarks on the Term "Parametric Models"

- The parametric model can be seen as a function $f : \mathcal{X} \times \Theta \to [0, \infty)$ such that

$$f(x, \theta) := p_\theta(x), \quad x \in \mathcal{X},\ \theta \in \Theta.$$

  We may say that f is a parametric model.
- Alternatively, regarding $\theta \in \Theta$ as a variable, we also say p_θ is a parametric model for simplicity.

Parametric Approach to Density Estimation

- The parametric model $\mathcal{P}_\Theta$ should be designed so that the unknown density p belongs to $\mathcal{P}_\Theta$, i.e., $p \in \mathcal{P}_\theta$;

    - $p \in P_\theta = \{p_\theta \mid \theta \in \Theta\}$ is equivalent to the existence of some $\theta^* \in \Theta$ such that
    $$p = p_{\theta^*} \in \mathcal{P}_\Theta.$$
    - We may call such θ^* the true parameter (vector).

- Therefore the model $\mathcal{P}_\Theta$ should reflect our knowledge/belief about the unknown p.

Parametric Approach to Density Estimation

- If $p \in \mathcal{P}_\Theta = \{p_\theta \mid \theta \in \Theta\}$, we say that the model $\mathcal{P}_\Theta$ is correctly specified.

  - In this case, estimation of the unknown density $p = p_{\theta^*}$ can be done by estimating the true parameter θ^* from the data $X_1, \ldots, X_n$.

- If $p \notin \mathcal{P}_\Theta = \{p_\theta \mid \theta \in \Theta\}$, we say that the model $\mathcal{P}_\Theta$ is misspecified.

Example: Gaussian Models

- Recall that the density function of a Gaussian distribution on $\mathcal{X} = \mathbb{R}$ is given by

$$p_{\text{gauss}}(x; \mu, \sigma^2) := \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \quad x \in \mathbb{R}$$

where

- $\mu \in \mathbb{R}$ is the mean of p_{gauss}
- $\sigma^2 > 0$ is the variance of p_{gauss}.

Example: Gaussian Density Models

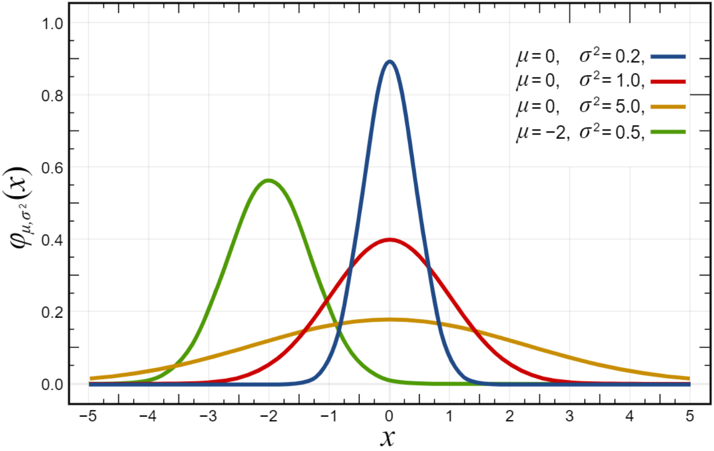


Figure 1: Gaussian density functions; From Wikipedia "Normal distribution."

Example: Gaussian Models

There are several ways to define a probabilistic model.

1. Parametrizing the mean

- Assume that we know/believe that the variance of the unknown density p is σ^2.
- Then we can define a parametric model p_θ by treating the mean μ as a parameter θ:
$$p_\theta(x) := p_{\text{gauss}}(x; \theta, \sigma^2).$$
- In this case, the parameter set may be defined as $\Theta := [-a, a] \subset \mathbb{R}$ for some $a > 0$.

Remarks

- Note that the definition of the parameter set Θ is a part of the model.
- e.g., the choice of the interval $[-a, a]$ implicitly represents our belief that the mean μ of p should satisfy $\mu \in [-a, a]$.

Example: Gaussian Models

2. Parametrizing both the mean and variance

- We can treat both mean μ and variance σ^2 as parameters.
- In this case, we can define a parametric model p_θ as

$$P_\theta(x) := p_{\mathrm{gauss}}(x; \theta_1, \theta_2).$$

where

$$\theta := (\theta_1, \theta_2) \in \Theta \subset \mathbb{R} \times (0, \infty).$$

- The parameter set may be defined as

$$\Theta := [-a, a] \times [b, c] \subset \mathbb{R} \times (0, \infty)$$

for some $a, b, c > 0$.

Example: Gaussian Models

- By using the Gaussian model p_θ, we implicitly makes several assumptions about the unknown p:

Assumptions about the true p made in the Gaussian model

1. There is only one mode (or the "bump") in the density p .
2. $X \sim p$ may take an arbitrarily large value, but with an exponentially small probability.
3. $X \sim p$ takes both positive and negative values.
4. All the moments of p exist: $-\infty < \mathbb{E}_{X \sim p}[X^k] < \infty$ for all $k \in \mathbb{N}$.

- Gaussian models have been widely used in practice.

— This is because there are several mathematically and computationally convenient properties (we'll see this soon).

Example: Gaussian Mixture Models

- Assume instead that we know/believe that there two bumps in the true density p.

- Then the use of the above Gaussian model might be inappropriate.
- We can instead consider a two-component Gaussian mixture model:

$$p_\theta(x) := \frac{1}{2} p_{\text{gauss}}(x; \theta_1, \theta_2) + \frac{1}{2} p_{\text{gauss}}(x; \theta_3, \theta_4), \quad x \in \mathbb{R}$$

where

$$\theta := (\theta_1, \theta_2, \theta_3, \theta_4) \in \Theta \subset \mathbb{R} \times (0, \infty) \times \mathbb{R} \times (0, \infty).$$

Outline

Maximum Likelihood Estimation

- **Maximum likelihood estimation (MLE)** is a classic but still widely used approach to estimating the parameter of a parametric model, advocated by [Fisher, 1922].

- The approach defines an estimator of the true parameter θ^* (in the correctly specified case) as a maximizer of the likelihood function.

Notation

In this lecture, we will use the notation

$$\arg\max_{\theta\in\Theta} A(\theta) = \left\{\theta^* \in \Theta \mid A(\theta^*) = \max_{\theta\in\Theta} A(\theta)\right\}$$

as a set of elements in Θ that maximize the objective function $A(\theta)$.

- Thus, if there are multiple maximizers of $A(\theta)$, then $\arg\max_{\theta\in\Theta} A(\theta)$ consists of multiple elements.

($\arg\min_{\theta\in\Theta} A(\theta)$ is defined in a similar way.)

Likelihood Function

- Let $X_1, \ldots, X_n \in \mathcal{X} \subset \mathbb{R}^d$ be i.i.d. data.

Likelihood Function

For a parametric model $\mathcal{P}_\Theta := \{p_\theta(x) \mid \theta \in \Theta\}$, the likelihood function $\ell_n : \Theta \to [0, \infty)$ for the data $X_1, \ldots, X_n$ is defined by:

$$\ell_n(\theta) := \prod_{i=1}^{n} p_\theta(X_i), \quad \theta \in \Theta.$$

Remarks

- $\ell_n(\theta)$ is a function of the parameter vector $\theta \in \Theta$ (with $X_1, \ldots, X_n$ being fixed).
- $\ell_n(\theta)$ is not a probability density function of $\theta \in \Theta$.
  In fact, its integral may not be 1:
  $\int \ell_n(\theta) d\theta = \int \left(\prod_{i=1}^{n} p_\theta(X_i)\right) d\theta \neq 1.$

Maximum Likelihood Estimation (MLE)

- Let $X_1, \ldots, X_n \sim p$ be i.i.d. data from the unknown density function p.

- Let $\ell_n(\theta) := \prod_{i=1}^n p_\theta(X_i)$ be the likelihood function.

Maximum Likelihood Estimation (MLE)

- Assume that there exists a true parameter $\theta^* \in \Theta$ such that $p = p_\theta^*$ (i.e., the correctly specified case $p \in \mathcal{P}_\Theta = \{p_\theta \mid \theta \in \Theta\}$).
- MLE defines an estimate $\hat{\theta}_n$ of the true parameter $\theta^* \in \Theta$ as a solution to the following optimization problem:

$$\hat{\theta}_n \in \arg\max_{\theta \in \Theta} \ell_n(\theta) := \left\{ \theta' \in \Theta \mid \ell_n(\theta') = \max_{\theta \in \Theta} \ell_n(\theta) \right\}$$

- i.e., the estimate $\hat{\theta}_n$ is a maximizer of the likelihood function:

$$\ell_n(\hat{\theta}_n) = \max_{\theta \in \Theta} \ell_n(\theta).$$

Maximum Likelihood Estimation: Intuition

- We may interpret a parametric model p_θ as a conditional probability density function on $\mathcal{X}$ given $\theta \in \Theta$:

$$p(x \mid \theta) := p_\theta(x), \quad x \in \mathcal{X},\ \theta \in \Theta.$$

- Thus, the likelihood function may be interpreted as the conditional joint probability density of i.i.d. observations $X_1, \ldots, X_n$:

$$\ell_n(\theta) = \prod_{i=1}^{n} p_\theta(X_i) = \prod_{i=1}^{n} p(X_i \mid \theta).$$

— Note that the product form is due to the independence assumption of $X_1, \ldots, X_n$.

- Thus the MLE may be interpreted as searching for the parameter vector θ^* that maximizes the conditional probability (density) of the data $X_1, \ldots, X_n$.

- This interpretation of the likelihood function becomes important in Bayesian inference (we'll see this in a coming lecture)

MLE as Maximizing the Log Likelihood Function

- MLE can be equivalently defined as a maximizer of the log likelihood:

$$\hat{\theta} \in \arg\max_{\theta \in \Theta} \ell_n(\theta) = \arg\max_{\theta \in \Theta} \log \ell_n(\theta)$$

- This is because the logarithm is a monotonically increasing function:

$$\log(t) > \log(s) \iff t > s > 0.$$

- The log likelihood function is often easier to work with in practice, because the product becomes the sum.

$$\log \ell_n(\theta) = \log \prod_{i=1}^{n} p_\theta(X_i) = \sum_{i=1}^{n} \log p_\theta(X_i).$$

- We'll also see the use of log likelihood leads to a deeper understanding of MLE [Akaike, 1998].

Example: MLE with a Gaussian Density Model

- Consider a Gaussian density model on $\mathcal{X} = \mathbb{R}$, with a parametrized mean $\mu = \theta$ and a fixed variance $\sigma^2 > 0$:

$$p_\theta(x) := p_{\text{gauss}}(x; \theta, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\theta)^2}{2\sigma^2}\right)$$

- Assume that i.i.d. data $X_1, \ldots, X_n$ are given.

Example: MLE with a Gaussian Density Model

- Then the log likelihood function is given as

$$
\begin{aligned}
\log \ell_n(\theta) &:= \sum_{i=1}^{n} \log p_{\text{gauss}}(X_i; \theta, \sigma^2) \\
&= \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp \left(-\frac{(X_i - \theta)^2}{2\sigma^2} \right) \right) \\
&= \sum_{i=1}^{n} \left(\log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) - \frac{(X_i - \theta)^2}{2\sigma^2} \right) \\
&= n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) - \sum_{i=1}^{n} \frac{(X_i - \theta)^2}{2\sigma^2}.
\end{aligned}
$$

Example: MLE with a Gaussian Density Model

- To obtain the maximizer, compute the derivative w.r.t. θ and equate it to 0:

$$\frac{d \log \ell_n(\theta)}{d\theta} = \sum_{i=1}^{n} \frac{(X_i - \theta)}{\sigma^2} = 0.$$

- Solving this leads to the maximum likelihood estimator for the mean:

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

- This is the empirical average of $X_1, \ldots, X_n$!

Exercise

- Think about why the empirical average is obtained as MLE for the Gaussian model.
(Hint: recall that the empirical average can be given as a solution to the least-squares problem).

Example: MLE with a Gaussian Density Model

Exercise

- Consider the Gaussian model with both mean $\mu = \theta_1$ and variance $\sigma^2 = \theta_2$ parametrized:

$$p_\theta(x) := p_{\mathrm{gauss}}(x; \theta_1, \theta_2) = \frac{1}{\sqrt{2\pi\theta_2^2}} \exp\left(-\frac{(x-\theta_1)^2}{2\theta_2^2}\right)$$

- Show that the MLE for $\theta = (\theta_1, \theta_2)$ with i.i.d. observations $X_1, \ldots, X_n$ is given by

$$\hat{\theta} = (\hat{\theta}_1, \hat{\theta}_2) = \left(\frac{1}{n}\sum_{i=1}^{n} X_i,\ \frac{1}{n}\sum_{i=1}^{n}(X_i - \hat{\theta}_1)^2\right).$$

Illustration

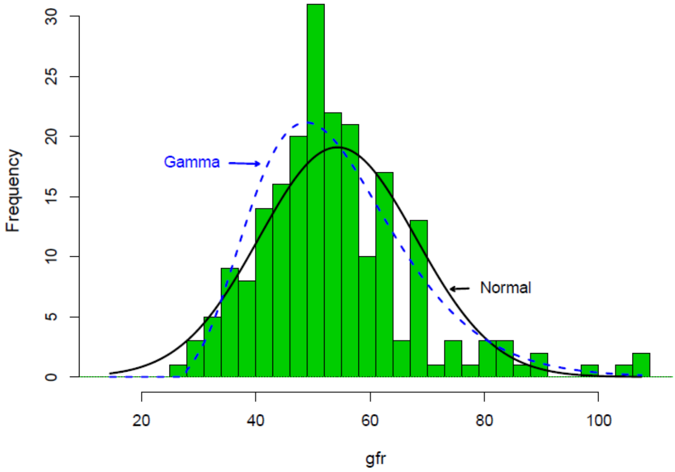


Figure 2: [Efron and Hastie, 2016, Fig 4.1]

Maximum Likelihood Estimation (MLE)

- In general, this optimization problem of MLE has no analytical solution (e.g., consider Gaussian mixture models)

- In that case, one needs to use numerical optimization. e.g.,

  - Gradient descent (see the Optim course for details.)
  - Expectation-Maximization (EM) algorithm.

- In this lecture, we'll study statistical properties of MLE, assuming that we can obtain the maximizer $\hat{\theta}_n$.

Outline

MLE as Kullback-Leibler (KL) Divergence Minimization

- Here we'll see an interpretation of MLE as searching for the parameter $\theta \in \Theta$ that minimizes the KL divergence between the true density p and the model density p_θ [Akaike, 1998].

- This interpretation is very important, because it provides an understanding of the MLE in the misspecified case $p \notin \mathcal{P}_\Theta$:

- To describe this, we'll look at the definition and properties of the KL divergence.

Kullback-Leibler (KL) Divergence

- KL divergence quantifies the discrepancy between two probability density functions.

Kullback-Leibler (KL) Divergence

- Let p and q be probability density functions on $\mathcal{X} \subset \mathbb{R}^d$ such that $p(x)/q(x) < \infty$ for all $x \in \mathcal{X}$.
- Then the KL divergence between p and q is defined as

$$
\begin{aligned}
KL(p||q) &:= \int p(x) \log \frac{p(x)}{q(x)} dx \\
&= \int p(x) \log p(x) dx - \int p(x) \log q(x) dx.
\end{aligned}
$$

Intuition: KL Divergence as a Discrepancy Measure

- If $KL(p\|q)$ is large, then p and q are very different;
- If $KL(p\|q)$ is small, then p and q are similar.

Properties of the KL Divergence

Nonnegativity

- The KL divergence only take non-negative values: for any density functions p and q,

$$KL(p\|q) \geq 0.$$

- This can be seen as follows:

$$\begin{aligned} KL(p\|q) &= \int p(x) \log\left(\frac{p(x)}{q(x)}\right) dx = -\int p(x) \log\left(\frac{q(x)}{p(x)}\right) dx \\ &\geq -\log\left(\int p(x) \frac{q(x)}{p(x)} dx\right) \\ &= -\log\left(\int q(x) dx\right) = -\log(1) = 0 \end{aligned}$$

where the inequality follows from Jensen's inequality and $\log(t)$ being a convex function of $t > 0$ (see e.g.,[Berger, 1985, Sec 1.8]).

Properties of the KL Divergence

KL Divergence as a Discrepancy

- $KL(p\|q) = 0$ if and only if $p = q$ (almost everywhere).

-"if" part can be shown easily: If $p = q$, we have

$$KL(p\|q) = \int p(x) \log \frac{p(x)}{q(x)} dx = \int p(x) \log(1) dx = 0.$$

Asymmetry of the KL Divergence

- That the KL divergence is not symmetric: in general,

$$KL(p\|q) \neq KL(q\|p)$$

- Therefore, KL divergence is not a distance (metric) between probability density functions. (A distance measure needs to be symmetric).

Properties of the KL Divergence

- KL divergence has its origin in Information Theory.

- Indeed, the KL divergence can be written as

$$
\begin{aligned}
KL(p|||q) &:= \int p(x) \log \frac{p(x)}{q(x)} dx \\
&= -\underbrace{\int p(x) \log \frac{1}{p(x)} dx}_{\text{Entropy of } p} + \underbrace{\int p(x) \log \frac{1}{q(x)} dx}_{\text{Cross Entropy of } p \text{ and } q}
\end{aligned}
$$

- For details see e.g. [Gray, 2011] and the InfoTheo course.

Example: KL Divergence between Gaussians

- Consider the KL divergence between two Gaussian densities p and q on $\mathcal{X} := \mathbb{R}$.

KL Divergence between Univariate Gaussians

- Let $p(x) := p_{\mathrm{gauss}}(x; \mu_p, \sigma_p^2)$ with mean $\mu_p \in \mathbb{R}$ and variance $\sigma_p^2 > 0$;
- Let $q(x) := p_{\mathrm{gauss}}(x; \mu_q, \sigma_q^2)$ with mean $\mu_q \in \mathbb{R}$ and variance $\sigma_q^2 > 0$.
- Then the KL divergence between p and q is given by

$$KL(p\|q) = \frac{1}{2}\left(\frac{(\mu_p - \mu_q)^2}{\sigma_q^2} + \log\left(\frac{\sigma_q^2}{\sigma_p^2}\right) + \frac{\sigma_p^2}{\sigma_q^2} - 1\right)$$

Exercise. Prove this.

Example: KL Divergence between Gaussians

- For instance, consider the equal variance case $\sigma_p^2 = \sigma_q^2 =: \sigma^2$.

- Then, the KL divergence simplifies to

$$KL(p\|q) = \frac{1}{2}\left(\frac{(\mu_p - \mu_q)^2}{\sigma^2} + \log\left(\frac{\sigma^2}{\sigma^2}\right) + \frac{\sigma^2}{\sigma^2} - 1\right)$$
$$= \frac{(\mu_p - \mu_q)^2}{2\sigma^2}.$$

- We can make the following observations:

  - As difference between the means μ_p and μ_q approaches 0, the KL divergence converges to 0.

$$KL(p\|q) \to 0 \quad \text{as} \quad (\mu_p - \mu_q)^2 \to 0.$$

  - As the variance σ^2 increases, the KL divergence converges to 0

$$KL(p\|q) \to 0 \quad \text{as} \quad \sigma^2 \to \infty$$

MLE as KL Divergence Minimization

- We now look at a connection between MLE and KL divergence.

- The estimate $\hat{\theta}$ of MLE can be obtained as

$$\hat{\theta} \in \arg\max_{\theta \in \Theta} \log \ell_n(\theta) = \arg\max_{\theta \in \Theta} \log \prod_{i=1}^{n} p_\theta(X_i)$$

$$= \arg\max_{\theta \in \Theta} \sum_{i=1}^{n} \log p_\theta(X_i) = \arg\max_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \log p_\theta(X_i).$$

- The objective function in the last expression is the empirical average of the log density $\log p_\theta(x)$ with the i.i.d. data $X_1, \ldots, X_n \sim p$:

$$\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(X_i).$$

MLE as KL Divergence Minimization

- Thus, we can interpret the objective function of MLE as an empirical approximation to the expected log density:

$$\frac{1}{n}\sum_{i=1}^{n}\log p_\theta(X_i) \approx \mathbb{E}_{X\sim p}[\log p_\theta(X)] = \int (\log p_\theta(x))p(x)dx.$$

where the expectation is with respect to the true unknown density, $X \sim p$.

- Thus, under an appropriate identifiability condition (introduced later), we may expect that

$$\hat{\theta}_n \approx \theta^* \in \arg\max_{\theta\in\Theta} \int p(x)\log p_\theta(x)dx.$$

where $\theta^* \in \Theta$ is a maximizer of the expected log density.

- (We use the the notation θ^* as for the "true parameter" intentionally, for a reason that will be clear later).

MLE as KL Divergence Minimization

- We show that this maximizer θ^* is the minimizer of the KL divergence between the true density p and the model density p_θ:

$$
\begin{aligned}
\theta^* &\in \arg\max_{\theta\in\Theta} \int p(x)\log p_\theta(x)dx \\
&= \arg\min_{\theta\in\Theta} -\int p(x)\log p_\theta(x)dx \\
&= \arg\min_{\theta\in\Theta} -\int p(x)\log p_\theta(x)dx + \int p(x)\log p(x)dx \\
&= \arg\min_{\theta\in\Theta} \int p(x)\left(-\log p_\theta(x) + \log p(x)\right)dx \\
&= \arg\min_{\theta\in\Theta} \int p(x)\log\frac{p(x)}{p_\theta(x)}dx \\
&= \arg\min_{\theta\in\Theta} KL(p\|p_\theta).
\end{aligned}
$$

MLE as KL Divergence Minimization

- Thus, we have:

$$\theta^* \in \arg\max_{\theta \in \Theta} \int p(x) \log p_\theta(x) dx = \arg\min_{\theta \in \Theta} KL(p \| p_\theta).$$

- Therefore, the estimate $\hat{\theta}_n$ of MLE

$$\hat{\theta}_n \in \arg\max_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \log p_\theta(X_i)$$

can be seen as an approximation to the minimizer of the KL divergence:

$$\theta^* \in \arg\min_{\theta \in \Theta} KL(p \| p_\theta)$$

- We will look at closely the conditions required for this interpretation to be valid.

- These are conditions required for MLE to "succeed", thus providing a guideline for the use of MLE in practice.

Outline

Consistency of MLE

- We saw that MLE may be interpreted as an estimator of the optimal parameter θ^* given by

$$\theta^* \in \arg\max_{\theta \in \Theta} \int p(x) \log p_\theta(x) dx = \arg\min_{\theta \in \Theta} KL(p \| p_\theta).$$

- We'll investigate the consistency of the estimate $\hat{\theta}_n$ in estimating such θ^* in a large sample limit $n \to \infty$.

  - This is based on [White 82]; see this paper for details.

- The purpose is to clarify conditions under which MLE "works well."

- To this end, we'll introduce several assumptions (= conditions).

Assumptions on the Data Distribution

Assumption 1 (Data and the True Density)

The data $X_1, \ldots, X_n \in \mathcal{X} \subset \mathbb{R}^d$ are i.i.d. with a distribution P with a density function p.

Assumptions on the Parametric Model

Assumption 2 (Model)

- The parameter set $\Theta \subset \mathbb{R}^q$ is compact.
  — i.e., Θ is a bounded and closed subset.
- For every $x \in \mathcal{X}$, the mapping

$$\theta \to p_\theta(x)$$

  is a continuous function of $\theta \in \Theta$.

Consequence of the Continuity Assumption

- The likelihood function $\ell_n(\theta) = \prod_{i=1}^n p_\theta(X_i)$ is a continuous function of $\theta \in \Theta$, because the mapping

$$\theta \to p_\theta(X_i)$$

is continuous for all $i = 1, \ldots, n$.

Assumptions on the Parametric Model

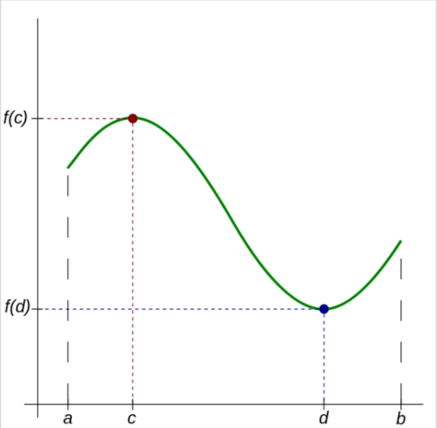
- Assumption 2 guarantees that the maximum of the likelihood function is bounded: i.e.,

$$\max_{\theta\in\Theta} \ell_n(\theta) = \max_{\theta\in\Theta} \prod_{i=1}^{n} p_\theta(X_i) < \infty.$$

This follows from

1. The likelihood function $\ell_n(\theta)$ is a continuous function of $\theta \in \Theta$;
2. Θ is compact;
3. **Extreme value theorem** (a general fact): a continuous function on a compact domain is bounded.

Assumptions on the Parametric Model



A continuous function $f(x)$ on the closed interval $[a, b]$ showing the absolute max (red) and the absolute min (blue).

Figure 3: From Wikipedia "Extreme value theorem"

Assumptions on the Parametric Model

- Thus, Assumption 2 guarantees that MLE

$$\hat{\theta}_n \in \arg\max_{\theta \in \Theta} \ell_n(\theta)$$

is well-defined.

- If Assumption 2 is not satisfied, then we may have

$$\max_{\theta \in \Theta} \ell_n(x) = \infty$$

- In this case, MLE $\hat{\theta}_n \in \arg\max_{\theta \in \Theta} \ell_n(x)$ is not well-defined.

Example where MLE is not Well-Defined

- Consider a 2-component Gaussian mixture model;

$$p_\theta(x) = \frac{1}{2} p_{\mathrm{gauss}}(x; \theta_1, \theta_2) + \frac{1}{2} p_{\mathrm{gauss}}(x; \theta_3, \theta_4),$$

with

$$\theta := (\theta_1, \theta_2, \theta_3, \theta_4) \in \Theta \subset \mathbb{R} \times (0, \infty) \times \mathbb{R} \times (0, \infty).$$

- Define the parameter set Θ as

$$\Theta := [-a, a] \times (0, c] \times [-a, a] \times (0, c]$$

for constants $a, c > 0$.

- In this case, Θ is not closed and thus not compact.

- Therefore Assumption 2 is not satisfied.

Example where MLE is not Well-Defined

- We'll show that in this case the maximum of the likelihood function is unbounded:

$$\max_{\theta \in \Theta} \ell_n(\theta) = \infty,$$

and thus MLE is not well-defined.

Example where MLE is not Well-Defined

- Define $\theta_1 := X_k$ for with $k \in \{1, \dots, n\}$ arbitrary, and fix θ_3 and θ_4.

$$
\begin{aligned}
p_\theta(X_k) &= \frac{1}{2} p_{\mathrm{gauss}}(X_k; \theta_1, \theta_2) + \frac{1}{2} p_{\mathrm{gauss}}(X_k; \theta_3, \theta_4) \\
&= \frac{1}{2} \frac{1}{\sqrt{2\pi\theta_2^2}} \exp\left(-\frac{(X_k - \theta_1)^2}{2\theta_2^2} \right) + \frac{1}{2} p_{\mathrm{gauss}}(X_k; \theta_3, \theta_4) \\
&= \frac{1}{2} \frac{1}{\sqrt{2\pi\theta_2^2}} + \frac{1}{2} p_{\mathrm{gauss}}(X_k; \theta_3, \theta_4).
\end{aligned}
$$

- Taking the limit $\theta_2 \to +0$ (i.e., the variance θ_2 going to 0), we have

$$
\lim_{\theta_2 \to +0} p_\theta(X_k) = \lim_{\theta_2 \to +0} \left(\frac{1}{2} \frac{1}{\sqrt{2\pi\theta_2^2}} + \frac{1}{2} p_{\mathrm{gauss}}(X_k; \theta_3, \theta_4) \right) = \infty.
$$

- The limit $\theta_2 \to +0$ can be taken, because $\theta_2 \in (0, c]$.

Example where MLE is not Well-Defined

- On the other hand, for all $i \neq k$ we have

$$
\begin{aligned}
p_\theta(X_i) &= \frac{1}{2} p_{\text{gauss}}(X_i; \theta_1, \theta_2) + \frac{1}{2} p_{\text{gauss}}(X_i; \theta_3, \theta_4) \\
&\geq \frac{1}{2} p_{\text{gauss}}(X_i; \theta_3, \theta_4).
\end{aligned}
$$

- Therefore,

$$
\begin{aligned}
\lim_{\theta_2 \to +0} \ell_n(\theta) &= \lim_{\theta_2 \to +0} \prod_{i=1}^{n} p_\theta(X_i) = \lim_{\theta_2 \to +0} p_\theta(X_k) \prod_{i \neq k}^{n} p_\theta(X_i) \\
&\geq \left(\lim_{\theta_2 \to +0} p_\theta(X_k) \right) \prod_{i \neq k} \frac{1}{2} p_{\text{gauss}}(X_i; \theta_3, \theta_4) = \infty.
\end{aligned}
$$

This implies that

$$
\max_{\theta \in \Theta} \ell_n(\theta) \geq \lim_{\theta_2 \to +0} \ell_n(\theta) = \infty.
$$

Example where MLE is not Well-Defined

- This example shows that MLE is not always well-defined.

- We need to be careful about how the parameter set Θ is defined.

Exercise

Construct other examples where MLE is not well-defined.

Assumptions for the KL Divergence to be Well-Defined

Assumption 3 (The existence of the KL divergence)

- The true density $p(x)$ satisfies

$$-\infty < \int p(x) \log p(x) dx < \infty.$$

- For the model $p_\theta(x)$, there exists a function $g : \mathcal{X} \to [0, \infty)$ such that

$$|\log p_\theta(x)| \leq g(x) \quad \text{for all } x \in \mathcal{X} \text{ and } \theta \in \Theta$$

and

$$\int g(x) p(x) dx < \infty.$$

Assumptions for the KL Divergence to be Well-Defined

- The latter condition implies that

$$\left|\int p(x)\log p_\theta(x)dx\right| < \int p(x)|\log p_\theta(x)|dx$$
$$\leq \int p(x)g(x)dx < \infty.$$

- Therefore, the above conditions imply that the KL divergence

$$KL(p\|p_\theta) = \int p(x)\log\frac{p(x)}{p_\theta(x)}dx$$
$$= \int p(x)\log p(x)dx - \int p(x)\log p_\theta(x)dx$$

is finite and thus well-defined.

Exercise

- Construct examples of p and p_θ for which the KL divergence cannot be defined.

Assumption for the Identifiability

Assumption 4 (Identifiability)

- Expected log density $\int p(x) \log p_\theta(x) dx$ has a unique maximizer $\theta^* \in \Theta$: i.e.,

$$\int p(x) \log p_{\theta^*}(x) dx > \int p(x) \log p_\theta(x) dx \quad \text{for all } \theta \in \Theta \text{ with } \theta \neq \theta^*.$$

- In other words, θ^* is the unique minimizer of the KL-divergence:

$$\begin{aligned} KL(p \| p_{\theta^*}) &= \int p(x) \log p(x) dx - \int p(x) \log p_{\theta^*}(x) dx \\ &< \int p(x) \log p(x) dx - \int p(x) \log p_\theta(x) dx = KL(p \| p_\theta) \\ &\quad \text{for all } \theta \in \Theta \text{ with } \theta \neq \theta^*. \end{aligned}$$

- In this case, we call the model $P_\Theta = \{p_\theta \mid \theta \in \Theta\}$ is identifiable with respect to p.

Assumption for the Identifiability

- If Assumption 4 (identifiability) is true, the notation

$$\theta^* = \arg\max_{\theta \in \Theta} \int p(x) \log p_\theta(x) dx = \arg\min_{\theta \in \Theta} KL(p \| p_\theta)$$

is justified (because the "argmax" only consists of one element, θ^*).

- Assumption 4 enables us to define θ^* as the quantity of interest (or the estimand) in statistical estimation.

- Thus, we can discuss the "consistency" of the MLE $\hat{\theta}_n \to \theta^*$ as $n \to \infty$.

- This will be important in particular

  - when we are interested in the optimal parameter θ^* itself; and
  - when we want to perform hypothesis testing regarding θ^*.

Interpretation of the Optimal Parameter θ^*

- Let's consider what the optimal parameter θ^* is.

- Assume that the KL divergence between the true unknown density p and the optimal model density p_{θ^*} is zero:

$$KL(p \| p_{\theta^*}) = 0.$$

- In this case,

- We have $p = p_{\theta^*}$, because $KL(p \| p_\theta^*) = 0$ if and only if $p = p_{\theta^*}$.
- Therefore, $p \in \mathcal{P}_\Theta = \{p_\theta \mid \theta \in \Theta\}$ i.e., the model $\mathcal{P}_\Theta$ is correctly specified.

- Thus, we can interpret θ^* as the true parameter in this case.

- The convergence of MLE $\hat{\theta}_n \to \theta^*$ implies that the MLE is consistent in estimating the true parameter θ^* .

Interpretation of the Optimal Parameter θ^*

Summary

- $KL(p \| p_{\theta^*}) = 0$ corresponds to the correctly specified case $p \in \mathcal{P}_\Theta$.
- Since $p = p_{\theta^*}$, the optimal parameter θ^* is interpreted as the true parameter.

Interpretation of the Optimal Parameter θ^*

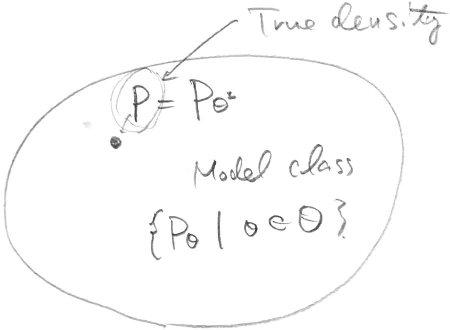


Figure 4: When $KL(p \| p_{\theta^*}) = 0$ (correctly specified case)

Interpretation of the Optimal Parameter θ^*

- Assume the KL divergence between the true density p and the optimal model density p_{θ^*} is larger than zero:

$$KL(p \| p_{\theta^*}) = \min_{\theta \in \Theta} KL(p \| p_\theta) > 0,$$

- In this case,

- we have $p \neq p_{\theta^*}$, i.e., the optimal model density p_{θ^*} does not match the true density p;
- thus $p \notin \mathcal{P}_\Theta = \{p_\theta \mid \theta \in \Theta\}$, i.e., the model $\mathcal{P}_\Theta$ is misspecified.

- In this case, we can interpret p_{θ^*} as the best approximation to the true density p as measured by the KL divergence.

- Thus, we can interpret θ^* as the parameter that gives the best approximation of the model $\mathcal{P}_\Theta$ to the true p.

Interpretation of the Optimal Parameter θ^*

Summary

- $KL(p\|p_{\theta^*}) > 0$ corresponds to the misspecified case $p \notin \mathcal{P}_\Theta$.
- Since $KL(p\|p_{\theta^*}) = \min_{\theta \in \Theta} KL(p\|p_\theta)$, the optimal parameter θ^* is interpreted as the parameter that gives the best approximation p_{θ^*} to the true density p under the KL divergence.

Interpretation of the Optimal Parameter θ^*

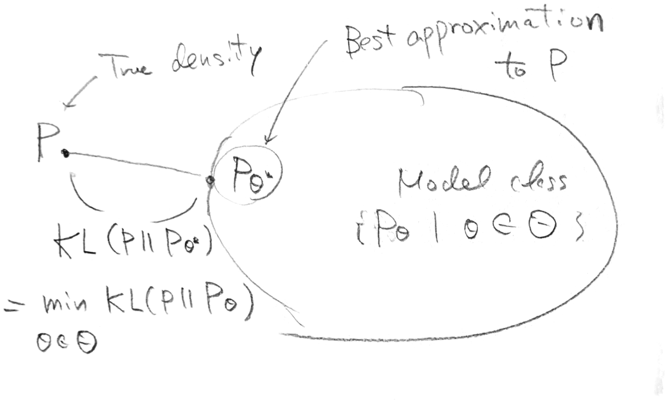


Figure 5: When $KL(p \| p_{\theta^*}) > 0$ (model misspecification).

Example where the Model is not Identifiable

- Consider a 2-component Gaussian mixture model;

$$p_\theta(x) = \frac{1}{2} p_{\mathrm{gauss}}(x; \theta_1, \theta_2) + \frac{1}{2} p_{\mathrm{gauss}}(x; \theta_3, \theta_4)$$

with

$$\theta = (\theta_1, \theta_2, \theta_3, \theta_4) \in \Theta \subset \mathbb{R} \times (0, \infty) \times \mathbb{R} \times (0, \infty).$$

- Define the parameter set Θ by

$$\Theta := [-a, a] \times [b, c] \times [-a, a] \times [b, c]$$

for constants $a, b, c > 0$.

- The model is not identifiable, because switching (θ_1, θ_2) and (θ_3, θ_4) produces the same density function.

Example where the Model is not Identifiable

- To show this, let

$$(\mu_1, \sigma_1^2) \in [-a, a] \times [b, c], \quad (\mu_2, \sigma_2^2) \in [-a, a] \times [b, c]$$

be arbitrary constants such that $\sigma_1^2 \neq \sigma_2^2$.

- Then, for $\theta^* := (\mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$, we have

$$p_{\theta^*}(x) = \frac{1}{2} p_{\mathrm{gauss}}(x; \mu_1, \sigma_1^2) + \frac{1}{2} p_{\mathrm{gauss}}(x; \mu_2, \sigma_2^2)$$

- For $\tilde{\theta}^* := (\mu_2, \sigma_2^2, \mu_1, \sigma_1^2)$

$$p_{\tilde{\theta}^*}(x) = \frac{1}{2} p_{\mathrm{gauss}}(x; \mu_2, \sigma_2^2) + \frac{1}{2} p_{\mathrm{gauss}}(x; \mu_1, \sigma_1^2)$$

- Thus, we have

$$p_{\theta^*} = p_{\tilde{\theta}^*} \quad \text{while} \quad \theta^* \neq \tilde{\theta}^*.$$

- Therefore the mixture model with this parameter set Θ is not identifiable.

Example where the Model is not Identifiable

- A simple trick to make this model identifiable is to restrict the parameter set Θ.

- For instance, if we define the parameter set as

$$\Theta := \{(\theta_1, \theta_2, \theta_3, \theta_4) \in [-a, a] \times [b, c] \times [-a, a] \times [b, c] \mid \theta_2 < \theta_4\}$$

then the mixture model becomes identifiable.

- This corresponds to assuming that one mixture component has a smaller variance than the other.

Exercise

Construct other examples where the model is not identifiable.

MLE Consistency Theorem

Theorem: Consistency of MLE (Theorem 2.2 of [White, 1982])

- Suppose that Assumptions 1, 2, 3 and 4 are satisfied.
- Let

$$\hat{\theta}_n \in \arg\max_{\theta \in \Theta} \ell_n(\theta) = \arg\max_{\theta \in \Theta} \prod_{i=1}^{n} p_\theta(X_i)$$

  be the MLE with i.i.d. data $X_1, \ldots, X_n \sim p$.
- Let $\theta^* \in \Theta$ be the optimal parameter

$$\theta^* = \arg\max_{\theta \in \Theta} \int p(x) \log p_\theta(x) dx = \arg\min_{\theta \in \Theta} KL(p \| p_\theta)$$

  .
- Then $\hat{\theta}_n$ converges to θ^* almost surely: i.e.,

$$\Pr(\lim_{n \to \infty} \hat{\theta}_n = \theta^*) = 1.$$

MLE Consistency Theorem

The proof idea is that

1. First show that

$$\frac{1}{n}\sum_{i=1}^{n}\log p_\theta(X_i) \to \int p(x)\log p_\theta(x)dx \quad \text{as} \quad n \to \infty$$

uniformly for all $\theta \in \Theta$.

2. Then conclude that

$$\hat{\theta}_n \in \arg\max_{\theta\in\Theta}\sum_{i=1}^{n}\log p_\theta(X_i) \to \theta^* = \arg\max_{\theta\in\Theta^*}\int p(x)\log p_\theta(x)dx.$$

as $n \to \infty$.

Outline

Conclusions

- MLE can be understood as searching for a model density that best approximates the true density in terms of the KL divergence.

- MLE makes sense also in the misspecified case where the true density does not belong to the model class.

- MLE is not always consistent; we need conditions = assumptions.

- These conditions provide a guideline for designing your parametric model.

Conclusions

More generic takeaways:

- A role of convergence analysis is to understand conditions under which the method of interest works well.

- Even the MLE - one of the simplest approaches - requires several conditions.

- So please always try to understand conditions under which your favorite statistical/ML method should work!

Further Readings

- [Fisher, 1922, Section 6].
- [White, 1982]
- [Efron and Hastie, 2016, Chapter 4]

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