Parameter Estimation

Distances Between Distributions

1. **Total Variation Distance**: The total variation distance between distributions P and Q, with density functions p and q, is defined to be

$$TV(P,Q) = \sup_{A \subset E} |\mathbb{P}_p(A) - \mathbb{P}_q(A)|.$$

This is equivalent to half the L^1 distance between p and q:

$$TV(P,Q) = \frac{1}{2} \int_{E} |p(x) - q(x)| dx.$$

- (a) This is a genuine metric.
- (b) Unfortunately, it is hard to estimate.
- 2. Kullback-Leibler Divergence: The Kullback-Leibler (known as relative entropy in Information Theory) divergence between P and Q is defined to be

$$KL(P||Q) = \int_{E} p(x) \log \left(\frac{p(x)}{q(x)}\right) dx,$$

where we assign the value ∞ if the support of p is not contained in the support of q (if it is, then anywhere q = 0, we will also have p = 0 and thus the points at which the integrand is not defined will all be removable discontinuities).

- (a) While positive semi-definite, KL-divergence is not a true metric, since it is anti-symmetric. It also fails to satify a trangle inequality.
- (b) It is, however, an expectation. Hence, it can be replaced with a sample mean and estimated.
 - Professor Rigollet calls the act of replating an expectation with a sample mean (i.e., the application of LLN) "the statistical hammer." The implication here is that it's our simplest (and often only) tool.

Examples

- 1. Let $X_n = \text{Poi}(1/n)$ and let δ_0 be a point mass centered at 0. Then $TV(X_n, \delta_0) \to 0$.
- 2. Let P = Bin(n, p), Q = Bin(n, q), where $p, q \in (0, 1)$, and write their densities with one function

$$f(p,k) = \binom{n}{k} p^k (1-p)^{n-k},$$

and similarly for f(n,q). Then it is actually a pretty straightforward calculation to show that

$$KL(P||Q) = np \cdot \log\left(\frac{p}{q}\right) + (n - np) \cdot \log\left(\frac{1 - p}{1 - q}\right).$$

3. Let P = N(a, 1) and let Q = N(b, 1). Then (also pretty straightforward to calculate):

$$KL(P||Q) = \frac{1}{2}(a-b)^2.$$

Maximum Likelihood Estimation

Definitions

1. Let $X_1, X_2, ..., X_n$ be an *iid* sample from a distribution with density $f(x; \theta)$. The *Likelihood* of the sample is

$$L(X_1, X_2, \dots, X_n) = \prod_{i=1}^{n} f(X_i; \theta).$$

2. The log-likelihood function, denoted $\ell(\theta)$ is

$$\ell(\theta) = \log(L(X_1, X_2, \dots, X_n; \theta)).$$

Note we write ℓ as a random function of θ .

3. The Fisher Information is defined to be

$$I(\theta) = E \left[\nabla \ell(\theta) (\nabla \ell(\theta))^T \right] - E \left[\nabla \ell(\theta) \right] E \left[\nabla \ell(\theta) \right]^T = -E \left[\mathbf{H} \ell(\theta) \right],$$

where in this case the likelihood is of a one-element sample, and the bold **H** denotes the Hessian operator. In one dimension, this reduces to

$$I(\theta) = -E(\ell''(\theta)).$$

Equivalently, we also have

$$I(\theta) = Var(\ell'(\theta)).$$

This latter definition is usually harder to work with, but has a more direct connection to maximum likelihood estimators.

Throughout, we will be discussing ways to estimate the value of a "true" parameter θ^* of a distribution \mathbb{P}_{θ^*} , given a model $(E, \{\mathbb{P}_{\theta} : \theta \in \Theta\})$. A noble goal might be to build an estimator $\widehat{TV}(P_{\theta}, P_{\theta^*})$ and compute the argmin using this estimator. However, TV distance is hard to estimate in general, so we use KL-divergence instead. Since this function is an expectation, it can be replaced by a sample mean (using LLN), and is therefore easy to estimate.

For the rest of this section, suppose we are estimating a distribution $\mathbb{P} = \mathbb{P}_{\theta^*}$ with a parametric family of distributions $\{\mathbb{P}_{\theta} : \theta \in \Theta\}$. We will proceed to do this by estimating the minimizer (argmin) of $KL(\mathbb{P}_{\theta}, \mathbb{P})$, which is θ^* , by the positive semidefiniteness (or nonnegative definiteness?) of KL.

The strategy for doing so will involve first estimating KL divergence and finding the minimizer of that estimator \widehat{KL} . That the argmin of \widehat{KL} converges to the argmin of KL follows from "nice analytic properties" of these functions. I'm guessing that KL is at least C^1 and the convergence is relatively strong.

Estimating KL Divergence

Recall that $KL(\mathbb{P}_{\theta}, \mathbb{P})$ is an expectation: if f_{θ} and f are the densities of \mathbb{P}_{θ} and \mathbb{P} , respectively, then

$$KL(\mathbb{P}, \mathbb{P}_{\theta}) = E_{\mathbb{P}}\left(\log\left(\frac{f(x)}{f_{\theta}(x)}\right)\right) = E_{\mathbb{P}}(\log(f(x))) - E_{\mathbb{P}}(\log(f_{\theta}(x))).$$

As a function $\theta \mapsto KL(f_{\theta}, f)$, this has the form

$$KL(\mathbb{P}, \mathbb{P}_{\theta}) = "constant" - E_{\mathbb{P}}(\log(f_{\theta}(x))).$$

Thus, by LLN, we have

$$\widehat{KL}(\mathbb{P}, \mathbb{P}_{\theta}) = "\text{constant}" - \frac{1}{n} \sum_{i=1}^{n} \log(f_{\theta}(X_i)).$$

Finding the Minimum of \widehat{KL}

Starting with the above equation, we have

$$\min_{\theta \in \Theta} \widehat{KL}(\mathbb{P}, \mathbb{P}_{\theta}) \Leftrightarrow \min_{\theta \in \Theta} -\frac{1}{n} \sum_{i=1}^{n} \log(f_{\theta}(X_{i}))$$

$$\Leftrightarrow \max_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \log(f_{\theta}(X_{i}))$$

$$\Leftrightarrow \max_{\theta \in \Theta} \log\left(\prod_{i=1}^{n} p_{\theta}(X_{i})\right)$$

$$\Leftrightarrow \max_{\theta \in \Theta} \prod_{i=1}^{n} p_{\theta}(X_{i}).$$

Therefore, the minimizer of \widehat{KL} is the maximum likelihood estimator $\widehat{\theta}$ of θ^* . Furthermore (avoiding a bunch of details necessary for this implication), we have

$$\hat{\theta} \stackrel{(p)}{\rightarrow} \theta^*$$
.

Examples of Maximum Likelihood Estimators

1. **TODO**

The Asymptotic Variance of MLE

The MLE is not only consistent, but also satisfies a central limit theorem:

$$\sqrt{n}(\hat{\theta} - \theta^*) \stackrel{(d)}{\to} N(0, V(\theta^*)),$$

where $V(\theta^*)$ represents the asymptotic variance of $\hat{\theta}$. But what is this asymptotic variance?!? Turns out that under some mild conditions, the asymptotic variance of $\hat{\theta}$ is known.

Theorem Assume the following.

- 1. θ^* is identifiable.
- 2. θ^* is an interior point of Θ .
- 3. The Fisher information matrix $I(\theta)$ is invertible in a neighborhood of θ^* .
- 4. All the functions involved are "nice".
- 5. The support of \mathbb{P}_{θ} does not depend on θ .

Then

$$V(\hat{\theta}) = I(\theta^*)^{-1}.$$

Proof Write $\ell_i(\theta) = \log f_{\theta}(X_i)$. We start with a couple of observations:

1. Since $\hat{\theta}$ is the unique maximizer of $\log(L_n(X_1, X_2, \dots, X_n; \theta))$,

$$\frac{d}{d\theta} \Big|_{\theta=\hat{\theta}} \sum_{i=1}^{n} \ell_i = \sum_{i=1}^{n} \ell_i(\hat{\theta}) = 0.$$

2. Since θ^* is the unique minimizer of $KL(\mathbb{P}_{\theta}, \mathbb{P})$ and this differs from $E(\ell(\theta))$ by a constant, we have

$$E(\ell'(\theta^*)) = \frac{d}{d\theta}\Big|_{\theta=\theta^*} E(\ell(\theta)) = 0.$$

Now, we start with a Taylor expansion at θ^* :

$$0 = \sum_{i=1}^{n} \ell'_{i}(\hat{\theta}) = \sum_{i=1}^{n} \left[\ell'_{i}(\theta^{*}) + (\hat{\theta} - \theta^{*})\ell''_{i}(\theta^{*}) + \cdots \right].$$

Therefore scaling and applying observation 1, we have

$$0 = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left[\left(\ell'_{i}(\theta^{*}) - E[\ell'_{i}(\theta^{*})] \right) + (\hat{\theta} - \theta^{*}) \ell''_{i}(\theta^{*}) + \cdots \right]$$

$$\approx \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left(\ell'_{i}(\theta^{*}) - E[\ell'_{i}(\theta^{*})] \right) + \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\hat{\theta} - \theta^{*}) \ell''_{i}(\theta^{*})$$

$$= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left(\ell'_{i}(\theta^{*}) - E[\ell'_{i}(\theta^{*})] \right) + \sqrt{n} (\hat{\theta} - \theta^{*}) \cdot \frac{1}{n} \sum_{i=1}^{n} \ell''_{i}(\theta^{*}).$$

By CLT, the term on the left converges to $N(0, I(\theta^*))$. By LLN, the term $n^{-1} \sum_i \ell_i''(\theta^*)$ converges to $E(\ell''(\theta^*)) = -I(\theta^*)$. Therefore, rearranging, we have

$$I(\theta^*) \cdot \sqrt{n}(\hat{\theta} - \theta^*) \stackrel{(d)}{\rightarrow} N(0, I(\theta^*)),$$

therefore,

$$\sqrt{n}(\hat{\theta} - \theta^*) \stackrel{(d)}{\to} N(0, I(\theta^*)^{-1}).$$

Remark: This proof only works in one dimension. In higher dimensions, there is a lack of commutativity that results in a more complicated expression in the end. (**TODO:** Write up something about it)

Remark: Recall the original definition of Fisher information as the Hessian of log-likelihood. This adds geometric intuition to the result: If the log-likelihood is more tightly curved at θ^* , then MLE will vary less around the maximum and vice versa. The word "information" is also more than superficial with this in mind; i.e., more "information" iff less variance, which translates to tighter confidence intervals around MLE.

Examples of Fisher Information

1. TODO: Match the MLE examples above.

Method of Moments

M-Estimation