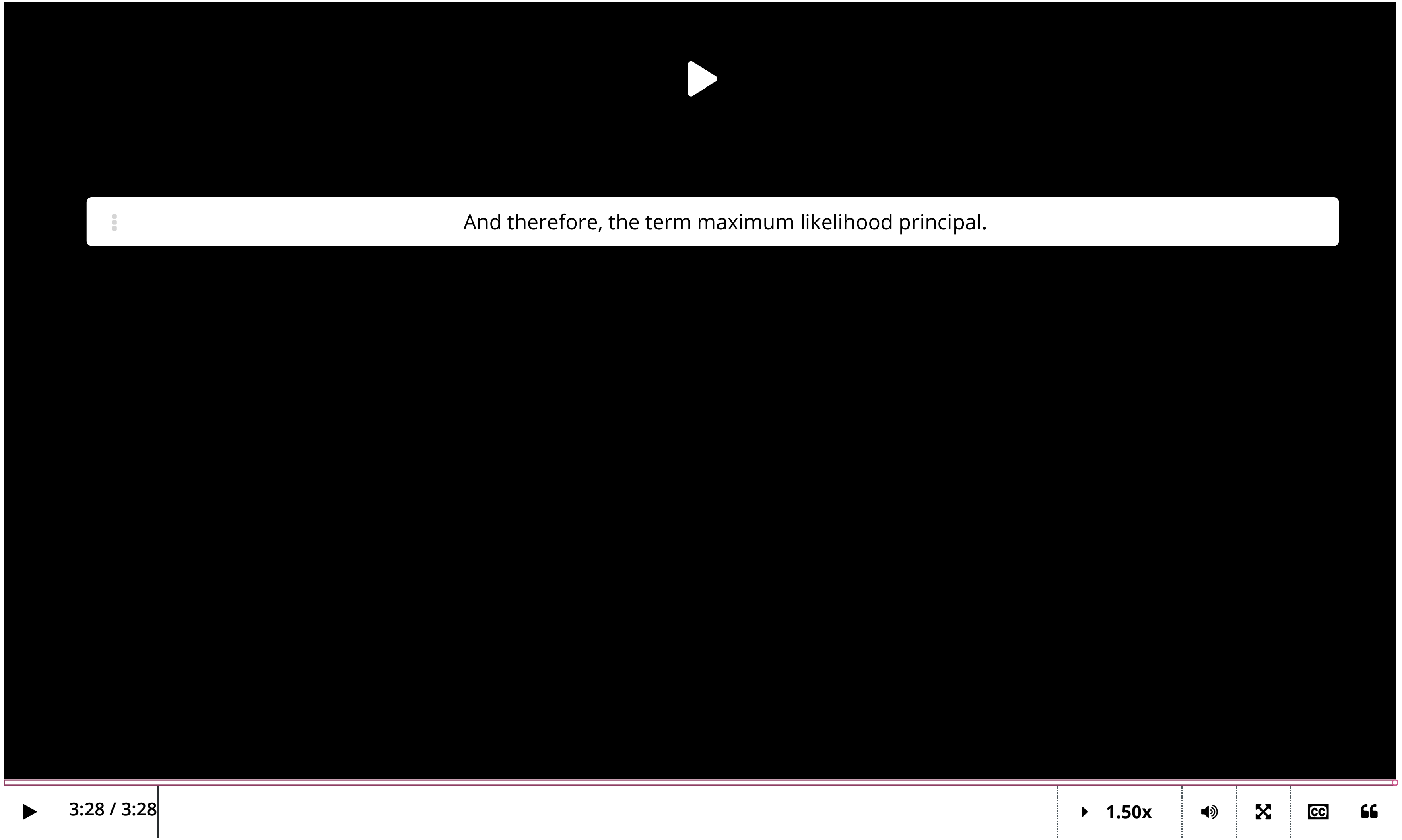
13. Parameter Estimation via KL Divergence

Deriving the Maximum Likelihood Estimator



And therefore, the term maximum likelihood principal.

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The next four problems concern the following statistical set-up.

You observe discrete random variables

$$X_1, \ldots, X_n \overset{iid}{\sim} P_{\theta^*}$$

where θ^* is the true parameter. You construct an associated statistical model $(E, \{P_\theta\}_{\theta \in \mathbb{R}})$. The sample space E is discrete.

Intuitively, your goal is to find an estimator $\hat{\theta}_n \in \mathbb{R}$ so that the distributions $P_{\hat{\theta}_n}$ and P_{θ^*} are close. Precisely, you want to find an estimator $\hat{\theta}_n \in \mathbb{R}$ so that the quantity

$$\mathrm{KL}\left(P_{\theta^*}, P_{\hat{\theta}_n}\right)$$

is as small as possible.

This approach will naturally lead to the construction of the **maximum likelihood estimator** .

Finding a Minimizer of KL Divergence

1/1 point (graded)

Consider the optimization problem in which we minimize the KL divergence between P_{θ^*}, the true distribution, and P_θ. Formally, we want to solve

$$\min_{\theta \in \mathbb{R}} \mathrm{KL}\left(P_{\theta^*}, P_\theta\right).$$

We are not so much interested in the minimum value attained by the objective function $\mathrm{KL}\left(P_{\theta^*}, P_\theta\right)$, but rather the value of θ where the minimum is attained. We refer to such a θ as a **minimizer** .

Let's suppose that there is a unique minimizer for the above optimization problem– *i.e.*, if m is the minimum value of $\mathrm{KL}\left(P_{\theta^*}, P_\theta\right)$, there is only one point $\theta_{\min}$ such that

$$m = \mathrm{KL}\left(P_{\theta^*}, P_{\theta_{\min}}\right).$$

For which θ is the minimum value of $\mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right)$ attained? (Equivalently, what is $\theta_{\min}$?)

● θ^*

○ θ

○ 0

○ None of the above.

✓

Solution:

The KL divergence is nonnegative, so $\mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right) \geq 0$. The right-hand side is achieved if we set $\theta = \theta^* : \mathrm{KL}\left(P_{\theta^*}, P_{\theta^*}\right) = 0$. Since the minimizer is unique by assumption, we conclude that the minimum value is attained at $\theta = \theta^*$.

Remark: The assumption that there is a unique minimizer holds if we are given that the parameter θ is identified. Here is why: since KL divergence is definite, $\mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right) = 0$ if and only if P_{θ^*} and P_{θ} are the same distribution. And if θ is identified, this implies that $\theta = \theta^*$.

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ℹ Answers are displayed within the problem

Can we Minimize KL Divergence Directly?

2/2 points (graded)

Let's use the same statistical set-up as above. Recall that you have access to the iid samples $X_1, \ldots, X_n$. You use these samples to build an estimator $\hat{\theta}_n$. Can you compute

$$\mathrm{KL}\left(P_{\hat{\theta}_n}, P_{1/2}\right)$$

without knowing θ^*, the true parameter?

● Yes

○ No

✓

Can you compute

$$\mathrm{KL}\left(P_{\theta^*}, P_{1/2}\right)$$

without knowing θ^*?

○ Yes

● No

✓

Solution:

In general, we can compute $\mathrm{KL}\left(\mathbf{P}, \mathbf{Q}\right)$ if and only if we know both distributions $\mathbf{P}$ and Q. Moreover, by our statistical model, we can compute P_θ if and only if we know the real number θ. Putting these last two facts together, we can compute

$$\mathrm{KL}\left(P_{\hat{\theta}_n}, P_{1/2}\right)$$

because $\hat{\theta}_n$ is known–it is an estimator so its expression does not depend on θ^*, the true parameter. However, regardless of how many samples we take, we cannot compute $\mathrm{KL}\left(P_{\theta^*}, P_{1/2}\right)$ exactly because the distribution P_{θ^*} is unknown.

Remark: Since we cannot even compute the function $\mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right)$ for general θ, this implies that the optimization problem

$$\min_{\theta \in \mathbb{R}} \mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right)$$

cannot be solved exactly, regardless of the number of samples we have. So to estimate the minimizer of this optimization problem (which is the true parameter θ^*) we will have to consider an approximation for $\mathrm{KL}\left(P_{\theta^*}, P_{\theta}\right)$.

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Finding the Minimizer for an Approximation of KL Divergence

1/1 point (graded)

We use the same statistical set-up as above. Recall that $X_1, \ldots, X_n \overset{iid}{\sim} P_{\theta^*}$. Let p_θ be the pmf of P_θ.

Which of the following is a (weakly) **consistent** estimator for

$$\mathbb{E}_{\theta^*}\left[\ln p_\theta\left(X\right)\right] = \sum_{x \in E} p_{\theta^*} \ln p_\theta\left(x\right) \ ?$$

○ $\frac{1}{n}\sum_{i=1}^{n} X_i$

● $\frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right)$

○ $\frac{1}{n}\sum_{i=1}^{n} \ln\left(p_{\theta^*}\left(X_i\right)\right) - \frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right)$

○ $\theta^* - \mathbb{E}_{\theta^*}\left[\ln p_{\theta^*}\right]$

✓

Solution:

By the law of large numbers, $\frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right) \to \mathbb{E}_{\theta^*}\left[\ln p_\theta\right]$ in probability. Hence, the second choice is correct.

Remark 1: The KL divergence between P_{θ^*} and P_θ can be written

$$\mathrm{KL}\left(P_{\theta^*}, P_\theta\right) = \sum_{x\in E} p_{\theta^*} \ln p_{\theta^*}\left(x\right) - \sum_{x\in E} p_{\theta^*} \ln p_\theta\left(x\right) = \mathbb{E}_{\theta^*}\left[\ln p_{\theta^*}\left(X\right)\right] - \mathbb{E}_{\theta^*}\left[\ln p_\theta\left(X\right)\right]$$

where $X \sim P_{\theta^*}$.

Remark 2: While we can't find θ that minimizes $\mathrm{KL}\left(P_{\theta^*}, P_\theta\right)$, we can find θ that minimizes

$$\hat{\mathrm{KL}}\left(P_{\theta^*}, P_\theta\right) := \mathbb{E}_{\theta^*}\left[\ln p_{\theta^*}\right] - \frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right).$$

Here's why: the first term on the RHS, $\mathbb{E}_{\theta^*}\left[\ln p_{\theta^*}\right]$, does not depend on θ. Hence, the θ that minimizes $\hat{\mathrm{KL}}\left(P_{\theta^*}, P_\theta\right)$ is the same as the θ that minimizes $-\frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right).$

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Deriving the Maximum Likelihood Estimator

1/1 point (graded)

We use the same statistical set-up as above. Recall that p_θ is the pmf of P_θ and $X_1, \ldots, X_n \overset{iid}{\sim} P_{\theta^*}$.

Suppose that $\theta_{\min}$ is a minimizer for the function

$$f\left(\theta\right) := -\frac{1}{n}\sum_{i=1}^{n} \ln\left(p_\theta\left(X_i\right)\right)$$

Which of the following functions is also minimized at $\theta_{\min}$?

○ $g_1\left(\theta\right) = -\prod_{i=1}^{n} p_\theta\left(X_i\right)$

○ $g_2\left(\theta\right) = 25 - \prod_{i=1}^{n} p_\theta\left(X_i\right)$

○ $g_3(\theta) = h(\theta^*) - \prod_{i=1}^n p_\theta(X_i)$ where h is a function of θ^* that does **not** depend on θ.

○ $g_4(\theta) = \theta^* - \prod_{i=1}^n p_\theta(X_i)$

● All of the above

✓

Solution:

Observe that rescaling by n does not change where the minimum of a function is attained. Hence, $f(\theta)$ and $nf(\theta)$ have the same minimizer. Next, by the addition property of logarithms,

$$nf(\theta) = \sum_{i=1}^{n} \ln(p_\theta(X_i)) = \ln\left(\prod_{i=1}^{n} p_\theta(X_i)\right).$$

Since $\ln$ is an increasing function, the function

$$\theta \mapsto \prod_{i=1}^{n} p_\theta(X_i)$$

has the same minimizer as $\ln\left(\prod_{i=1}^n p_\theta(X_i)\right)$. Thus the first choice is correct.

Moreover, the second and third choices are also correct. Whenever we have an optimization problem

$$\min_{\theta\in\mathbb{R}} C + g(\theta)$$

where C does not depend on θ, then the above will have the same minimizer as the optimization problem

$$\min_{\theta\in\mathbb{R}} g\left(\theta\right).$$

In the second choice, $C = 25$ (which is independent of θ), and in the third choice, $C = h\left(\theta^*\right)$ (which by assumption is independent of θ).

Remark 1: The quantity

$$\hat{\theta}_n{:=}\text{maximizer of } \prod_{i=1}^{n} p_\theta\left(X_i\right)$$

is referred to as the **maximum likelihood estimator** . Note that this is the same as the estimator

$$\hat{\theta}_n{:=}\text{minimizer of } \quad -\frac{1}{n}\sum_{i=1}^{n}\ln\left(p_\theta\left(X_i\right)\right)$$

considered in Remark 2 in the solution of the previous problem.

Remark 2: Under certain technical conditions, the maximum likelihood estimator is guaranteed to (weakly) converge to the true parameter θ^* .

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