

# Lecture #5: some properties of the KL

Last lecture, we proposed algorithms with (pseudo) regrets bounded as

$$R_T \leq c \sum_{k, \Delta_k > 0} \frac{\ln T}{\Delta_k} \quad (\text{instance dependent regret})$$

Is it possible to do better?

This lecture focuses on lower bounding the achievable regret by any algorithm

For that we consider a model where the rewards distributions belong to some **known** distribution set  $\mathcal{D}$ .

$$\text{ie } \forall k \in [K], v_k \in \mathcal{D}$$

unknown  $\nearrow$   $v_k$   $\leftarrow$  known

One can show matching upper and lower bounds (with associated strategies):

$$R_T \text{ is at best of order } \left( \sum_{k, \Delta_k > 0} \frac{\Delta_k}{K \inf(v_k, \mu^*, \mathcal{D})} \right) \ln T$$

where

$$K \inf(v_k, \mu^*, \mathcal{D}) = \inf \left\{ \text{KL}(v_k, v') \mid v' \in \mathcal{D}, \mathbb{E}[v'] > \mu^* \right\}$$

Kullback-Leibler divergence

We will only prove the lower bound part

(and the upper bound in exercise session/homework for two specific cases).

• Case 1:  $\mathcal{D} = \left\{ \mathcal{N}(\mu, \sigma^2) \mid \mu \in \mathbb{R} \right\}$

then

$$\text{King}(\nu_k, \mu^*, \mathcal{D}) = \frac{\Delta_k^2}{2\sigma^2}$$

Best possible regret of order  $2\sigma^2 \sum_{k, \Delta_k > 0} \frac{\ln T}{\Delta_k}$

UCB has regret  $\leq 32\sigma^2 \sum_{k, \Delta_k > 0} \frac{\ln T}{\Delta_k}$

↳ optimal up to constant factor  
can be made optimal with finer version

• Case 2:  $\mathcal{D} = \left\{ \text{Ber}(p) \mid p \in [0, 1] \right\}$

then

$$\text{King}(\nu_k, \mu^*, \mathcal{D}) = \mu_k \ln \frac{\mu_k}{\mu^*} + (1 - \mu_k) \ln \frac{1 - \mu_k}{1 - \mu^*}$$

**But** before proving the lower bound, I guess that some reminder of basic and non-basic results about KL divergences would be needed!

## Definition

let  $P, Q$  be two probability measures over  $(\Omega, \mathcal{F})$

$$KL(P, Q) = \begin{cases} +\infty & \text{if } P \text{ is not absolutely continuous wrt } Q \\ \int_{\Omega} \left( \frac{dP}{dQ} \ln \left( \frac{dP}{dQ} \right) \right) dQ = \int_{\Omega} \ln \left( \frac{dP}{dQ} \right) dP & \text{if } \underline{P \ll Q}. \end{cases}$$

$Q(A) = 0 \Rightarrow P(A) = 0$

## Basic Facts

- existence of the defining integral when  $P \ll Q$ , because  $\Psi: x \mapsto x \ln x$  is bounded from below on  $[0, +\infty)$
- $KL(P, Q) \geq 0$  and  $KL(P, Q) = 0$  if and only if  $P = Q$ .  
indeed,  $\Psi$  is strictly convex. Jensen's inequality indicates that

$$KL(P, Q) = \int_{\Omega} \psi\left(\frac{dP}{dQ}\right) dQ \geq \psi\left(\int_{\Omega} \frac{dP}{dQ} dQ\right) = \psi(1) = 0, \text{ with}$$

equality if and only if  $\frac{dP}{dQ}$  is  $Q$ -almost surely constant, i.e.  $P=Q$ .

A useful rewriting:

Assume  $P \ll Q$  and let  $\nu$  be any probability measure over  $(\Omega, \mathcal{F})$  with  $P \ll \nu$ ,  $Q \ll \nu$ . Denote  $f = \frac{dP}{d\nu}$ ,  $g = \frac{dQ}{d\nu}$ ,

$$\text{Then } KL(P, Q) = \int_{\Omega} \ln\left(\frac{f}{g}\right) f d\nu.$$

see proof in exercise session 3.

useful when  $P$  and  $Q$  both admit densities over a classical reference measure (eg Lebesgue).

Lemma (data processing inequality)

Let  $P, Q$  be two probability measures over  $(\Omega, \mathcal{F})$ .

Let  $X: (\Omega, \mathcal{F}) \rightarrow (\Omega', \mathcal{F}')$  be any random variable.

Denote by  $P^X$  and  $Q^X$  the laws of  $X$  under  $P$  and  $Q$ .

$$\text{Then } KL(P^X, Q^X) \leq KL(P, Q)$$

Proof: we can assume  $P \ll Q$ , since otherwise  $KL(P, Q) = +\infty$  and it holds.

We show that we then have  $P^x \ll Q^x$ , with  $\frac{dP^x}{dQ^x} = \underbrace{E_Q \left[ \frac{dP}{dQ} \mid X = \cdot \right]}_{=: \gamma(X) = E_Q \left[ \frac{dP}{dQ} \mid X \right]}$

Indeed, for all  $B \in \mathcal{F}'$ ,

$$P^x(B) = P(X \in B) = \int_{\Omega} \mathbb{1}_B(X) \frac{dP}{dQ} dQ \stackrel{\text{tower rule}}{=} \int_{\Omega} \mathbb{1}_B(X) E_Q \left[ \frac{dP}{dQ} \mid X \right] dQ$$

$$= \int_{\Omega} \mathbb{1}_B(X) \gamma(X) dQ = \int_{\Omega'} \mathbb{1}_B \gamma dQ^x$$

by def of  $Q^x$

Therefore,  $KL(P^x, Q^x) = \int_{\Omega'} \gamma \ln \gamma dQ^x = \int_{\Omega} \gamma(X) \ln \gamma(X) dQ$

$$= \int_{\Omega} \left( E_Q \left[ \frac{dP}{dQ} \mid X \right] \ln \left( E_Q \left[ \frac{dP}{dQ} \mid X \right] \right) \right) dQ$$

$$\leq \int_{\Omega} E_Q \left[ \frac{dP}{dQ} \ln \frac{dP}{dQ} \mid X \right] dQ$$

$\psi$  is convex,  
conditional Jensen inequality

$$\stackrel{\text{tower rule}}{=} \int_{\Omega} \frac{dP}{dQ} \ln \frac{dP}{dQ} dQ = KL(P, Q) \quad \square$$

## References

• the proof above is due to Ali and Silvey ('66),  
but it's far from being well-known.

• Typical proofs in the more recent literature:

- either focus on the discrete case (Cover and Thomas, 2006)

- or use the duality/variational formula for the KL (Massart 2007,  
Boucheron, Lugosi, Massart 2013)

• The joint convexity of KL, given below, is typically proved in a tedious way, relying on the joint convexity of  $(x, y) \in \mathbb{R}_+^2 \mapsto \left(\frac{x}{y} \ln \frac{x}{y}\right)$ .  
We may see it instead as a consequence of the data processing inequality.

### Corollary (joint convexity of KL)

For all probability distributions  $P_1, P_2$  and  $Q_1, Q_2$  over the same measurable space  $(\Omega, \mathcal{F})$  and all  $\lambda \in (0, 1)$ :

$$\text{KL}((1-\lambda)P_1 + \lambda P_2, (1-\lambda)Q_1 + \lambda Q_2) \leq (1-\lambda) \text{KL}(P_1, Q_1) + \lambda \text{KL}(P_2, Q_2).$$

Proof: we augment  $(\Omega, \mathcal{F})$  into  $(\Omega', \mathcal{F}')$  where

$$\Omega' = \Omega \times \{1, 2\}$$

$$\mathcal{F}' = \mathcal{F} \otimes \{ \{1\}, \{2\}, \{1, 2\} \}$$

we define the random pair  $(X, J)$  by the projections  $X: \Omega \times \{1, 2\} \rightarrow \mathcal{X}$   
 $(\omega, j) \mapsto \omega$   
 and  $J: \Omega \times \{1, 2\} \rightarrow \{1, 2\}$   
 $(\omega, j) \mapsto j$

Let  $\mathbb{P}$  be a probability measure on  $(\mathcal{X}, \mathcal{F})$  such that:

$$\begin{cases} J \sim 1 + \text{Ber}(\lambda) \\ X|J=j \sim \mathbb{P}_j \end{cases} \quad (\text{and a similar def for } \mathbb{Q} \text{ with } \mathbb{Q}_1, \mathbb{Q}_2)$$

that is  $\forall j \in \{1, 2\}, \forall A \in \mathcal{F}, \mathbb{P}(A \times \{j\}) = ((1-\lambda) \mathbb{1}_{\{j=1\}} + \lambda \mathbb{1}_{\{j=2\}}) \mathbb{P}_j(A)$

Now,  $\mathbb{P}^X = (1-\lambda) \mathbb{P}_1 + \lambda \mathbb{P}_2$

$\mathbb{Q}^X = (1-\lambda) \mathbb{Q}_1 + \lambda \mathbb{Q}_2$

and *as we prove below*  $KL(\mathbb{P}, \mathbb{Q}) = (1-\lambda) KL(\mathbb{P}_1, \mathbb{Q}_1) + \lambda KL(\mathbb{P}_2, \mathbb{Q}_2)$  so that the

result follows from the data processing inequality.

Indeed, we may assume with no loss of generality for  $\lambda \in (0, 1)$  that  $\mathbb{P}_1 \ll \mathbb{Q}_1, \mathbb{P}_2 \ll \mathbb{Q}_2$ , so that  $\mathbb{P} \ll \mathbb{Q}$  with

$$\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega, j) = \mathbb{1}_{\{j=1\}} \frac{d\mathbb{P}_1}{d\mathbb{Q}_1}(\omega) + \mathbb{1}_{\{j=2\}} \frac{d\mathbb{P}_2}{d\mathbb{Q}_2}(\omega)$$

This entails that:

$$KL(\mathbb{P}, \mathbb{Q}) = \int_{\mathcal{X}^1} \left( \frac{d\mathbb{P}}{d\mathbb{Q}}(\omega, j) \ln \frac{d\mathbb{P}}{d\mathbb{Q}}(\omega, j) \right) d\mathbb{Q}(\omega, j)$$

$$= \int_{\Omega'} \left( \frac{dP_1}{dQ_1}(w) \ln \frac{dP_1}{dQ_1}(w) \right) \mathbb{1}_{\Omega \times \{1\}}(w_{ij}) dQ(w_{ij})$$

$$+ \int_{\Omega'} \left( \frac{dP_2}{dQ_2}(w) \ln \frac{dP_2}{dQ_2}(w) \right) \mathbb{1}_{\Omega \times \{2\}}(w_{ij}) dQ(w_{ij})$$

$$= \int_{\Omega} \left( \frac{dP_1}{dQ_1}(w) \ln \frac{dP_1}{dQ_1}(w) \right) (1-\lambda) dQ_1(w) + \dots$$

$$= (1-\lambda) KL(P_1, Q_1) + \lambda KL(P_2, Q_2) \quad \square$$

### Proposition (KL for product measures, independent case)

Let  $(\Omega, \mathcal{F})$  and  $(\Omega', \mathcal{F}')$  be two measurable spaces.

Let  $P, Q$  be two probability measures over  $(\Omega, \mathcal{F})$

$P', Q'$   $(\Omega', \mathcal{F}')$

and denote by  $P \otimes P'$  and  $Q \otimes Q'$  the product distributions over  $(\Omega \times \Omega', \mathcal{F} \otimes \mathcal{F}')$ . Then

$$KL(P \otimes P', Q \otimes Q') = KL(P, Q) + KL(P', Q')$$



Proof we have  $P \otimes P' \ll Q \otimes Q' \iff (P \ll Q \text{ and } P' \ll Q')$ , so we can

assume that all  $\ll$  statements hold. Then

$$\frac{d(P \otimes P')}{d(Q \otimes Q')} = \frac{dP}{dQ} \frac{dP'}{dQ'}$$

(this is a fundamental result in measure theory and of the best characterizations of independence).

Therefore by Tonelli

$$KL(P \otimes P', Q \otimes Q') = \int_{\Omega \times \Omega'} \left( \frac{dP}{dQ} \frac{dP'}{dQ'} \ln \left( \frac{dP}{dQ} \frac{dP'}{dQ'} \right) \right) d(Q \otimes Q')$$

$\int f \cdot g \geq 0$ , then



$$\int (f+g) d\mu = \int f d\mu + \int g d\mu$$

$$= \int_{\Omega'} \left( \int_{\Omega} \left( \frac{dP}{dQ} \ln \frac{dP}{dQ} \right) dQ \right) \frac{dP'}{dQ'} dQ'$$

$KL(P, Q)$

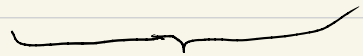
$KL(P, Q)$

here we apply Tonelli again

$$f = \frac{dP}{dQ} \left( \frac{dP}{dQ} \ln \frac{dP}{dQ} + \frac{1}{\epsilon} \right)$$

$$g = \frac{dP'}{dQ'} \left( \frac{dP'}{dQ'} \ln \frac{dP'}{dQ'} + \frac{1}{\epsilon} \right) \quad \text{here}$$

+ similar term with  $\ln \frac{dP'}{dQ'}$



$KL(P', Q')$

□

Consequence (Gaussian, Merand, Stoltz 2016)

Data-processing inequality with expectations of random variables.

Let  $X : (\Omega, \mathcal{F}) \rightarrow ([0, 1], \mathcal{B}([0, 1]))$  be any  $[0, 1]$ -valued random variable

Then, denoting by  $E_P[X]$  and  $E_Q[X]$  the respective expectations of  $X$  under  $P$  and  $Q$ , we have:

$$E_p[X] \ln \frac{E_p[X]}{E_q[X]} + (1 - E_p[X]) \ln \frac{1 - E_p[X]}{1 - E_q[X]} = \text{KL}(\text{Ber}(E_p[X]), \text{Ber}(E_q[X])) \leq \text{KL}(P, Q).$$

Proof: we denote by  $\mu$  the Lebesgue measure over  $[0, 1]$  and augment the underlying measurable space into  $(\Omega \times [0, 1], \mathcal{F} \otimes \mathcal{B}([0, 1]))$ , over which we consider the product-distributions  $P \otimes \mu$  and  $Q \otimes \mu$ .

For any event  $E \in \mathcal{F} \otimes \mathcal{B}([0, 1])$ , we have by the data processing inequality:

$$\underbrace{\text{KL}((P \otimes \mu)^{\mathbb{1}_E}, (Q \otimes \mu)^{\mathbb{1}_E})}_{\text{Ber}(P \otimes \mu)(E)} \leq \text{KL}(P \otimes \mu, Q \otimes \mu) = \text{KL}(P, Q) + \text{KL}(\mu, \mu) = \text{KL}(P, Q).$$

The proof is concluded by picking  $E \in \mathcal{F} \otimes \mathcal{B}([0, 1])$  such that  $P \otimes \mu(E) = E_p[X]$  and  $Q \otimes \mu(E) = E_q[X]$ .

Is it possible?

Yes, taking  $E = \left\{ (\omega, x) \in \Omega \times [0, 1] : x \leq X(\omega) \right\} \in \mathcal{F} \otimes \mathcal{B}([0, 1])$  as  $X$  is measurable.

By Tonelli's theorem:

$$P \otimes \mu(E) = \int_{\Omega} \left( \int_{[0, 1]} \mathbb{1}_{\{x \leq X(\omega)\}} d\mu(x) \right) dP(\omega) = \int_{\Omega} X(\omega) dP(\omega) \quad \text{and same for } Q. \quad \square$$

The chain rule - A generalization of the decomposition of the KL between product-distributions.

we will need it in a special case only, when the joint distributions follow from one of the marginal distributions via a stochastic kernel.

Definition Let  $(\Omega, \mathcal{F})$  and  $(\Omega', \mathcal{F}')$  be two measurable spaces; we denote by  $\mathcal{P}(\Omega', \mathcal{F}')$  the set of probability measures over  $(\Omega', \mathcal{F}')$ . A (regular) stochastic kernel  $K$  is a mapping  $(\Omega, \mathcal{F}) \rightarrow \mathcal{P}(\Omega', \mathcal{F}')$   
 $\omega \mapsto K(\omega, \cdot)$   
such that  $\forall B \in \mathcal{F}', \omega \mapsto K(\omega, B)$  is  $\mathcal{F}$ -measurable

Now consider two such kernels  $K$  and  $L$ , and two probability measures  $P$  and  $Q$  on  $(\Omega, \mathcal{F})$ . Then  $KP$  and  $LQ$  defined below are probability measures over  $(\Omega \times \Omega', \mathcal{F} \otimes \mathcal{F}')$ , by some extension theorem (Caratheodory)

$$\forall A \in \mathcal{F}, \forall B \in \mathcal{F}', \quad KP(A \times B) = \int_{\Omega} \underbrace{\mathbb{1}_A(\omega) K(\omega, B)}_{\text{is indeed measurable}} dP(\omega)$$

$$LQ(A \times B) = \int_{\Omega} \mathbb{1}_A(\omega) L(\omega, B) dQ(\omega)$$

An extension of Fubini (Tonelli) theorem

### Lemma

Let  $\psi: \Omega \times \Omega' \rightarrow \mathbb{R}$  be either  $\mathcal{F} \otimes \mathcal{F}'$  measurable and  $\geq 0$   
or  $KP$ -integrable.

Then  $w \mapsto \int_{\Omega'} \varphi(w, w') K(w, dw')$  is  $\mathcal{F}$ -measurable and  $\int_{\Omega \times \Omega'} \varphi dK \mathbb{P} = \int_{\Omega} \left( \int_{\Omega'} \varphi(w, w') K(w, dw') \right) d\mathbb{P}(w)$

including measurability of  $w \mapsto \int \varphi(w, \cdot) K(w, d\cdot)$  by regularity of  $K$

Proof (sketch): The result is true for  $\varphi = \mathbb{1}_{A \times B}$  by definition of  $K \mathbb{P}$ .

Extension to  $\mathbb{1}_E$  for any  $E \in \mathcal{F} \otimes \mathcal{F}'$  by an argument of  $\sigma$ -algebra contained/monotone class theorem, using monotone convergence (including the  $w \mapsto \int_{\Omega'} \dots$  measurability)

Extension to  $\begin{cases} \varphi \geq 0 \\ \varphi \in L^1 \end{cases}$  by monotone convergence

↓ actually with no loss of generality.

Theorem (chain rule for KL): Assume  $\mathbb{P} \ll \mathbb{Q}$

As soon as  $(*) K(w, \cdot) \ll L(w, \cdot)$  for  $\mathbb{Q}$ -almost all  $w \in \Omega$

with  $(**)$  the existence of a function  $g: (w, w') \mapsto \frac{dK(w, \cdot)}{dL(w, \cdot)}(w')$  being  $\mathcal{F} \otimes \mathcal{F}'$ -measurable,  $\hat{=}$  up to a  $L \mathbb{Q}$ -null set

Then 
$$KL(K \mathbb{P}, L \mathbb{Q}) = KL(\mathbb{P}, \mathbb{Q}) + \int_{\Omega} KL(K(w, \cdot), L(w, \cdot)) d\mathbb{P}(w)$$

where  $w \mapsto KL(K(w, \cdot), L(w, \cdot))$  is indeed  $\mathcal{F}$ -measurable and  $\geq 0$  so that the integral in the right-hand side is well defined.

Remark:

1) the assumptions  $(*)$  and  $(**)$  will be satisfied for the

applications we have in mind.

2) They can be relaxed: - it suffices to assume that  $\Omega'$  is a topological space with a countable base and  $\mathcal{F}'$  is the Borel  $\sigma$ -algebra.

i.e. there exists some countable collection  $(O_m)_{m \geq 1}$  of open sets of  $\Omega'$  such that each open set  $V$  of  $\Omega'$  can be written

$$V = \bigcup_{i: O_i \subset V} O_i, \text{ that is, as a countable union of elements of}$$

$(O_m)_{m \geq 1}$

Ex:  $\Omega'$  a separable metric space  $\rightarrow$  we will consider

$$\Omega' = [0, 1] \times (\mathbb{R} \times [0, 1])^{\mathbb{N}}$$

Proof

\* by bi-measurability of  $g|ng$ , and since  $g|ng$  is lower bounded,

or immediate extension of

the previous lemma can be applied to get  $w \mapsto \int_{\Omega'} g(w, \cdot) \ln(g(w, \cdot)) L(w, d\cdot)$   
 $= KL(K(w, \cdot), L(w, \cdot))$

is  $\mathcal{F}$ -measurable and  $\geq 0$

\* We assume  $P \ll Q$ , let  $f = \frac{dP}{dQ}$ . What can we say about  $(w, w') \mapsto f(w) g(w, w')$ ?

$$\int \mathbb{1}_{A \times B}(w, w') f(w) g(w, w') dLQ(w, w') = \int_{\Omega} \left( \int_{\Omega'} \mathbb{1}_B(w') g(w, w') L(w, dw') \right) \mathbb{1}_A(w) f(w) dQ(w)$$

extension of Tonelli

$$= \int_{\Omega'} \mathbb{1}_B(\omega') K(\omega, d\omega') = K(\omega, B)$$

$$= \int_{\Omega} \underbrace{\mathbb{1}_A(\omega)}_{\mathcal{F}\text{-measurable}} \underbrace{K(\omega, B)}_{d\mathbb{P}(\omega)} f(\omega) d\mathbb{Q}(\omega) = \mathbb{K}\mathbb{P}(A \times B) \quad \text{by def of } \mathbb{K}\mathbb{P}$$

By Radon-Nikodym's theorem:  $\frac{d\mathbb{K}\mathbb{P}}{dL\mathbb{Q}} = fg$   $L\mathbb{Q}$ -as

• It is easily seen that  $\mathbb{K}\mathbb{P} \ll L\mathbb{Q} \Rightarrow \mathbb{P} \ll \mathbb{Q}$  (in all cases, even without  $(*)$  and  $(**)$ )

$$\text{indeed } L\mathbb{Q}(A \times \Omega') = \mathbb{Q}(A)$$

$$\mathbb{K}\mathbb{P}(A \times \Omega') = \mathbb{P}(A)$$

• Therefore under  $(*)$ ,  $(**)$ , we have  $\mathbb{K}\mathbb{P} \ll L\mathbb{Q} \Leftrightarrow \mathbb{P} \ll \mathbb{Q}$ .

$$\text{Then } \text{KL}(\mathbb{K}\mathbb{P}, L\mathbb{Q}) = \int_{\Omega \times \Omega'} (f(\omega)g(\omega, \omega') \ln(f(\omega)g(\omega, \omega'))) dL\mathbb{Q}(\omega, \omega').$$

$\Psi = fg \ln(fg)$  is lower bounded. The lemma (extension of Fubini-Tonelli extends to it):

$$\int (fg \ln(fg)) dL\mathbb{Q} = \int_{\Omega} f(\omega) \left( \int_{\Omega'} g(\omega, \omega') (\ln g(\omega, \omega') + \ln f(\omega)) L(\omega, d\omega') \right) d\mathbb{Q}(\omega)$$

(again we can use the translation by  $+\frac{1}{e}$  to justify this equality)

$$= \int_{\Omega} \left( \underbrace{\int_{\Omega'} g(\omega, \omega') \ln g(\omega, \omega') L(\omega, d\omega')}_{\text{KL}(K(\omega, \cdot), L(\omega, \cdot))} + \underbrace{\ln f(\omega) \int_{\Omega'} g(\omega, \omega') L(\omega, d\omega')}_{=1} \right) f(\omega) d\mathbb{Q}(\omega)$$

$$= \int_{\Omega} (\text{KL}(K(\omega, \cdot), L(\omega, \cdot)) + \ln(f(\omega))) p(\omega) dQ(\omega)$$

again, sum of two functions  
bounded from below

$$= \int_{\Omega} \underbrace{\text{KL}(K(\omega, \cdot), L(\omega, \cdot))}_{dP(\omega)} p(\omega) dQ(\omega) + \int_{\Omega} \underbrace{\ln(f(\omega))}_{\text{KL}(P, Q)} dQ(\omega)$$

□