Let's first complete the proof of the Lemma: ["Hoeffding-Azuma inequality with a random number of summands"]

Setting: Probability distributions $\nu_1, \dots \nu_K$ over $[0,1]$ with respective expectations $\mu_1, \dots \mu_K$

At each round, $I_t \in \{1, \dots K\}$ is picked in a $\sigma(Y_1, \dots Y_{t-1})$-measurable way

then Y_t is drawn independently at random according to ν_{I_t}, given I_t

ie: $Y_t \mid I_t \sim \nu_{I_t}$

We denote $N_a(t) = \sum_{s=1}^{t} \mathbb{1}_{\{I_s = a\}}$ and assume that each arm a was pulled once in the first K rounds, so that:

$$N_a(t) \geqslant 1 \qquad \forall t \geqslant K$$

Then, for $t \geqslant K$: $\hat{\mu}_{a,t} = \dfrac{1}{N_a(t)} \sum_{s=1}^{t} Y_s \mathbb{1}_{\{I_s = a\}}$

Lemma: $\forall \delta \in (0,1)$, $\mathbb{P}\left\{ \mu_a > \hat{\mu}_{a,t} - \sqrt{\dfrac{\ln(1/\delta)}{2 N_a(t)}} \right\} \geqslant 1 - t\delta$

(and a similar symmetric statement with $\mu_a < \hat{\mu}_{a,t} + \sqrt{\dots}$)

The proof will be based on the fact that $(Z_t)_{t \geqslant 0}$, where

$$Z_t = \sum_{s=1}^{t} (Y_s - \mu_a) \mathbb{1}_{\{I_s = a\}}$$

is a martingale wrt. $(\mathcal{F}_t) = (\sigma(Y_1, \dots Y_t))_{t \geqslant 0}$, which we already proved last time:

$$\mathbb{E}\big[(Y_t - \mu_a) \mathbb{1}_{\{I_t = a\}} \mid Y_1 \dots Y_{t-1} \big] = \mathbb{E}\big[(Y_t - \mu_a) \mathbb{1}_{\{I_t = a\}} \mid I_t, Y_1 \dots Y_{t-1} \big]$$

$$= \big(\mathbb{E}[Y_t \mid I_t, Y_1 \dots Y_{t-1}] - \mu_a \big) \mathbb{1}_{\{I_t = a\}}$$

where we used the bandit model

$$= (\mu_{I_t} - \mu_a) \mathbb{1}_{\{I_t = a\}} = 0 \quad \text{a.s.}$$

Remark: How does this bound compare to what the classical version of the Hoeffding-Azuma says?

Martingale increment $(Y_s - \mu_a) \mathbb{1}_{\{I_s = a\}}$ bounded between

$$a_t = -\mu_a \quad \text{and} \quad b_t = 1 - \mu_a$$

so that

(actually in the version I stated, I can take $\leqslant$ or $<$) $\quad (b_t - a_t)^2 = 1$

$$1 - t\delta \leqslant \mathbb{P}\left\{ Z_t < \sqrt{\frac{t}{2} \ln \frac{1}{t\delta}} \right\} = \mathbb{P}\left\{ N_a(t)\left(\hat{\mu}_{a,t} - \mu_a\right) < \sqrt{\frac{t}{2}\ln\frac{1}{t\delta}} \right\}$$

$$= \mathbb{P}\left\{ \hat{\mu}_{a,t} - \sqrt{\frac{t}{N_a(t)}} \sqrt{\frac{\ln(1/t\delta)}{2\, N_a(t)}} < \mu_a \right\}$$

versus the bound of our lemma: $1 - t\delta \leqslant \mathbb{P}\left\{ \hat{\mu}_{a,t} - \sqrt{\frac{\ln(1/\delta)}{2 N_a(t)}} < \mu_a \right\}$

The proposed deviations essentially differ from a $\sqrt{t/N_a(t)}$ factor, and it is so nice to get rid of it!

<u>Proof:</u> (1) We prove that $\forall x \in \mathbb{R}$, $\mathbb{E}\left[e^{x Z_t - x^2/8\, N_a(t)} \right] \leqslant 1$

We do so by showing that $M_t = \exp\left(x Z_t - \frac{x^2}{8} N_a(t) \right)$ is a supermartingale, so that $\mathbb{E}[M_t] \leqslant \mathbb{E}[M_0] = 1$.

<u>Indeed</u>, by the conditional version of Hoeffding's lemma,

$$\mathbb{E}\left[e^{x(Y_t - \mu_a)\mathbb{1}_{\{I_t = a\}}} \,\middle|\, \mathcal{F}_{t-1} \right] \leqslant e^{x^2/8} \quad \text{a.s.}$$

but we can do better!

Since I_t and thus also $\mathbb{1}_{\{I_t = a\}}$ are $\mathcal{F}_{t-1}$-measurable, we get:

$$\mathbb{E}\left[e^{x(Y_t - \mu_a)\mathbb{1}_{\{I_t=a\}}} \,\middle|\, \mathcal{F}_{t-1} \right] = \mathbb{E}\left[e^{x(Y_t - \mu_a)\mathbb{1}_{\{I_t=a\}}} \left(\mathbb{1}_{\{I_t = a\}} + \mathbb{1}_{\{I_t \neq a\}} \right) \,\middle|\, \mathcal{F}_{t-1} \right]$$

$$= \mathbb{E}\left[e^{x(Y_t - \mu_a)\mathbb{1}_{\{I_t=a\}}} \,\middle|\, \mathcal{F}_{t-1} \right] \mathbb{1}_{\{I_t=a\}} + e^0\, \mathbb{1}_{\{I_t \neq a\}}$$

given what we had before

$$\leqslant e^{x^2/8}\, \mathbb{1}_{\{I_t = a\}} + \mathbb{1}_{\{I_t \neq a\}} = \exp\left(\frac{x^2}{8} \mathbb{1}_{\{I_t = a\}} \right)$$

Put differently, $\mathbb{E}\left[e^{x(Y_t - \mu_a)\mathbb{1}_{\{I_t=a\}} - \frac{x^2}{8}\mathbb{1}_{\{I_t=a\}}} \,\middle|\, \mathcal{F}_{t-1} \right] \leqslant 1$

which entails that $\exp\left(x \sum_{s=1}^{t} (Y_s - \mu_a)\mathbb{1}_{\{I_s = a\}} - \frac{x^2}{8} \sum_{s=1}^{t} \mathbb{1}_{\{I_s = a\}} \right)$

$$= \exp\left(x Z_t - \frac{x^2}{8} N_a(t) \right) = M_t$$

is a supermartingale wrt $\mathcal{F}_t = \sigma(Y_1, \ldots Y_t)$.

(2) We prove that $\forall \varepsilon > 0$, $\forall \ell \geq 1$, $\mathbb{P}\{ Z_t \geq \varepsilon \text{ and } N_a(t) = \ell \} \leq \exp(-2\varepsilon^2/\ell)$

Indeed, by a Markov-Chernov bounding,

$\forall x > 0$,

$$\mathbb{P}\{ Z_t \geq \varepsilon \text{ and } N_a(t) = \ell \} \leq e^{-x\varepsilon} \, \mathbb{E}\left[e^{x Z_t} \mathbb{1}_{\{N_a(t)=\ell\}} \right]$$

$$= e^{-x\varepsilon + \frac{x^2 \ell}{8}} \, \mathbb{E}\left[e^{x Z_t - \frac{x^2}{8} N_a(t)} \mathbb{1}_{\{N_a(t)=\ell\}} \right]$$

$$\leq e^{-x\varepsilon + x^2\ell/8} \, \underbrace{\mathbb{E}\left[e^{x Z_t - \frac{x^2}{8} N_a(t)} \right]}_{\leq 1 \text{ by } (1)}$$

Optimizing over $x > 0$ (take $x = 4\varepsilon/\ell$) yields the claimed bound.

(3) Conclusion: we prove that $\mathbb{P}\left\{ \mu_a \leq \hat{\mu}_{at} - \sqrt{\dfrac{\ln(1/\delta)}{2 N_a(t)}} \right\} \leq t\delta$

Indeed, by distinguishing according to the values taken by $N_a(t)$:

$$\mathbb{P}\left\{ \mu_a \leq \hat{\mu}_{at} - \sqrt{\frac{\ln(1/\delta)}{2 N_a(t)}} \right\}$$

$$= \sum_{\ell=1}^{t} \mathbb{P}\left\{ N_a(t) = \ell \text{ and } \mu_a \leq \hat{\mu}_{at} - \sqrt{\ln(1/\delta)/2\ell} \right\}$$

$\Big(\sum_{\ell=1}^{t-K+1}$ would be enough $\Big)$

$$= \sum_{\ell=1}^{t} \mathbb{P}\left\{ N_a(t) = \ell \text{ and } \frac{Z_t}{N_a(t)} \geq \sqrt{\ln(1/\delta)/2\ell} \right\}$$

$$= \sum_{\ell=1}^{t} \mathbb{P}\left\{ N_a(t) = \ell \text{ and } Z_t \geq \sqrt{\ell \ln(1/\delta)/2} \right\}$$

by (2)

$$\leq \sum_{\ell=1}^{t} \exp\Big(-2 \big(\ell \ln(1/\delta)/2 \big) / \ell \Big) = t\delta.$$

<u>Two notes</u> on this proof:

* We noted last week that the conditional version of Hoeffding's lemma (based on Proof #2) could be generalized into

X bounded random variable, U, V two $\mathcal{G}$-measurable random variables with $U \leq X \leq V$

then $\forall s \in \mathbb{R}$, $\ln \mathbb{E}\left[e^{sX} \mid \mathcal{G} \right] \leqslant s\, \mathbb{E}[X \mid \mathcal{G}] + \frac{s^2}{8}(V-U)^2$

(Because of the proof technique relying on weights with denominators $1/_{V-U}$, it is safer to assume $V-U>0$ as, eg, by replacing U and V by $U-\varepsilon$ and $V+\varepsilon$ if needed and letting $\varepsilon \searrow 0$; so at the end of the day we may drop the $V-U>0$ as condition.)

* This extension may be applied to

$$X_t = (Y_t - \mu_a)\, \mathbb{1}_{\{I_t = a\}}$$
$$\mathcal{G} = \mathcal{F}_{t-1}$$
$$U_t = -\mu_a \, \mathbb{1}_{\{I_t = a\}}$$
$$V_t = (1-\mu_a)\, \mathbb{1}_{\{I_t = a\}}$$

and directly entails

$$\mathbb{E}\left[e^{s(Y_t - \mu_a)\mathbb{1}_{\{I_t=a\}}} \mid \mathcal{F}_{t-1} \right] \leqslant \exp\left(\frac{s^2}{8}\, \mathbb{1}_{\{I_t = a\}} \right)$$

without the need for the

$$1 = \mathbb{1}_{\{I_t = a\}} + \mathbb{1}_{\{I_t \neq a\}}$$

trick used in Step (1).

* The question is: Don't we have a generalized version of the Hoeffding-Azuma inequality with such predictable ranges $V_t - U_t$?

Yes we do have something in terms of constant upper bounds $V_t - U_t \leqslant \Delta_t \in \mathbb{R}$ as

But $V_t - U_t = \mathbb{1}_{\{I_t = a\}}$ can only be bounded by $\Delta_t = 1$

So I think that Steps (2) and (3) are needed

Stochastic bandits : What about arms indexed by a continuum?

Setting 1 : Arms indexed by $x \in A$, where A is some possibly large set

With each arm $x \in A$ is associated a probability distribution ν_x over $\mathbb{R}$ s.t. $E(\nu_x)$ exists

At each round, the decision-maker picks $I_t \in A$, gets a reward Y_t drawn at random according to ν_{I_t} (given I_t); and this is the only feedback she gets.

Definition : $f : x \in A \longmapsto E(\nu_x)$ is the mean-payoff function

Regret : $\overline{R}_T = T \sup_{x \in A} f(x) - E\left[\sum_{t=1}^{T} Y_t\right]$

Setting 2 : [special case] $\longrightarrow$ Noisy optimization of a function.

We fix $f : A \to \mathbb{R}$

The noise is given by a sequence of iid random variables $\varepsilon_1, \varepsilon_2, \ldots$

When $I_t \in A$ is picked, $Y_t = f(I_t) + \varepsilon_t$

↳ Special case of setting #1 where ν_x is the distribution of $f(x) + \varepsilon_1$ (all these distributions have the same shape given by the common distribution of the ε_j)

We of course need conditions for the regret to be minimized.

Definition : Let $\mathcal{F}$ be a set of possible bandit problems $\underline{\nu} = (\nu_x)_{x \in A}$

The regret can be controlled (in a non-uniform way) against $\mathcal{F}$ if:

there exists a strategy s.t. $\forall \underline{\nu} \in \mathcal{F}$, $\overline{R}_T = o(T)$.

we also say that $(A, \mathcal{F})$ is tractable

Ex: $\mathcal{A} = \{1, \dots K\}$ and $\underbrace{\mathcal{F} = \left(\mathcal{P}([0,1])\right)^K}_{\text{the case of finitely many arms with bounded distributions}}$, the set of all K-tuples of probability distributions over $[0,1]$

→ UCB does the job.

Counter-example: $\mathcal{A} = [0,1]$ and $\mathcal{F} = \underbrace{\left(\mathcal{P}([0,1])\right)^{[0,1]}}$

↑ illustrating that continuity is a minimal requirement.

all bandit problems $(\nu_x)_{x\in[0,1]}$ with distributions ν_x having support $[0,1]$.

Indeed: Consider $(\delta_0)_{x\in[0,1]}$ the bandit problem in which each arm x is associated with the Dirac mass on 0

Fix any strategy: it gets $Y_t = 0 \quad \forall t$ and uses a sequence of (possibly) random choices I_t, $t \geq 1$

Since probability distributions can only have at most countably many atoms, $\mathcal{Y} = \{x\in[0,1] : \exists t \mid \mathbb{P}\{I_t = x\} > 0 \text{ under } (\delta_0)_{x\in[0,1]}\}$

is countable. In particular, $[0,1]\setminus\mathcal{Y}$ is non empty.

But the strategy behaves the same under the problem $(\nu'_x)_{x\in[0,1]}$ in which $\begin{cases} \nu'_x = \delta_0 & \forall x \neq x_0 \\ \nu'_{x_0} = \delta_1 & \text{for one fixed } x_0 \in [0,1]\setminus\mathcal{Y} \end{cases}$

With probability 1, it thus never hits x_0.

Therefore, $Y_t = 0$ a.s. $\forall t$ and $\overline{R}_T = T - \mathbb{E}\left[\sum_{t=1}^{T} Y_t\right] = T$.

Actually, continuity is sufficient for the regret to be controlled, as long as $\mathcal{A}$ is not too large.

Theorem: Let $\mathcal{A}$ be a metric space and let $\mathcal{F}^{\text{cont}}$ be the set of bandit problems $(\nu_x)_{x\in\mathcal{A}}$

with: → $\forall x$, ν_x is a distribution over $[0,1]$

→ a continuous mean-payoff function $f : x \mapsto \mathbb{E}(\nu_x)$

The regret can be controlled against $\mathcal{F}^{cont}$ if and only if A is separable.

Corollary. Let $\mathcal{F}^{all}$ be the family of all bandit models $(\nu_x)_{x\in A}$ with distributions ν_x over $[0,1]$. Then the regret against $\mathcal{F}^{all}$ can be controlled if and only if A is at most countable.

let A be any set.

Before we prove these facts, consider the following more concrete example, in which, by strengthening the regularity requirement on the mean-payoff function, we can even get rates.

Exercise: (Lipschitz bandits) Let $A = [0,1]$ and let $\mathcal{F}^{Lip}$ be the family of bandit models $(\nu_x)_{x\in[0,1]}$ with distributions ν_x over $[0,1]$ and with mean-payoff functions that are Lipschitz.

Exhibit a strategy based on UCB + a sequence of discretizations of $[0,1]$ into K bins (to be refined over time) such that:

$$\forall \nu \in \mathcal{F}^{Lip}, \qquad \overline{R}_T \leq \left(3L + 6\sqrt{8\ln T + 2}\right)T^{2/3} + 2$$

where L is the Lipschitz constant of the mean-payoff function of ν

Hint: First, prove a performance bound by splitting $[0,1]$ into $[(i-1)/K, i/K]$ with $i = 1, \dots, K$ for a fixed K, where each bin $[(i-1)/K, i/K]$ plays the role of an i in a bandit problem with finitely many arms. Then discuss how to pick K over the time, as we do in the next proof.

Proof of the Corollary:

We endow A with the discrete topology, ie, chose the distance $d(x,y) = \mathbb{1}_{\{x\neq y\}}$. Then:

1. All applications $f: A \to \mathbb{R}$ are continuous
2. A is separable if and only if A is at most countable.

Proof of the Theorem: It relies on the possibility or impossibility of uniform exploration of the arms

1) If $\mathcal{A}$ is separable: let $(x_n)_{n\in\mathbb{N}}$ be a collection of points in $\mathcal{A}$ that is dense

We pick actions in a triangular fashion:

Regime 1: UCB based on $x_1\, x_2$ (fresh start) : $I_1^{(1)} \ldots I_4^{(1)}$

⋮

Regime r: UCB based on $x_1\, x_2 \ldots x_r$ (fresh start) $I_1^{(r)} \ldots I_{(r+1)^2}^{(r)}$

⋮

In Regime r: (starts at time $S_r + 1 = 2^2 + \cdots r^2 + 1$)

$$(r+1)^2 \max_{s\leq r} f(x_s) - \mathbb{E}\left[\sum_{t=S_r+1}^{S_r+(r+1)^2} Y_t\right] \qquad (*)$$

$$\leq c\sqrt{r^3 \ln r}$$

c: well-chosen numerical constant

$\sqrt{r^3 \ln r}$: order of magnitude of the distribution-free regret bound for UCB on $(r+1)^2$ steps with r arms (we saw this bound as an exercise)

Now, let $\varepsilon > 0$ and let $\tilde{r}_\varepsilon \in \mathbb{N}^*$ s.t. $\mu_{x_{\tilde{r}_\varepsilon}} \geq \sup_{\mathcal{A}} f - \varepsilon$

($\tilde{r}_\varepsilon$ exists by separability of $\mathcal{A}$ and continuity of f)

In particular, $\max_{s\leq \tilde{r}_\varepsilon} f(x_s) \geq \sup_{\mathcal{A}} f - \varepsilon \qquad (**)$

We denote by r_T the index of the regime where T lies:

we have that S_r is of the order of r^3

thus that r_T is of the order of $T^{1/3}$

in particular, $r_T = O(T^{1/3})$

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The regret can be decomposed (for T large enough) as

$$\overline{R}_T = T \sup_{\mathcal{A}} f - \mathbb{E}\left[\sum_{t=1}^{T} Y_t\right] = \text{sum of the regrets of each regime}$$

$$= \underbrace{\sum_{r=1}^{\tilde{r}_\varepsilon - 1} (r+1)^2}_{\substack{\text{initial regimes,}\\ \text{regret bounded}\\ \text{by their lengths}\\ = O(1)}} + \underbrace{\sum_{r=\tilde{r}_\varepsilon}^{r_T - 1} \left((r+1)^2 \varepsilon + c\sqrt{r^3 \ln r} \right)}_{\text{cf. bounds } (*) \text{ and } (**)} + \underbrace{(r_T+1)^2}_{\substack{\text{regime } r_T\\ \text{may be}\\ \text{incomplete}}}$$

$$\leqslant T\varepsilon + c \sum_{r=\tilde{r}_\varepsilon}^{r_T - 1} r^{3/2} \sqrt{\ln r_T} \qquad = O(T^{2/3})$$

$$\leqslant T\varepsilon + O\left(r_T^{5/2} \sqrt{\ln r_T} \right)$$

$$= T\varepsilon + O\left(T^{5/6} \sqrt{\ln T} \right)$$

All in all, $\displaystyle \limsup \frac{\overline{R}_T}{T} \leqslant \varepsilon$, which is true $\forall \varepsilon > 0$,

that is, $\displaystyle \lim \frac{\overline{R}_T}{T} = 0$ as requested.

2) If $\mathcal{A}$ is not separable:

* We use the following characterization of separability (which relies on Zorn's lemma):

> A metric space $\mathcal{X}$ is separable if and only if it contains no uncountable subset $\mathcal{D}$ s.t.
> $$\rho = \inf\{ d(x,y) : x,y \in \mathcal{D}\} > 0.$$

In particular, if $\mathcal{A}$ is not separable, there exist an uncountable subset $\mathcal{D} \subset \mathcal{A}$ and $\rho > 0$ such that the balls $B(a, \rho/2)$, with $a \in \mathcal{D}$, are all disjoint.

↳ No probability distribution over $\mathcal{A}$ can give a positive mass to all these balls.

* We consider the bandit models $\nu^{(a)}$ inducing mean-payoff functions
$$f^{(a)} : x \in \mathcal{A} \longmapsto \left(1 - \frac{d(x,a)}{\rho/2}\right)^{+} ;$$ in particular, $\nu^{(a)}_x = \delta_0$ for $x \notin B(a, \rho/2)$.

↑ $f^{(a)}$ is indeed continuous.

We proceed as in the example showing the necessity of continuity when $\mathcal{A} = [0,1]$ and consider the bandit model $(\delta_0)_{x\in\mathcal{A}}$, as well as any strategy and the laws induced by the I_t under this model: let q_t be the law of I_t under $(\delta_0)_{x\in\mathcal{A}}$ and let $q = \sum_{t \geq 1} \frac{1}{2^t} q_t$.

[as only countably many balls can have a positive mass under q

↳ There exists $a \in \mathcal{A}$ s.t. $q\big(B(a,\rho/2)\big) = 0$, that is, s.t.,
$$\forall t \geq 1, \qquad \mathbb{P}\Big(I_t \in B(a,\rho/2) \text{ under } (\delta_0)_{x\in\mathcal{A}} \Big) = 0.$$

The considered strategy is therefore such that the I_t have the same distribution under $(\delta_0)_{x\in\mathcal{A}}$ and $\nu^{(a)}$. In particular, $\mathbb{E}\left[\sum_{t=1}^{T} Y_t\right] = 0$ in both cases, but in the latter case, $\sup f^{(a)} = 1$, so that $\overline{R}_T = T$ against $\nu^{(a)}$. The regret is not controlled against $\nu^{(a)} \in \mathcal{F}^{\mathrm{cont}}$.

[Back to K-armed bandits]

Overview of the next topic: Fix a model $\mathcal{D}$, known to the decision-maker, i.e. a collection of probability distributions over $\mathbb{R}$ with an expectation.

Assume that $\nu_1, \ldots \nu_K$ are unknown but that the decision-maker knows $\nu_j \in \mathcal{D}$ $\forall j$.

What are the best bounds on $\overline{R}_T = T\mu^* - \mathbb{E}\left[\sum_{t=1}^{T} Y_t\right]$?

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

$$\overline{R}_T \text{ is at best of the order of } \left(\sum_{a : \Delta_a > 0} \frac{\Delta_a}{\mathcal{K}_{\inf}(\nu_a, \mu^*, \mathcal{D})}\right) \ln T$$

where

$$\mathcal{K}_{\inf}(\nu_a, \mu^*, \mathcal{D}) = \inf \left\{ \mathrm{KL}(\nu_a, \nu'_a) : \begin{array}{l} \nu'_a \in \mathcal{D} \\ \mathbb{E}(\nu'_a) > \mu^* \end{array} \right\}$$

Kullback-Leibler divergence

expectation of ν'_a

We will only prove the lower bound part

but not discuss the strategy, called KL-UCB, to achieve the bound. } it's just a matter of time, we would need about 3h to discuss this strategy

|| * But * before we do that, I guess that some reminder of basic and non-basic results about KL divergences would be needed!

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The Kullback-Leibler divergence: definition and basic properties.

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

$$\mathrm{KL}(\mathbb{P},\mathbb{Q}) = \begin{cases} +\infty & \text{if } \mathbb{P} \text{ is not absolutely continuous wrt } \mathbb{Q} \\ \displaystyle\int_\Omega \left(\frac{d\mathbb{P}}{d\mathbb{Q}} \ln \frac{d\mathbb{P}}{d\mathbb{Q}} \right) d\mathbb{Q} = \int_\Omega \left(\ln \frac{d\mathbb{P}}{d\mathbb{Q}} \right) d\mathbb{P} & \text{if } \mathbb{P} \ll \mathbb{Q} \end{cases}$$

Basic facts:

- Existence of the defining integral when $\mathbb{P} \ll \mathbb{Q}$: because $\varphi : x \mapsto x \ln x$ is bounded from below on $[0, +\infty)$

- $\mathrm{KL}(\mathbb{P},\mathbb{Q}) \geq 0$ and $\mathrm{KL}(\mathbb{P},\mathbb{Q})$ if and only if $\mathbb{P} = \mathbb{Q}$:

It suffices to consider the case $\mathbb{P} \ll \mathbb{Q}$: because φ is strictly convex, Jensen's inequality indicates that

$$\mathrm{KL}(\mathbb{P},\mathbb{Q}) = \int_\Omega \varphi\left(\frac{d\mathbb{P}}{d\mathbb{Q}}\right) d\mathbb{Q} \geq \varphi\Bigg(\underbrace{\int_\Omega \frac{d\mathbb{P}}{d\mathbb{Q}} \, d\mathbb{Q}}_{=1} \Bigg) = 0,$$

with equality if and only if $\frac{d\mathbb{P}}{d\mathbb{Q}}$ is $\mathbb{Q}$-as constant, ie, $\mathbb{P} = \mathbb{Q}$

Exercise: A useful rewriting. Prove the following result:

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

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

Beware: with the usual measure-theoretic conventions, if $x \neq 0$ and $y = 0$, then $x \neq y \dfrac{x}{y}$

↳ you therefore need to proceed with care!

Lemma (contraction of entropy; also known as data-processing inequality):

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

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

Denote by $\mathbb{P}^X$ and $\mathbb{Q}^X$ the laws of X under $\mathbb{P}$ and $\mathbb{Q}$.

Then:

$$\mathrm{KL}(\mathbb{P}^X, \mathbb{Q}^X) \leqslant \mathrm{KL}(\mathbb{P}, \mathbb{Q}).$$

Proof: We may assume that $\mathbb{P} \ll \mathbb{Q}$, otherwise $\mathrm{KL}(\mathbb{P},\mathbb{Q}) = +\infty$ and the inequality is true. We show that we then have

$$\mathbb{P}^X \ll \mathbb{Q}^X, \quad \text{with} \quad \frac{d\mathbb{P}^X}{d\mathbb{Q}^X} = \mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X = \cdot \right] \overset{\text{not.}}{=} \gamma$$

ie, $\gamma(X) = \mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X \right]$.

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

$$\mathbb{P}^X(B) = \mathbb{P}\{X \in B\} = \int_\Omega \mathbb{1}_B(X) \frac{d\mathbb{P}}{d\mathbb{Q}} \, d\mathbb{Q} \overset{\text{tower rule}}{=} \int_\Omega \mathbb{1}_B(X) \, \mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X \right] d\mathbb{Q}$$

$$\overset{\text{not.}}{=} \int_\Omega \mathbb{1}_B(X) \, \gamma(X) \, d\mathbb{Q} \underset{\substack{\text{by} \\ \text{definition of } \mathbb{Q}^X}}{=} \int_{\Omega'} \mathbb{1}_B \, \gamma \, d\mathbb{Q}^X.$$

Therefore,

$$\mathrm{KL}(\mathbb{P}^X, \mathbb{Q}^X) = \int_{\Omega'} \gamma \ln \gamma \, d\mathbb{Q}^X = \int_\Omega \gamma(X) \ln \gamma(X) \, d\mathbb{Q}$$

$$\underset{\text{definition of } \gamma}{=} \int_\Omega \left(\mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X \right] \ln \mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X \right] \right) d\mathbb{Q}$$

$$\underset{\text{conditional version of Jensen's inequality}}{\leqslant} \int_\Omega \mathbb{E}_{\mathbb{Q}}\left[\frac{d\mathbb{P}}{d\mathbb{Q}} \ln \frac{d\mathbb{P}}{d\mathbb{Q}} \,\Big|\, X \right] d\mathbb{Q}$$

$$\underset{\text{tower rule}}{=} \int_\Omega \left(\frac{d\mathbb{P}}{d\mathbb{Q}} \ln \frac{d\mathbb{P}}{d\mathbb{Q}} \right) d\mathbb{Q} = \mathrm{KL}(\mathbb{P}, \mathbb{Q})$$

References : • The proof above is due to Ali and Silvey (1966), 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, which we discuss below, is typically proved in a tedious way, relying on the rewriting of Exercise 1 and the joint convexity of $(x,y) \in [0,+\infty)^2 \longmapsto \left(\frac{x}{y} \ln \frac{x}{y}\right) y$

We may see it instead as a consequence of the data-processing inequality :

Corollary (joint convexity of KL) : For all probability distributions $\mathbb{P}_1$, $\mathbb{P}_2$ and $\mathbb{Q}_1$, $\mathbb{Q}_2$ over the same measurable space $(\Omega, \mathcal{F})$, and all $\alpha \in (0,1)$,

$$\mathrm{KL}\big((1-\alpha)\mathbb{P}_1 + \alpha\mathbb{P}_2, (1-\alpha)\mathbb{Q}_1 + \alpha\mathbb{Q}_2\big) \leqslant (1-\alpha)\,\mathrm{KL}(\mathbb{P}_1, \mathbb{Q}_1) + \alpha\,\mathrm{KL}(\mathbb{P}_2, \mathbb{Q}_2)$$

Proof : We augment $(\Omega, \mathcal{F})$ into $(\Omega \times \{1,2\}, \mathcal{F}')$ where
$$\mathcal{F}' = \mathcal{F} \otimes \big\{\emptyset, \{1\}, \{2\}, \{1,2\}\big\}$$

We define the random pair (X, J) by the projections
$$X : (\omega, j) \mapsto \omega \quad \text{and} \quad J : (\omega, j) \mapsto j$$

Let $\mathbb{P}$ be a probability measure on $(\Omega \times \{1,2\}, \mathcal{F}')$ such that
$$\begin{cases} J \sim 1 + \mathrm{Ber}(\alpha) \\ X \mid J=j \sim \mathbb{P}_j \end{cases}$$
(and a similar definition for $\mathbb{Q}$ based on $\mathbb{Q}_1$, $\mathbb{Q}_2$)

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

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

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

and (as we prove below) $\mathrm{KL}(\mathbb{P},\mathbb{Q}) = (1-\alpha)\,\mathrm{KL}(\mathbb{P}_1,\mathbb{Q}_1) + \alpha\,\mathrm{KL}(\mathbb{P}_2,\mathbb{Q}_2)$
so that the result follows from the data-processing inequality.

Indeed: we may assume with no loss of generality, given $\alpha\in(0,1)$, that $\mathbb{P}_1 \ll \mathbb{Q}_1$ and $\mathbb{P}_2 \ll \mathbb{Q}_2$, 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

$$\mathrm{KL}(\mathbb{P},\mathbb{Q}) = \int_{\Omega\times\{1,2\}} \left(\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,j)\ \ln\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,j)\right) d\mathbb{Q}(\omega,j)$$

we just use that for $f \geq$ a constant, $\int f\,d\mu = \int f\mathbb{1}_A\,d\mu + \int f\mathbb{1}_{A^c}\,d\mu$, whether f is integrable or not

$$= \int_{\Omega\times\{1,2\}} \left(\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,1)\ \ln\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,1)\right) \underbrace{\mathbb{1}_{\Omega\times\{1\}}(\omega,j)\ d\mathbb{Q}(\omega,j)}_{\text{on } \Omega\times\{1\},\ d\mathbb{Q} \text{ is } \alpha\, d\mathbb{Q}_1}$$
$$+ \int_{\Omega\times\{1,2\}} \left(\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,2)\ \ln\frac{d\mathbb{P}}{d\mathbb{Q}}(\omega,2)\right)\mathbb{1}_{\Omega\times\{2\}}(\omega,j)\ d\mathbb{Q}(\omega,j)$$

$$= \underbrace{\int_{\Omega}\left(\frac{d\mathbb{P}_1}{d\mathbb{Q}_1}(\omega)\ \ln\frac{d\mathbb{P}_1}{d\mathbb{Q}_1}(\omega)\right)}_{=\mathrm{KL}(\mathbb{P}_1,\mathbb{Q}_1)} \alpha\, d\mathbb{Q}_1(\omega) + \underbrace{\int \cdots}_{\mathrm{KL}(\mathbb{P}_2,\mathbb{Q}_2)}$$

<u>KL for product measures.</u> ($\leftrightarrow$ The independent case)

<u>Proposition:</u> Let $(\Omega,\mathcal{F})$ and $(\Omega',\mathcal{F}')$ be two measurable spaces,
let $\mathbb{P},\mathbb{Q}$ be two probability measures over $(\Omega,\mathcal{F})$
$\mathbb{P}',\mathbb{Q}'$ over $(\Omega',\mathcal{F}')$
and denote by $\mathbb{P}\otimes\mathbb{P}'$ and $\mathbb{Q}\otimes\mathbb{Q}'$ the product distributions over $(\Omega\times\Omega',\ \mathcal{F}\otimes\mathcal{F}')$. Then:

$$\mathrm{KL}(\mathbb{P}\otimes\mathbb{P}',\ \mathbb{Q}\otimes\mathbb{Q}') = \mathrm{KL}(\mathbb{P},\mathbb{Q}) + \mathrm{KL}(\mathbb{P}',\mathbb{Q}')$$