

Lec 3 : f - divergence

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Defn. (f -divergence, Csiszár '63)

Let $f: (0, \infty) \rightarrow \mathbb{R}$ be convex with $f(1) = 0$. The f -divergence between two distributions P and Q on the same space is

$$D_f(P \parallel Q) = \mathbb{E}_Q \left[f\left(\frac{dP}{dQ}\right) \right].$$

Remark: 1. Some defn. additionally assumes that $f'(1) = 0$. This is WLOG.

$f(x)$ and $f(x) + c(x-1)$ give the same f -divergence.

2. If $\frac{dP}{dQ} = 0$, define $f(0) := f(0+)$;

If $P \neq Q$, define $D_f(P \parallel Q) = \int_{q=0}^1 q f\left(\frac{P}{q}\right) dq + f(\infty) P(q=0)$,
with $f'(\infty) := \lim_{x \rightarrow \infty} \frac{f(x)}{x}$.

Examples $\star 1$: $f(x) = \frac{1}{2}|x-1|$: $D_f(P \parallel Q) = \text{TV}(P, Q) = \frac{1}{2} \int |dP - dQ|$
(total variation (TV) distance)

$\star 2$: $f(x) = (\sqrt{x} - 1)^2$: $D_f(P \parallel Q) = H^2(P, Q) = \int (\sqrt{dP} - \sqrt{dQ})^2$
(squared Hellinger distance)

$\star 3$: $f(x) = x \log x$: $D_f(P \parallel Q) = D_{KL}(P \parallel Q) = \int dP \log \frac{dP}{dQ}$

$\star 4$: $f(x) = (x-1)^2$: $D_f(P \parallel Q) = \chi^2(P \parallel Q) = \int \frac{(dP - dQ)^2}{dQ}$
(χ^2 divergence)

5. $f(x) = \frac{1-x}{2(1+x)}$: $D_f(P \parallel Q) = L_C(P, Q) = \frac{1}{2} \int \frac{(dP - dQ)^2}{dP + dQ}$
(Le Cam distance)

6. $f(x) = x \log x + (x+1) \log \frac{2}{x+1}$: $D_f(P \parallel Q) = JS(P, Q) = D_{KL}(P \parallel \frac{P+Q}{2}) + D_{KL}(Q \parallel \frac{P+Q}{2})$
(Jensen-Shannon divergence)

Basic properties. ① $D_f(P \parallel Q) \geq 0$

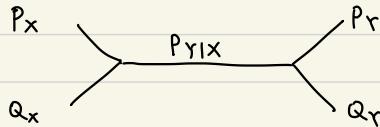
Pf. $D_f(P \parallel Q) = \mathbb{E}_Q \left[f\left(\frac{dP}{dQ}\right) \right] \geq f\left(\mathbb{E}_Q \left[\frac{dP}{dQ} \right]\right) = f(1) = 0$

② $(P, Q) \mapsto D_f(P \parallel Q)$ is jointly convex.

Pf. For convex f , the perspective transform $\mathbb{R}_+^2 \ni (x, y) \mapsto y f(\frac{x}{y})$ is also convex.

Check Hessian:
$$\begin{bmatrix} \frac{1}{y} f''(\frac{x}{y}) & -\frac{x}{y^2} f''(\frac{x}{y}) \\ -\frac{x}{y^2} f''(\frac{x}{y}) & \frac{x^2}{y^3} f''(\frac{x}{y}) \end{bmatrix} \succeq 0.$$
 □

③ Data processing inequality: $D_f(P_X \parallel Q_X) \geq D_f(P_Y \parallel Q_Y)$



Pf. Follow from joint convexity (similar to the KL proof) □

Why f -divergence? Binary hypothesis testing.

Recall the simple hypothesis testing problem:

Null $H_0: X \sim P$

Alternative $H_1: X \sim Q$

Test: $T: X \rightarrow \{0, 1\}$

Type I error: $P(T(X) = 1)$

Type II error: $Q(T(X) = 0)$

Thm.

$$\inf_T \left(P(T(X) = 1) + Q(T(X) = 0) \right) = 1 - TV(P, Q)$$

Pf. Easy to show $TV(P, Q) = \sup_A P(A) - Q(A)$

(\leq) Take $T(X) = 1(X \notin A)$ for A attaining the supremum;

(\geq) Take $A = \{T(X) = 0\}$. □

Remark: ① $TV(P, Q) = 0$: $P = Q$, totally indistinguishable

② $TV(P, Q) = 1$: $P \perp Q$, perfectly distinguishable

③ $TV(P, Q) < 1$: partially indistinguishable

(Important quantity for establishing minimax lower bounds later)

Why not just TV ?

① $TV(P, Q)$ can be hard to compute

② TV does not tensorize; e.g. $TV(P^{\otimes n}, Q^{\otimes n}) \leq n TV(P, Q)$ is the best possible inequality in general, but is often loose.

Example. How large is $TV(Ber_n(\frac{1}{2})^{\otimes n}, Ber_n(\frac{1}{2} + \delta)^{\otimes n})$?

Using $TV(P^{\otimes n}, Q^{\otimes n}) \leq n TV(P, Q)$: $n\delta$ upper bound

Using Pinsker's inequality: $TV(P^{\otimes n}, Q^{\otimes n}) \leq \sqrt{\frac{1}{2} D_{KL}(P^{\otimes n} \| Q^{\otimes n})}$
 $= \sqrt{\frac{n}{2} D_{KL}(P \| Q)} = O(\sqrt{n}\delta)$!

Popular f -divergences that tensorize:

① H^2 : $1 - \frac{1}{2} H^2(\prod_i P_i, \prod_i Q_i) = \prod_i (1 - \frac{1}{2} H^2(P_i, Q_i))$

② KL : $D_{KL}(\prod_i P_i \| \prod_i Q_i) = \sum_i D_{KL}(P_i \| Q_i)$

③ χ^2 : $\chi^2(\prod_i P_i \| \prod_i Q_i) + 1 = \prod_i (\chi^2(P_i \| Q_i) + 1)$.

Remark (optional): All of them follow from the tensorization of Rényi divergences

i.e. $D_\lambda(\prod_i P_i \| \prod_i Q_i) = \sum_i D_\lambda(P_i \| Q_i)$, with

$$D_\lambda(P \| Q) \triangleq \frac{1}{\lambda-1} \log \mathbb{E}_Q \left[\left(\frac{dP}{dQ} \right)^\lambda \right].$$

For $\lambda = \frac{1}{2}, 1, 2$, D_λ corresponds to H^2 , KL and χ^2 .

Similarities and differences between f -divergences

Locally χ^2 -like: when $f''(1)$ exists and $P \approx Q$:

$$\begin{aligned} D_f(P \parallel Q) &= \mathbb{E}_Q \left[f \left(\frac{dP}{dQ} \right) \right] \\ &\approx \mathbb{E}_Q \left[\underbrace{f(1)}_{=0} + f'(1) \left(\frac{dP}{dQ} - 1 \right) + \frac{f''(1)}{2} \left(\frac{dP}{dQ} - 1 \right)^2 \right] \\ &= \frac{f''(1)}{2} \chi^2(P \parallel Q). \end{aligned}$$

In parametric models: Fisher information: if $(P_\theta)_{\theta \in \Theta}$ is a "regular" parametric model with $\theta \in \mathbb{R}^d$, then for $h \in \mathbb{R}^d$ and $t \approx 0$:

$$\begin{aligned} \chi^2(P_{\theta+th} \parallel P_\theta) &= \int \frac{(f_{\theta+th} - f_\theta)^2}{f_\theta} \mu(dx) \quad (\text{assume } \frac{dP_\theta}{d\mu} = f) \\ &\approx t^2 h^T \int \frac{(\dot{f}_\theta)^2}{f_\theta} \mu(dx) h \quad (\dot{f}_\theta(x) = \frac{\partial f}{\partial \theta}(x)) \\ &=: t^2 h^T I(\theta) h, \end{aligned}$$

where $I(\theta) \in \mathbb{R}^{d \times d}$ is the Fisher information:

$$\begin{aligned} I(\theta) &= \int \frac{(\dot{f}_\theta)^2}{f_\theta} d\mu = \mathbb{E}[(\nabla_\theta \log f_\theta(x)) (\nabla_\theta \log f_\theta(x))^T] \\ &= \mathbb{E}[-\nabla_\theta^2 \log f_\theta(x)]. \end{aligned}$$

f -divergence as "average statistical information"

In binary hypothesis testing, if $P(H_0) = \pi \in (0, 1)$, then the Bayes error is

$$\begin{aligned} B_\pi(P, Q) &= \inf_T (\pi P(T(X)=1) + (1-\pi) Q(T(X)=0)) \\ &= \int (\pi dP \wedge (1-\pi) dQ) \quad (x \wedge y := \min\{x, y\}) \end{aligned}$$

The statistical information is the difference between "a priori" and "a posteriori" Bayes losses:

$$I_{\pi}(P, Q) = \pi \wedge (1-\pi) - B_{\pi}(P, Q),$$

which is a f -divergence with $f_{\pi}(t) = \pi \wedge (1-\pi) - (\pi t) \wedge (1-\pi)$.

Thm (Liese & Vajda '06). For any f -divergence, \exists a measure Γ_f on $(0, 1)$ s.t.

$$D_f(P \parallel Q) = \int_0^1 I_{\pi}(P, Q) \Gamma_f(d\pi). \quad \forall P, Q.$$

Remark: every f -divergence is an "average" statistical information, with different weights on π .

Pf. $f(1) = 0$, and WLOG assume $f'(1) = 0$. Then

$$\begin{aligned} f(t) &= \int_1^t (t-x) f''(dx) && (\text{For } f \in C^2, f''(dx) = f''(x) dx; \\ &\stackrel{\text{check}}{=} \int_0^t (x-t \wedge x) f''(dx) && \text{in general, any convex function gives} \\ &\quad + \int_t^\infty (t-x \wedge x) f''(dx). && \text{rise to a "measure" } f''(dx) \end{aligned}$$

Define $\tilde{f}(t) = \int_0^t (x-t \wedge x) f''(dx) + \int_t^\infty (1-t \wedge x) f''(dx)$, then

$$\mathbb{E}_a[(f - \tilde{f})(\frac{dP}{dQ})] = \mathbb{E}_a\left[\int_0^\infty \left(\frac{dP}{dQ} - 1\right) f''(dx)\right] = 0.$$

On the other hand,

$$1 \wedge x - t \wedge x = (1+x) \left(\frac{1}{1+x} \wedge \frac{x}{1+x} - \frac{t}{1+x} \wedge \frac{x}{1+x} \right) = (1+x) f_{\frac{1}{1+x}}(t),$$

so

$$\begin{aligned} \int_0^\infty (1+x) I_{\frac{1}{1+x}}(P, Q) f''(dx) &= \mathbb{E}_a\left[\int_0^\infty (1+x) f_{\frac{1}{1+x}}\left(\frac{dP}{dQ}\right) f''(dx)\right] \\ &= \mathbb{E}_a\left[\tilde{f}\left(\frac{dP}{dQ}\right)\right] = \mathbb{E}_a\left[f\left(\frac{dP}{dQ}\right)\right] = D_f(P \parallel Q), \end{aligned}$$

and $P_f(\pi)$ is the pushforward measure of $(1+x) f''(dx)$ by the map

$$x \in (0, \infty) \mapsto \frac{1}{1+x} \in (0, 1)$$

□

Different guarantees on contiguity

Def (contiguity) $\{P_n\}$ is contiguous w.r.t. $\{Q_n\}$ (written as $\{P_n\} \triangleleft \{Q_n\}$)
if $Q_n(A_n) \rightarrow 0$ implies $P_n(A_n) \rightarrow 0$.

Clearly, $TV(P_n, Q_n) \rightarrow 0$ implies $\{P_n\} \triangleleft \{Q_n\}$.

In comparison, $KL(P_n \parallel Q_n) \leq C$ already establishes contiguity, as

$$P_n(A_n) \log \frac{P_n(A_n)}{e Q_n(A_n)} \leq KL(P_n \parallel Q_n) \leq C \quad (\text{see Lec 2})$$

$\chi^2(P_n \parallel Q_n) \leq C$ leads to an even stronger guarantee:

$$\frac{(P_n(A_n) - Q_n(A_n))^2}{Q_n(A_n)(1 - Q_n(A_n))} \stackrel{\text{PPI}}{\leq} \chi^2(P_n \parallel Q_n) \leq C$$
$$\Rightarrow P_n(A_n) \leq Q_n(A_n) + \sqrt{C \cdot Q_n(A_n)}.$$

Therefore, different f -divergences have different powers in establishing contiguity results, due to different growth of $f(t)$ as $t \rightarrow \infty$. In this context, a popular choice is to upper bound $\chi^2(P_n \parallel Q_n)$, known as the "second moment method" in random graph theory & property testing (Lec 8).

Dual representations of f -divergence

Similar to KL, f -divergences also admit dual representations.

Def (convex conjugate): for a convex function f on \mathbb{R} , its convex conjugate is defined as

$$f^*(y) = \sup_x (xy - f(x)).$$

- Properties : ① f^* is convex ;
 ② $f^{**} = f$;
 ③ Young's inequality : $f(x) + f^*(y) \geq xy$.

The following result is then immediate :

Thm.

$$D_f(P \parallel Q) = \sup_{g: \mathbb{E}_Q[g] < \infty} \mathbb{E}_P g - \mathbb{E}_Q[f^* \circ g].$$

Pf.

$$\begin{aligned} D_f(P \parallel Q) &= \mathbb{E}_Q \left[f\left(\frac{dP}{dQ}\right) \right] = \mathbb{E}_Q \left[\sup_y y \frac{dP}{dQ} - f^*(y) \right] \\ &= \sup_{g: x \rightarrow R} \mathbb{E}_P g - \mathbb{E}_Q[f^* \circ g]. \quad \blacksquare \end{aligned}$$

Example 1 (TV), When $f(x) = \frac{1}{2}|x-1|$, $f^*(y) = \begin{cases} y & \text{if } |y| \leq \frac{1}{2} \\ +\infty & \text{if } |y| > \frac{1}{2} \end{cases}$, so

$$TV(P, Q) = \sup_{\|g\|_\infty \leq \frac{1}{2}} \mathbb{E}_P g - \mathbb{E}_Q g = \frac{1}{2} \sup_{\|g\|_\infty \leq 1} |\mathbb{E}_P g - \mathbb{E}_Q g|.$$

Example 2 (KL), When $f(x) = x \log x$, $f^*(y) = e^{y-1}$, so

$$D_{KL}(P \parallel Q) = \sup_g \mathbb{E}_P g - \mathbb{E}_Q e^{g-1} = \sup_g \mathbb{E}_P g - (\mathbb{E}_Q e^g - 1).$$

As $\mathbb{E}_Q e^0 - 1 \geq \log \mathbb{E}_Q e^0$, this is weaker than Donsker-Varadhan.

A way to recover Donsker-Varadhan is

$$\begin{aligned} D_{KL}(P \parallel Q) &= \sup_g \sup_{a \in R} \mathbb{E}_P[g+a] - \mathbb{E}_Q e^{g+a-1} \\ &= \sup_g \left(\mathbb{E}_P[g] - \underbrace{\inf_{a \in R} (\mathbb{E}_Q e^{g+a-1} - a)}_{= \log \mathbb{E}_Q e^g} \right) \\ &= \log \mathbb{E}_Q e^g, \text{ by taking } a = 1 - \log \mathbb{E}_Q e^g. \end{aligned}$$

Example 3 (X^2): When $f(x) = (x-1)^2$, $f^*(y) = y + \frac{y^2}{4}$, so

$$X^2(P \parallel Q) = \sup_g \mathbb{E}_P[g] - \mathbb{E}_Q[g + \frac{g^2}{4}]$$

$$= \sup_g \sup_{\lambda \in \mathbb{R}} \mathbb{E}_P[\lambda(g+c)] - \mathbb{E}_Q[\lambda(g+c) + \frac{\lambda^2(g+c)^2}{4}]$$

$$= \sup_g \frac{(\mathbb{E}_P[g] - \mathbb{E}_Q[g])^2}{\text{Var}_Q[g]}.$$

Corollary (Hammersley-Chapman-Robbins (HCR) lower bound)

In a parametric family $(P_\theta)_{\theta \in \mathbb{R}}$, if an estimator $\hat{\theta}$ is unbiased, then

$$\text{Var}_\theta(\hat{\theta}) \geq \sup_{\theta' \neq \theta} \frac{(\theta - \theta')^2}{X^2(P_{\theta'} \parallel P_\theta)}.$$

In particular, by taking $\theta' \rightarrow \theta$, it recovers the Cramér-Rao bound

$$\text{Var}_\theta(\hat{\theta}) \geq \frac{1}{I(\theta)}.$$

Example 4 (JS): When $f(x) = x \log x + (x+1) \log \frac{2}{x+1}$, $f^*(y) = \begin{cases} -\log(2-e^y), & y < \log 2 \\ +\infty, & y \geq \log 2 \end{cases}$

$$JS(P, Q) = \sup_{g \leq \log 2} \mathbb{E}_P[g] + \mathbb{E}_Q[\log(2-e^g)]$$

$$= \sup_{0 < h < 1} \mathbb{E}_P[\log h] + \mathbb{E}_Q[\log(1-h)] + \log 2.$$

So generative adversarial networks (GAN) aim to minimize

$$\min_G \text{JS}(P, P_{G(z)}) = \min_G \sup_D \mathbb{E}_{x \sim P} [\log D(x)] + \mathbb{E}_{z \sim N} [\log(1 - D(G(z)))]$$

\uparrow generator \uparrow data distribution \uparrow noise \uparrow discriminator

Joint range: given two f -divergences, how to prove inequalities between them?

(For example, is there a general paradigm to prove Pinsker's inequality

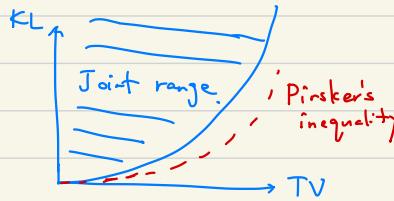
$$2\text{TV}(P, Q) \leq D_{KL}(P \parallel Q) ?$$

Def (Joint range): Fix two f -divergences $D_f(P \parallel Q)$ and $D_g(P \parallel Q)$.

Define: $R = \{ (D_f(P \parallel Q), D_g(P \parallel Q)) : P, Q \text{ general prob. measures} \}$

$R_k = \{ (D_f(P \parallel Q), D_g(P \parallel Q)) : P, Q \text{ prob. measures on } [k] \}$.

Example (TV vs. KL):



Thm (Harremoës-Vajda'11) $R = \text{conv}(R_2) = R_4$.

Implication: to establish inequalities between D_f and D_g , suffices to prove them for $P = (p, 1-p)$ and $Q = (q, 1-q)$!

Pf (of a simpler case $P \ll Q$)

① $R \subseteq \text{conv}(R_2)$: Fix any point $(D_f(P \parallel Q), D_g(P \parallel Q)) \in R$.

Then $L = \frac{dP}{dQ}$ is a RV in $[0, \infty)$ with $\mathbb{E}_Q[L] = 1$, and

$$(D_f(P \parallel Q), D_g(P \parallel Q)) = (\mathbb{E}_Q[f(L)], \mathbb{E}_Q[g(L)]).$$

Next consider the set C of all prob. measures on $[0, \infty)$ with mean 1.

For $\mu \in C$, we associate a point $(\mathbb{E}_\mu f(L), \mathbb{E}_\mu g(L)) \in R$.

Clearly C is convex, and

extremal points of $C = \{ \text{distributions with mean 1 and support size } 2 \}$.

(i.e. all points x that cannot be expressed as $x = \lambda y + (1-\lambda)z$ with $y, z \in C$, $\lambda \in (0, 1)$)

In fact, if A_1, A_2, A_3 form a partition of $[0, \infty)$, and

$$\mu = \lambda_1 \mu_1 + \lambda_2 \mu_2 + \lambda_3 \mu_3, \quad \lambda_i > 0, \quad \text{supp}(\mu_i) \subseteq A_i.$$

Then the probability and mean constraints only require

$$\begin{cases} \lambda_1 + \lambda_2 + \lambda_3 = 1, \\ \lambda_1 m(\mu_1) + \lambda_2 m(\mu_2) + \lambda_3 m(\mu_3) = 1, \end{cases}$$

which is a line containing $(\lambda_1, \lambda_2, \lambda_3)$. So μ cannot be an extremal point.

Now by Choquet-Bishop-de Leeuw, any $\mu \in C$ can be written as a convex combination of extremal points of C , i.e. $R \subseteq \text{conv}(R_2)$.

Thm (Choquet-Bishop-de Leeuw): if C is a metrizable convex compact subset of a locally convex topological vector space, then $C = \text{conv}(\text{extremal}(C))$.

② $\text{conv}(R_2) \subseteq R_4$: by Carathéodory theorem below, any point of $\text{conv}(R_2) \subseteq \mathbb{R}^2$ (which is connected) can be written as a convex combination of 2 points of R_2 , which belongs to R_4 .

Thm (Carathéodory): Let $S \subseteq \mathbb{R}^d$ and $x \in \text{conv}(S)$. Then there exists $S' = \{x_1, \dots, x_k\}$ s.t. $x \in \text{conv}(S')$, with

① $k \leq d+1$ in general;

② $k \leq d$ if S has at most d connected components.



Examples of inequalities:

① TV vs. H^2 : $\frac{H^2}{2} \leq TV \leq \sqrt{H^2(1 - \frac{H^2}{4})}$ (also the joint range)

② TV vs. KL: $TV^2 \leq \frac{1}{2} KL$

$$TV \leq 1 - \frac{1}{2} \exp(-KL)$$

③ KL vs. X^2 : $KL \leq \log(1 + X^2)$ (also the joint range)

Special topic: chain rule for H^2

Thm (Jayram '09) For all P_{X^n}, Q_{X^n} :

$$H^2(P_{X^n}, Q_{X^n}) \leq C \sum_{i=1}^n \mathbb{E}_P [H^2(P_{X_{i|X^{i-1}}}, Q_{X_{i|X^{i-1}}})],$$

with $C = \prod_{i=1}^{\infty} \frac{1}{1-2^{-i}} \approx 3.46$.

The proof is surprisingly combinatorial. First, it suffices to prove the case $n=2^k$: for general $2^{k-1} < n \leq 2^k$, can consider $P_{2^k} = P_{X^n} \otimes P_0^{2^k-n}$, $Q_{2^k} = Q_{X^n} \otimes P_0^{2^k-n}$. The proof uses several properties of H^2 .

Lemma 1 (L^2 geometry). For arbitrary distributions P_0, \dots, P_m :

$$\frac{1}{m} \sum_{1 \leq i < j \leq m} H^2(P_i, P_j) \leq \sum_{i=1}^m H^2(P_i, P_0).$$

Pf. This result holds for all L^2 distance:

$$\frac{1}{m} \sum_{1 \leq i < j \leq m} \|P_i - P_j\|^2 \leq \sum_{i=1}^m \|P_i - P_0\|^2.$$

$$\begin{aligned} \text{In fact, } 2 \cdot \text{LHS} &= \frac{1}{m} \sum_{i,j=1}^m \|P_i - P_j\|^2 \\ &= \frac{1}{m} \sum_{i,j=1}^m \|P_i - P_0 - (P_j - P_0)\|^2 \\ &= \frac{1}{m} \sum_{i,j=1}^m (\|P_i - P_0\|^2 + \|P_j - P_0\|^2 - 2 \langle P_i - P_0, P_j - P_0 \rangle) \\ &= 2 \cdot \text{RHS} - \frac{2}{m} \left\| \sum_{i=1}^m (P_i - P_0) \right\|^2 \leq 2 \cdot \text{RHS}. \end{aligned}$$

Finally, note that

$$H^2(P, Q) = \int (\sqrt{P} - \sqrt{Q})^2$$

is indeed an L^2 distance.



Now for $A \subseteq [n]$, define interpolations

$$P^A = \prod_{i=1}^n (P_{x_i|x_{i-1}})^{1(i \notin A)} (Q_{x_i|x_{i-1}})^{1(i \in A)}.$$

Then $P^B = P_{X^n}$, $P^{[n]} = Q_{X^n}$.

Lemma 2 (cut-paste property) Let $a, b, c, d \in \{0, 1\}^n$ be the indicators of sets $A, B, C, D \subseteq [n]$. If $a+b = c+d$, then $H^2(P^A, P^B) = H^2(P^C, P^D)$.

PF.

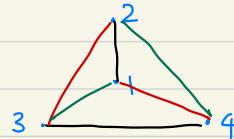
$$\begin{aligned} H^2(P^A, P^B) &= 2 - 2 \int \sqrt{P^A P^B} \\ &= 2 - 2 \int \sqrt{\prod_{i=1}^n P_{x_i|x_{i-1}}^{1-a_i+1-b_i} Q_{x_i|x_{i-1}}^{a_i+b_i}} \\ &= 2 - 2 \int \sqrt{\prod_{i=1}^n P_{x_i|x_{i-1}}^{1-c_i+1-d_i} Q_{x_i|x_{i-1}}^{c_i+d_i}} = H^2(P^C, P^D) \quad \square \end{aligned}$$

Lemma 3 (1-factorization of cliques) For even n , the complete graph K_n can be decomposed into $(n-1)$ edge-disjoint perfect matchings.
(i.e. round-robin tournaments)

Example of $n=4$.



A geometric construction:



Put node 1 in the center of a regular polygon with $(n-1)$ vertices. Use color i for $(1, i)$ and all edges perpendicular to $(1, i)$.

Completing the proof. For $n = 2^k$, prove by induction on $m = 0, 1, \dots, k$ that for any partition A_1, \dots, A_{2^m} of $[n]$ (each of size 2^{k-m}),

$$\sum_{i=1}^{2^m} H^2(P^{A_i}, P^\phi) \geq c_m \cdot H^2(P^{[n]}, P^\phi),$$

with $c_m = \prod_{i=1}^m (1 - 2^{-i})$.

Base $m = 0$: trivial.

Induction from $m-1$ to m :

$$\begin{aligned} \sum_{i=1}^{2^m} H^2(P^{A_i}, P^\phi) &\stackrel{\text{Lemma 1}}{\geq} \frac{1}{2^m} \sum_{1 \leq s < t \leq 2^m} H^2(P^{A_s}, P^{A_t}) \\ &\stackrel{\text{Lemma 2}}{=} \frac{1}{2^m} \sum_{1 \leq s < t \leq 2^m} H^2(P^{A_s \cup A_t}, P^\phi) \\ &\stackrel{\text{Lemma 3}}{=} \frac{1}{2^m} \sum_{a=1}^{2^m-1} \sum_{(s,t) \in E_a} H^2(P^{A_s \cup A_t}, P^\phi), \end{aligned}$$

where each E_a is a perfect matching of K_{2^m} . By induction hypothesis,

$$\sum_{i=1}^{2^m} H^2(P^{A_i}, P^\phi) \geq \frac{2^m-1}{2^m} c_{m-1} H^2(P^{[n]}, P^\phi) = c_m H^2(P^{[n]}, P^\phi).$$

Conclusion: choosing $m = k$ yields

$$\begin{aligned} H^2(P^{[n]}, P^\phi) &\leq \frac{1}{c_k} \sum_{i=1}^k H^2(P^{f_i}, P^\phi) \\ &= \frac{1}{c_k} \sum_{i=1}^k \mathbb{E}_P [H^2(P_{X_i|X^{i-1}}, Q_{X_i|X^{i-1}})]. \end{aligned}$$