Machine Learning B (2025)
Home Assignment 1

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Contents

1 Numerical comparison of kl inequality with its relaxations and with Hoeffding's inequality (40 points) [Yevgeny]

Bounds

We shall evaluate the following four bounds on p:

- Hoeffding: $\hat{p}_n + \sqrt{\frac{\ln\frac{1}{\delta}}{2n}}$
- The kl inequality: $\mathrm{kl}^{-1^+}(\hat{p}_n, \epsilon) = \max\{p : \mathrm{kl}(\hat{p}_n \| p) \leq \epsilon\}$
- Pinsker's relaxation: identical to Hoeffding according to eq. (2.12) in the lecture notes
- Refined Pinsker's: $\hat{p}_n + \sqrt{\frac{2\hat{p}_n \ln\frac{1}{\delta}}{n}} + \frac{2\ln\frac{1}{\delta}}{n}$

Plot of upper bounds

In figure 1 we plot the upper bounds.

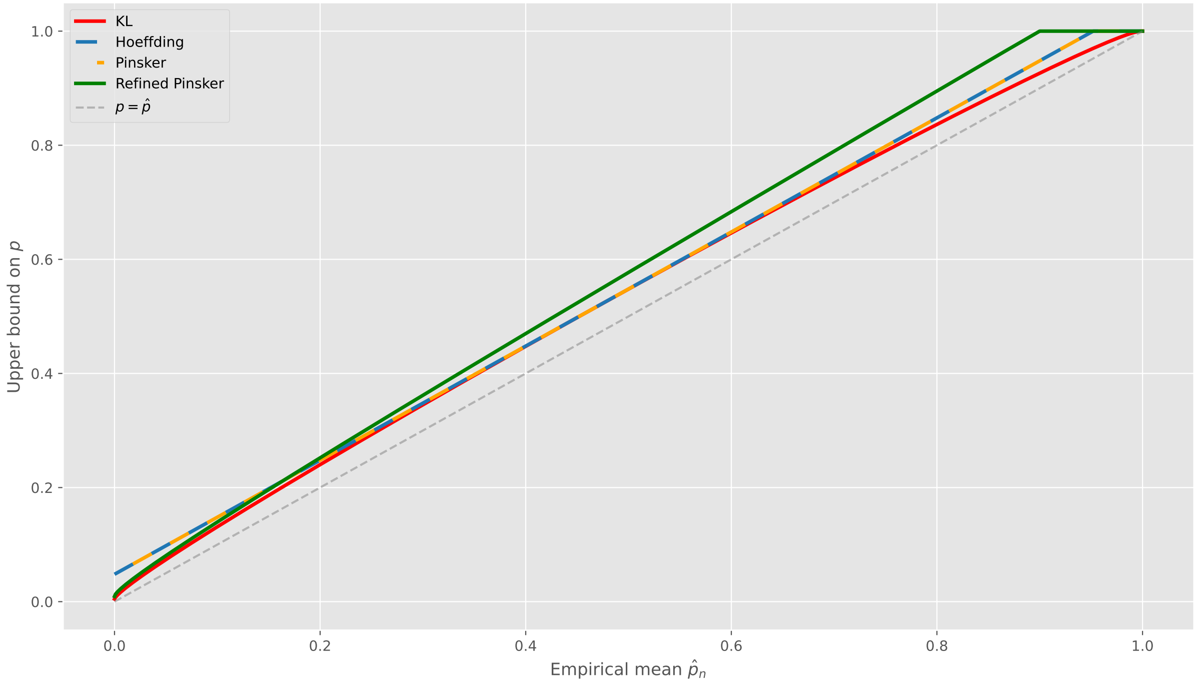


Figure 1: Upper bounds for $\hat{p}_n \in [0, 1]$

and in figure 2 we plot the same upper bounds ”zoomed in” on $\hat{p}_n \in [0, 0.1]$.

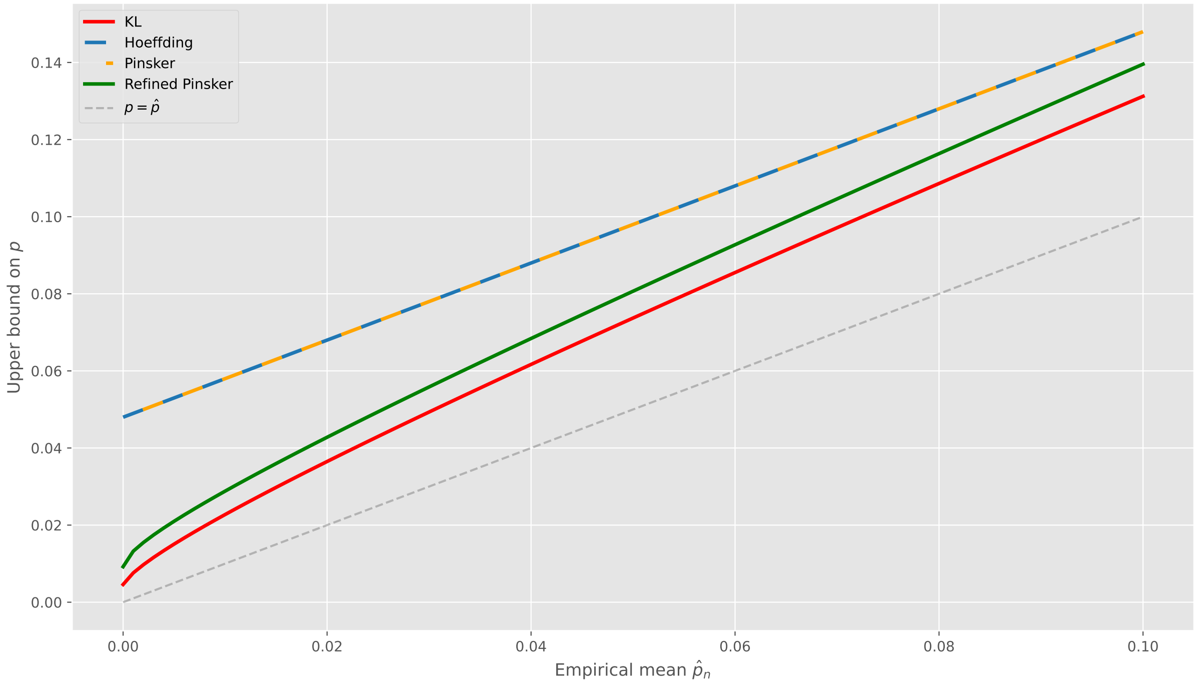


Figure 2: Zoomed upper bounds for $\hat{p}_n \in [0, 0.1]$

The implementation of the upper bound calculations are listed here 2.

Plot of lower bounds

The lower bounds are shown in figure 3.

Computation of upper and lower inverse of kl

Please see code listing 3 for the implementation of the upper inverse of kl. To compute the lower inverse of kl, we note that $\mathrm{kl}(a\|b) = \mathrm{kl}(1-a\|1-b)$ for all $a, b \in [0, 1]$. So $\mathrm{kl}(\hat{p}\|p) \leq \epsilon$ is equivalent to $\mathrm{kl}(1-\hat{p}\|1-p) \leq \epsilon$. For $q = 1-p$ the sets $\{p : \mathrm{kl}(\hat{p}\|p) \leq \epsilon\}$ and $\{q : \mathrm{kl}(1-\hat{p}\|q) \leq \epsilon\}$ are identical.

By the definition of the upper inverse we have

$$q^+ = \mathrm{kl}^{\text{-1}^+}(1-\hat{p}, \epsilon) = \max\{q \geq 1-\hat{p} : \mathrm{kl}(1-\hat{p}\|q) \leq \epsilon\}$$

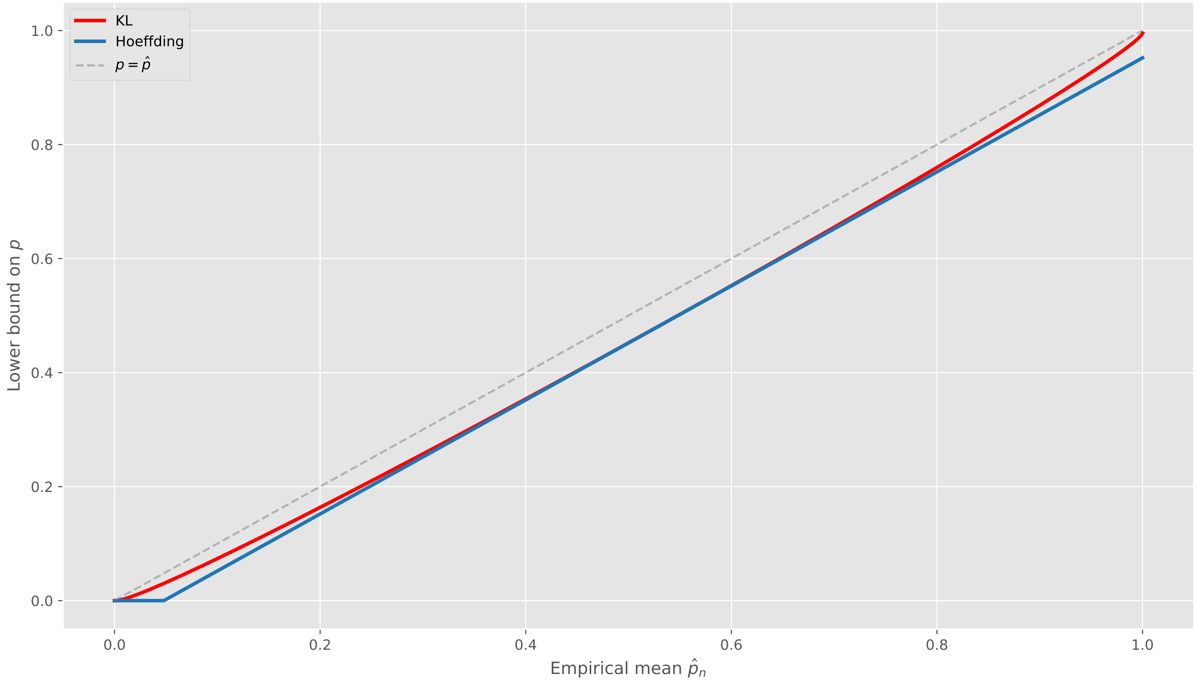


Figure 3: Lower bounds for $\hat{p}_n \in [0, 1]$

We now replace q with $1 - p$ to obtain

$$p^- = 1 - q^+ = 1 - \mathrm{kl}^{-1^+}(1 - \hat{p}, \epsilon) = \min\{p \leq \hat{p} : \mathrm{kl}(\hat{p} \| p) \leq \epsilon\} = \mathrm{kl}^{-1^-}(\hat{p}, \epsilon)$$

So the lower inverse can be obtained from the upper inverse through the code:

```
def kl_lower_bound_symm(p_hat, n, delta, **kw):
    return 1.0 - kl_upper_bound(1.0 - p_hat, n, delta, **kw)
```

Listing 1: Lower inverse

I also implemented the lower inverse using the same numerical approach as for the upper inverse and used property testing to verify that the two approaches produce same results.

Conclusion

kl is the tightest bound in the whole interval $[0, 1]$. As long as we are close to 0, refined Pinsker is only slightly worse than kl. Once we pass approximately $\hat{p}_n = 0.2$ Hoeffding is actually better than Refined Pinsker.

2 Occam's razor with kl inequality (30 points) [Yevgeny]

I have not be able to provide a direct proof of Occam's razor with kl inequality. As an alternative I used a "backward" approach going from the desired result moving backwards to the assumptions of the theorem. Using this approach I end up with the following inequality

$$\mathbb{P}(\mathrm{kl}(\hat{L}(h,S)\|L(h)) \geq \varepsilon) \leq e^{-n\varepsilon} \tag{1}$$

that should hold for any $\varepsilon > 0$. It looks like a kl-version of Chernoff's bound[1] but I have not be able to proof that it is correct. Assuming eq. 1 is correct the proof goes like this.

Theorem (Occam's kl-razor inequality)**.** *Let S be an i.i.d. sample of n points, let ℓ be a loss function bounded in the interval $[0,1]$, let $\mathcal{H}$ be countable and let $\pi(h)$ be such that it is independent of the sample S and satisfies $\pi(h) \geq 0$ for all h and $\sum_{h\in\mathcal{H}} \pi(h) \leq 1$. Let $\delta \in (0,1)$. Then*

$$\mathbb{P}\left(\exists h \in \mathcal{H} : \mathrm{kl}(\hat{L}(h,S)\|L(h)) \geq \frac{\ln \frac{1}{\pi(h)\delta}}{n}\right) \leq \delta.$$

Proof. Define for each hypothesis h:

$$\varepsilon_h = \frac{\ln \frac{1}{\pi(h)\delta}}{n}$$

Using eq. 1 this gives us:

$$\mathbb{P}\left(\mathrm{kl}(\hat{L}(h,S)\|L(h)) \geq \frac{\ln \frac{1}{\pi(h)\delta}}{n}\right) \leq e^{-n\cdot\frac{\ln\frac{1}{\pi(h)\delta}}{n}} = e^{-\ln\frac{1}{\pi(h)\delta}} = \pi(h)\delta$$

Now we apply the union bound over all $h \in \mathcal{H}$:

$$\begin{aligned}\mathbb{P}\left(\exists h \in \mathcal{H} : \mathrm{kl}(\hat{L}(h,S)\|L(h)) \geq \frac{\ln \frac{1}{\pi(h)\delta}}{n}\right) &\leq \sum_{h\in\mathcal{H}} \mathbb{P}\left(\mathrm{kl}(\hat{L}(h,S)\|L(h)) \geq \frac{\ln \frac{1}{\pi(h)\delta}}{n}\right) \\ &\leq \sum_{h\in\mathcal{H}} \pi(h)\delta = \delta \sum_{h\in\mathcal{H}} \pi(h) \leq \delta \cdot 1 = \delta\end{aligned}$$

where the second last inequality follows from the condition that $\sum_{h\in\mathcal{H}} \pi(h) \leq 1$. ■

Importance of $\pi(h)$ being independent of S

The critical step where we use the independence of $\pi(h)$ from the sample S is when applying the union bound. If $\pi(h)$ were to depend on S, we could not treat it as a fixed quantity when calculating the probability. Without independence, $\pi(h)$ becomes a random variable that depends on the same sample S we are using to compute $\hat{L}(h,S)$.

[1] See [MU05] for Chernoff bounds.

Corollary. *Under the assumptions of Theorem 3.38 (Occam's kl-razor inequality), the following holds:*

$$\mathbb{P}\left(\exists h \in \mathcal{H} : L(h) \geq \hat{L}(h,S) + \sqrt{\frac{2\hat{L}(h,S)\ln\frac{1}{\pi(h)\delta}}{n}} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right) \leq \delta. \tag{2}$$

Proof. From the above Theorem, with probability at least $1-\delta$, for all $h \in \mathcal{H}$:

$$\mathrm{kl}(\hat{L}(h,S)\|L(h)) < \frac{\ln\frac{1}{\pi(h)\delta}}{n}$$

For $p, q \in [0,1]$ with $p \leq q$, we can use the following lower bound on KL-divergence:

$$\frac{(q-p)^2}{2q} \leq \mathrm{kl}(p||q).$$

This is from corollary 2.31 (Refined Pinsker's inequality) in the lecture notes [Sel25]. Here we are interested in the case where $\hat{L}(h,S) \leq L(h)$, we can apply this with $p = \hat{L}(h,S) := \hat{L}$ and $q = L(h) := L$, where the last equality is simplification of the notation.

$$\frac{(L-\hat{L})^2}{2L} \leq \mathrm{kl}(\hat{L}||L)$$

Now theorem 3.38 give us, with probability at least $1-\delta$:

$$\frac{(L-\hat{L})^2}{2L} < \frac{\ln\frac{1}{\pi(h)\delta}}{n}$$

This is a quadratic inequality in L, that we can re-write to:

$$L^2 - L\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right) + \hat{L}^2 < 0$$

Using the quadratic formula, the solutions to $aL^2 + bL + c = 0$ with

$$a = 1, b = -\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right), \text{and } c = \hat{L}^2$$

are:

$$L = \hat{L} + \frac{\ln\frac{1}{\pi(h)\delta}}{n} \pm \sqrt{\frac{2\hat{L}\ln\frac{1}{\pi(h)\delta}}{n} + \frac{(\ln\frac{1}{\pi(h)\delta})^2}{n^2}}$$

Please see 3 for details on calculating the roots. For a quadratic inequality of the form $aL^2 + bL + c < 0$ with $a > 0$, the solution is between the two roots. We are looking for an upper bound for L, which will be the larger root:

$$L < \hat{L} + \frac{\ln\frac{1}{\pi(h)\delta}}{n} + \sqrt{\frac{2\hat{L}\ln\frac{1}{\pi(h)\delta}}{n} + \frac{(\ln\frac{1}{\pi(h)\delta})^2}{n^2}}$$

Using that for non-negative a and b we have $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$:

$$L < \hat{L} + \frac{\ln\frac{1}{\pi(h)\delta}}{n} + \sqrt{\frac{2\hat{L}\ln\frac{1}{\pi(h)\delta}}{n}} + \frac{\ln\frac{1}{\pi(h)\delta}}{n} = \hat{L} + \sqrt{\frac{2\hat{L}\ln\frac{1}{\pi(h)\delta}}{n}} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}$$

Hence with probability at least $1-\delta$, for all $h \in \mathcal{H}$:

$$L(h) < \hat{L}(h,S) + \sqrt{\frac{2\hat{L}(h,S)\ln\frac{1}{\pi(h)\delta}}{n}} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}$$

Using the complement event:

$$\mathbb{P}\left(\exists h \in \mathcal{H} : L(h) \geq \hat{L}(h,S) + \sqrt{\frac{2\hat{L}(h,S)\ln\frac{1}{\pi(h)\delta}}{n}} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right) \leq \delta$$

which is exactly the statement of the Corollary. ■

Discussion of the Corollary

This corollary provides important advantages over the original KL-divergence formulation:

1. It provides an explicit upper bound on the true loss $L(h)$ in terms of the empirical loss $\hat{L}(h,S)$

2. It clearly shows the convergence rate through the terms $\sqrt{\frac{2\hat{L}(h,S)\ln\frac{1}{\pi(h)\delta}}{n}}$ and $\frac{2\ln\frac{1}{\pi(h)\delta}}{n}$

3. The first term scales with $\sqrt{\frac{\hat{L}(h,S)}{n}}$, showing faster convergence for hypotheses with lower empirical error

3 Numerical comparison of the kl and split-kl inequalities (30 points) [Yevgeny]

We consider a ternary random variable X taking values $X \in \left\{0, \frac{1}{2}, 1\right\}$. Let

$$p_0 = \mathbb{P}\big(X = 0\big), \qquad p_{\frac{1}{2}} = \mathbb{P}\big(X = \tfrac{1}{2}\big), \qquad p_1 = \mathbb{P}\big(X = 1\big).$$

and set $p_0 = p_1 = (1 - p_{\frac{1}{2}})/2$, so that the probabilities of $X = 0$ and $X = 1$ are equal, and there is only one parameter $p_{\frac{1}{2}}$, which controls the probability mass of the central value.

We now want to compare the two bounds kl and split-kl as a function of $p_{\frac{1}{2}} \in [0, 1]$. The upper kl bound for $p - \hat{p}_n$ is given by

$$\mathrm{kl}^{-1^+}\Big(\hat{p}_n, \tfrac{\ln \frac{1}{\delta}}{n}\Big) - \hat{p}_n$$

and the split-kl bound is

$$b_0 + \sum_{j=1}^{K} \left(\alpha_j \ \mathrm{kl}^{-1^+}\Big(\hat{p}_{|j}, \frac{1}{n} \ln \frac{K}{\delta}\Big) - \hat{p}_{|j}\right), \tag{3}$$

where $\hat{p}_{|j} = \frac{1}{n} \sum_{i=1}^{n} X_{i|j}$ and $X_{i|j} = \mathbb{1}(X_i \geq b_j)$ denotes the elements of the binary decomposition of X_i.

For this experiment, we find that the domain is $b_0 = 0, b_1 = 0.5, b_2 = 1$ and the $K = 2$ segments are $\alpha_1 = \alpha_2 = \frac{1}{2}$. So eq. 3 simplifies to:

$$\tfrac{1}{2}\Big(\ \mathrm{kl}^{-1^+}(\hat{p}_{|1}, \epsilon) - \hat{p}_{|1}\Big) + \tfrac{1}{2}\Big(\ \mathrm{kl}^{-1^+}(\hat{p}_{|2}, \epsilon) - \hat{p}_{|2}\Big),$$

where $\epsilon = \frac{1}{n} \ln \frac{K}{\delta} = \frac{1}{n} \ln \frac{2}{\delta}$. In figure 3 we see a plot of kl and split-kl.

Brief discussion

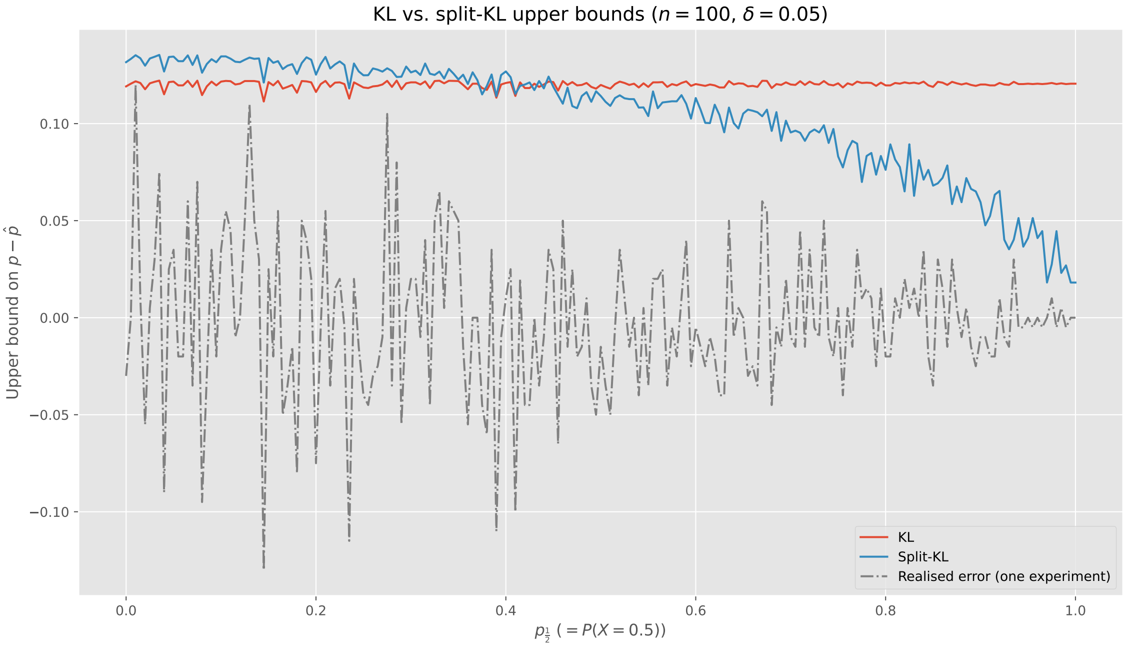
Because the true mean is fixed at 0.5 for every choice of $p_{1/2}$, the empirical mean fluctuates around 0.5, with variance depending on the shape of the distribution.

The dashed curve is the error realized in the single sample that was drawn for each $p_{1/2}$

Let us consider what happens when $p_{\frac{1}{2}} \to 1$. In that case most of the probability mass is pushed to the center value 0.5, and the two outcomes (0 and 1) become very rare since their probabilities $p0 = p1 = (1 - p_{\frac{1}{2}})/2 \to 0$. Consequently, the variance of X is given by $\mathrm{Var}(X) = 0.25(1 - p_{\frac{1}{2}}) \to 0$. Hence the empirical mean is in practice locked very tightly around the true mean 0.5 once $p_{\frac{1}{2}}$ gets closer to 1.

Split-kl decomposes X into the two binary indicators:

$$X_{|1} = \mathbb{1}(X \geq 0.5), \quad X_{|2} = \mathbb{1}(X \geq 1).$$



Their expectations are

$$p_{|1} = \mathbb{P}(X \geq 0.5) = 1 - p_0 \to 1,$$
$$p_{|2} = \mathbb{P}(X \geq 1.0) = p_1 \to 0$$

as $p_{\frac{1}{2}} \to 1$.

When a Bernoulli parameter is very close to 0 or 1, the kl-inverse difference $\text{kl}^{-1^+}(\hat{p}, \epsilon) - \hat{p}$ is proportional to $\hat{p}(1 - \hat{p})$ and therefore goes to zero.

For the split-kl bound these two tiny differences are multiplied by $\alpha_1 = \alpha_2 = 0.5$ and then added, so the whole bound collapses toward 0 as soon as X almost never takes the extreme values. That is why in figure 3 we observe a split-kl close to 0 for $p_{\frac{1}{2}}$ close to 1.

Python code

```
# kl
kl_upper = np.array([mlb.kl_upper_bound(ph, n, delta) for ph in p_hats])

# Hoeffding
epsilon = np.sqrt(np.log(1.0 / delta) / (2.0 * n))
hoeffding_upper = np.clip(p_hats + epsilon, 0.0, 1.0)

# Refined Pinsker’s inequality
last_term = 2.0 * np.log(1.0 / delta) / n
refined_pinsker_tmp = (
    p_hats + np.sqrt((2.0 * p_hats * np.log(1.0 / delta)) / n) +
   last_term
)
refined_pinsker = np.clip(refined_pinsker_tmp, 0.0, 1.0)
```

Listing 2: Upper bound calculations

```
def kl_upper_bound(p_hat, n, delta, tol=1e-12, max_iter=100):
    """
    Calculate the upper confidence bound using the Kullback-Leibler
   divergence.

    This function computes an upper bound p such that
    KL(p_hat, p) <= log(1/delta)/n, where p_hat is the empirical
   probability
    estimate, n is the sample size, and delta is the confidence level.

    Parameters
    ----------
    p_hat : float
        The empirical probability estimate in [0, 1].
    n : int
        Number of samples.
    delta : float
        Confidence level parameter in (0, 1).
        The bound holds with probability 1-delta.
    tol : float, optional
        Tolerance for the binary search convergence. Default is 1e-12.
    max_iter : int, optional
        Maximum number of iterations for the binary search. Default is
   100.

    Returns
    -------
    float
        The upper confidence bound p such that KL(p_hat, p) <= log(1/
   delta)/n.

    Notes
    -----
    Uses binary search to find the upper bound. Special cases are handled
    for
    p_hat = 0 and p_hat = 1.
    """
    eps = np.log(1.0 / delta) / n
    if p_hat <= 0.0:
        return 1.0 - np.exp(-eps)
    if p_hat >= 1.0:
        return 1.0
    lo, hi = p_hat, 1.0
    for _ in range(max_iter):
        mid = 0.5 * (lo + hi)
        if kl(p_hat, mid) > eps:
            hi = mid
        else:
            lo = mid
        if hi - lo < tol:
            break
    return hi
```

Listing 3: Upper inverse

Detailed calculation of quadratic roots

Using the quadratic formula, the solutions to $aL^2 + bL + c = 0$ with

$$a = 1, b = -\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right), \text{ and } c = \hat{L}^2$$

are:

$$L = \frac{\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right) \pm \sqrt{\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right)^2 - 4\hat{L}^2}}{2}$$

We simplify the discriminant:

$$\begin{aligned}\left(2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n}\right)^2 - 4\hat{L}^2 &= 4\hat{L}^2 + \frac{8\hat{L}\ln\frac{1}{\pi(h)\delta}}{n} + \frac{4(\ln\frac{1}{\pi(h)\delta})^2}{n^2} - 4\hat{L}^2 \\ &= \frac{8\hat{L}\ln\frac{1}{\pi(h)\delta}}{n} + \frac{4(\ln\frac{1}{\pi(h)\delta})^2}{n^2}\end{aligned}$$

Hence the roots are:

$$L = \frac{2\hat{L} + \frac{2\ln\frac{1}{\pi(h)\delta}}{n} \pm \sqrt{\frac{8\hat{L}\ln\frac{1}{\pi(h)\delta}}{n} + \frac{4(\ln\frac{1}{\pi(h)\delta})^2}{n^2}}}{2}$$

Simplifying:

$$L = \hat{L} + \frac{\ln \frac{1}{\pi(h)\delta}}{n} \pm \sqrt{\frac{2\hat{L}\ln \frac{1}{\pi(h)\delta}}{n} + \frac{(\ln \frac{1}{\pi(h)\delta})^2}{n^2}}$$

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