Upper bounds for average Bayes accuracy in terms of mutual information

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These are preliminary notes.

1 Introduction

Suppose X and Y are continuous random variables (or vectors) which have a joint distribution with density $p(x, y)$. Let $p(x) = \int p(x, y)dy$ and $p(y) = \int p(x, y)dx$ denote the respective marginal distributions, and $p(y|x) = p(x, y)/p(x)$ denote the conditional distribution.

Mutual information is defined

$$\mathrm{I}[p(x, y)] = \int p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dxdy.$$

ABE_k, or k-class Average Bayes accuracy is defined as follows. Let $X_1, ..., X_K$ be iid from $p(x)$, and draw Z uniformly from $1, .., k$. Draw $Y \sim p(y|X_Z)$. Then, the average Bayes accuracy is defined as

$$\mathrm{ABA}_k[p(x, y)] = \sup_f \Pr[f(X_1, ..., X_k, Y) = Z]$$

where the supremum is taken over all functions f. A function f which achieves the supremum is

$$f_{Bayes}(x_1, ..., x_k, y) = \mathrm{argmax}_{z \in \{1,...,k\}} p(y|x_z),$$

where an arbitrary rule can be employed to break ties. Such a function f_{Bayes} is called a *Bayes classification rule*. It follows that ABA_k is given explicitly by

$$\mathrm{ABA}_k = \frac{1}{k} \int \left[\prod_{i=1}^{k} p(x_i) dx_i \right] \int dy \max_i p(y|x_i),$$

as stated in the following theorem.

Theorem 1.1 *For a joint distribution $p(x, y)$, define*

$$ABA_k[p(x, y)] = \sup_f \Pr[f(x_1, ..., x_k, y) = Z]$$

where $X_1, ..., X_K$ are iid from $p(x)$, Z is uniform from $1, .., k$, and $Y \sim p(y|X_Z)$, and the supremum is taken over all functions $f : \mathcal{X}^k \times \mathcal{Y} \to \{1, ..., k\}$. Then,

$$ABA_k = \frac{1}{k} \int \left[\prod_{i=1}^{k} p(x_i) dx_i \right] \int dy \max_i p(y|x_i).$$

Proof. First, we claim that the supremum is attained by choosing

$$f(x_1, ..., x_k, y) = \mathrm{argmax}_{z \in \{1,...,k\}} p(y|x_z).$$

To show this claim, write

$$\sup_f \Pr[f(X_1, ..., X_k, Y) = Z] = \sup_f \frac{1}{k} \int p_X(x_1) \ldots p_X(x_k) p(y|x_{f(x_1,...,x_k,y)}) dx_1 \ldots dx_k dy$$

We see that maximizing $\Pr[f(X_1, ..., X_k, Y) = Z]$ over functions f additively decomposes into infinitely many subproblems, where in each subproblem we are given $\{x_1, ..., x_k, y\} \in \mathcal{X}^k \times \mathcal{Y}$, and our goal is to choose $f(x_1, ..., x_k, y)$ from the set $\{1, ..., k\}$ in order to maximize the quantity $p(y|x_{f(x_1,...,x_k,y)})$. In each subproblem, the maximum is attained by setting $f(x_1, ..., x_k, y) = \mathrm{argmax}_z p(y|x_z)$–and the resulting function f attains the supremum to the functional optimization problem. This proves the claim.

We therefore have

$$p(y|x_{f(x_1,...,x_k,y)}) = \max_{i=1}^{k} p(y|x_i).$$

Therefore, we can write

$$\begin{aligned}
\mathrm{ABA}_k[p(x,y)] &= \sup_f \Pr[f(X_1, ..., X_k, Y) = Z] \\
&= \frac{1}{k}\int p_X(x_1)\dots p_X(x_k)p(y|x_{f(x_1,\dots,x_k,y)})dx_1\dots dx_k dy. \\
&= \frac{1}{k}\int p_X(x_1)\dots p_X(x_k)\max_{i=1}^k p(y|x_i)dx_1\dots dx_k dy.
\end{aligned}$$

2 Problem formulation

Let $\mathcal{P}$ denote the collection of all joint densities $p(x, y)$ on finite-dimensional Euclidean space. For $\iota \in [0, \infty)$ define $C_k(\iota)$ to be the largest k-class average Bayes error attained by any distribution $p(x, y)$ with mutual information not exceeding ι:

$$C_k(\iota) = \sup_{p\in\mathcal{P}:\mathrm{I}[p(x,y)]\leq\iota} \mathrm{ABA}_k[p(x,y)].$$

A priori, $C_k(\iota)$ exists since ABA_k is bounded between 0 and 1. Furthermore, C_k is nondecreasing since the domain of the supremum is monotonically increasing with ι.

It follows that for any density $p(x, y)$, we have

$$\mathrm{ABA}_k[p(x,y)] \leq C_k(\mathrm{I}[p(x,y)]).$$

Hence C_k provides an upper bound for average Bayes error in terms of mutual information.

Conversely we have

$$\mathrm{I}[p(x,y)] \geq C_k^{-1}(\mathrm{ABA}_k[p(x,y)])$$

so that C_k^{-1} provides a lower bound for mutual information in terms of average Bayes error.

On the other hand, there is no nontrivial *lower* bound for average Bayes error in terms of mutual information, nor upper bound for mutual information in terms of average Bayes error, since

$$\inf_{p\in\mathcal{P}:\mathrm{I}[p(x,y)]\leq\iota} \mathrm{ABA}_k[p(x,y)] = \frac{1}{k}.$$

regardless of ι.

The goal of this work is to attempt to compute or approximate the functions C_k and C_k^{-1}.

3 Special case

We work out the special case where $p(x,y)$ lies on the unit square, and $p(x)$ and $p(y)$ are both the uniform distribution. Let $\mathcal{P}^{unif}$ denote the set of such distributions, and

$$C_k^{unif}(\iota) = \sup_{p(x,y)\in\mathcal{P}^{unif}:\mathrm{I}[p]\leq\iota} \mathrm{ABA}_k[p].$$

We prove the following result:

Theorem 3.1 *For any $\iota > 0$, there exists $c_\iota \geq 0$ such that defining*

$$Q_c(t) = \frac{\exp[ct^{k-1}]}{\int_0^1 \exp[ct^{k-1}]},$$

we have

$$\int_0^1 Q_{c_\iota}(t)\log Q_{c_\iota}(t)dt = \iota.$$

Then,

$$C_k^{unif} = \int_0^1 Q_{c_\iota}(t)t^{k-1}dt.$$

The proof depends on the following three lemmas.

Lemma 3.2 *Let $f(t)$ be an increasing function from $[a,b]\to\mathbb{R}$, where $a<b$, and let $g(t)$ be a bounded continuous function from $[a,b]\to\mathbb{R}$. Define the set*

$$A = \{t : f(t) \neq g(t)\}.$$

Then, we can write A as a countable union of intervals

$$A = \bigcup_{i=1}^{\infty} A_i$$

where A_i are mutually disjoint intervals of the form

- $[a_i, b_i]$,
- $(a_i, b_i]$,

- $[a_i, b_i)$,
- *or* (a_i, b_i)

with $a_i < b_i$, *and for each* i, *either* $f(t) > g(t)$ *for all* $t \in A_i$ *or* $f(t) < g(t)$ *for all* $t \in A_i$.

Lemma 3.3 *For any measure* G *on* $[0, \infty]$, *let* G^k *denote the measure defined by*

$$G^k(A) = G(A)^k,$$

and define

$$E[G] = \int x dG(x).$$

$$I[G] = \int x \log x dG(x)$$

and

$$\psi_k[G] = \int x d(G^k)(x).$$

Then, defining Q_c *and* c_ι *as in Theorem 1, we have*

$$\sup_{G: E[G]=1, I[G] \le \iota} \psi_k[G] = \int_0^1 Q_{c_\iota}(t) t^{k-1} dt.$$

Furthermore, the supremum is attained by a measure G *that has cdf equal to* Q_c^{-1}, *and thus has a density* g *with respect to Lesbegue measure.*

Lemma 3.4 *The map*

$$\iota \to \int_0^1 Q_{c_\iota}(t) t^{k-1} dt$$

is concave in $\iota > 0$.

Proof of Lemma 3.2. (This will appear in the appendix of the paper.)

The function $h(t) = f(t) - g(t)$ is measurable, since all increasing functions are measurable. Define $A^+ = \{t : f(t) > g(t)\}$ and $A^- = \{t : f(t) < g(t)\}$. Since A^+ and A^- are measurable subsets of $\mathbb{R}$, they both admit countable partitions $\mathcal{A}^+$ and $\mathcal{A}^-$ respectively consisting of open, closed, or half-open intervals. Define

$$\mathcal{A} = \mathcal{A}^+ \cup \mathcal{A}^-$$

and enumerate the elements

$$\mathcal{A} = \{A_i\}_{i=1}^{\infty}.$$

It remains to show that there are not isolated points in $\mathcal{A}$.

$\square$

Proof of Lemma 3.3. (This will appear in the appendix of the paper.)

Consider the quantile function $Q(t) = \inf_{x \in [0,1]} : G((-\infty, x]) \geq t$. $Q(t)$ must be a monotonically increasing function from $[0,1]$ to $[0,\infty)$.

We have

$$E[G] = \int_0^1 Q(t)dt$$

$$\psi_k[G] = \int_0^1 Q(t)x^{k-1}dt.$$

and

$$I[G] = \int_0^1 Q(t) \log Q(t)dt.$$

For any given ι, let P_ι denote the class of probability distributions G on $[0,\infty]$ such that $E[G] = 1$ and $-H[G] \leq \iota$. From Markov's inequality, for any $G \in P_\iota$ we have

$$G([x,\infty]) \leq x^{-1}$$

for any $x \geq 0$, hence P_ι is tight. From tightness, we conclude that P_ι is closed under limits with respect to weak convergence. Hence, since ψ_k is a continuous function, there exists a distribution $G^* \in P_\iota$ which attains the supremum

$$\sup_{G \in P_\iota} \psi_k[G].$$

Let $\mathcal{Q}_\iota$ denote the collection of quantile functions of distributions in P_ι. Then, $\mathcal{Q}_\iota$ consists of monotonic functions $Q : [0,1] \to [0,\infty]$ which satisfy

$$E[Q] = \int_0^1 Q(t)dt = 1,$$

and

$$I[Q] = \int_0^1 Q(t) \log Q(t)dt \leq \iota.$$

Let $\mathcal{Q}$ denote the collection of *all* quantile functions from measures on $[0, \infty]$. And letting Q^* be the quantile function for G^*, we have that Q^* attains the supremum

$$\sup_{Q \in \mathcal{Q}_\iota} \phi_k[Q] = \sup_{Q \in \mathcal{Q}_\iota} \int_0^1 Q(t) t^{k-1} dt.$$

Therefore, there exist Lagrange multipliers $\lambda \geq 0$ and $\nu \leq 0$ such that defining

$$\mathcal{L}[Q] = E[Q] + \lambda \phi_k[Q] + \nu I[Q] = \int_0^1 Q(t)(1 + \lambda \log Q(t) + \nu t^{k-1}) dt,$$

Q^* attains the infimum of $\mathcal{L}[Q]$ over *all* quantile functions,

$$\mathcal{L}[Q^*] = \inf_{Q \in \mathcal{Q}} \mathcal{L}[Q].$$

We now claim that for such λ and ν, we have

$$1 + \lambda + \lambda \log Q(t) + \nu t^{k-1} = 0.$$

Consider a perturbation function $\xi : [0, 1] \to \mathbb{R}$. We have

$$\mathcal{L}[Q + \xi] \approx \mathcal{L}[Q] + \int_0^1 \xi(t)(1 + \lambda + \lambda \log Q(t) + \nu t^{k-1}) dt$$

for small ξ. Define

$$\nabla Q^*(t) = (1 + \lambda + \lambda \log Q^*(t) + \nu t^{k-1}).$$

The function $\nabla Q^*(t)$ is a *functional derivative* of the Lagrangian. Note that if we were able to show that $\nabla Q^*(t) = 0$, as we might naively expect, this immediately yields

$$Q^*(t) = \exp[-\lambda^{-1} - 1 - \nu \lambda^{-1} t^{k-1}]. \quad (1)$$

However, the reason why we cannot simply assume $\nabla Q^*(t) = 0$ is because the optimization occurs on a constrained space. We will ultimately show that this is the case (up to sets of neglible measure), but some delicacy is needed.

First let us establish some properties of $\nabla Q^*(t)$. If we define $f(t) = 1 + \lambda + \lambda Q^*(t)$ and $g(t) = \nu t^{k-1}$, then f is increasing while g is continuous and stricly increasing. Therefore, as

$$\nabla Q^*(t) = f^+(t) - g(t),$$

we see that $\nabla Q^*(t)$ is a difference between two increasing functions.

Let B denote the set of points t such that $\nabla Q^*(t) \neq 0$. We would like to show that B is of measure zero, which would yield (1) up to neglible sets. What needs to be done is to show that $\nabla Q^*(t) = 0$ on a set of non-zero measure results in a contradiction. One can verify that for any t such that $\nabla Q^*(t) \neq 0$, one of the following four cases must apply.

- *Case 1:* $\nabla Q^*(t) \neq 0$ on an isolated point; i.e. for all neigborhoods N_t of t, $B \cap N_t$ is a set of measure zero.
- *Case 2:* $\nabla Q^*(t) \neq 0$ and there does not exist an interval such that $[a,b] \ni t$ is $\nabla Q^*(t)$ strictly positive or negative on the interval, but there does exist a neighborhood N_t of t such that $B \cap N_t$ has nonzero measure.
- *Case 3:* $\nabla Q^*(t) \neq 0$ and there exists an interval $[a,b] \ni t$ with $Q^*(a) < Q^*(b)$ such that $\nabla Q^*(t)$ is either strictly positive or negative on $[a,b]$.
- *Case 4:* $\nabla Q^*(t) \neq 0$ and there exists an interval $[a,b] \ni t$ with $Q^*(a) = Q^*(b)$ such that $\nabla Q^*(t)$ is either strictly positive or negative on $[a,b]$.

The set of all points t where case 1 applies is necessarily of zero measure. Therefore if B is non-negligible, there must exist t falling in one of the three other cases must occur. But we will show that each of cases 2 through 4 result in a contradiction.

Case 2.

Let N_t be a neighborhood of t such that $B \cap N_t$ has nonzero measure. Let S denote the set of points where

Case 3. Define

$$\xi^+(t) = I\{t \in [a,b]\}(Q(b) - Q(t))$$

and

$$\xi^-(t) = I\{t \in [a,b]\}(Q(a) - Q(t)).$$

, Observe that $Q + \epsilon\xi^+ \in \mathcal{Q}$ and $Q + \epsilon\xi^- \in \mathcal{Q}$ for any $\epsilon \in [0,1]$. Now, if $\nabla Q^*(t)$ is strictly positive on $[a,b]$, then for some $\epsilon > 0$ we would have $\mathcal{L}[Q^* + \epsilon\xi^-] < \mathcal{L}[Q^*]$, a contradiction. A similar argument with ξ^+ shows that $\nabla Q^*(t)$ cannot be stricly negative on $[a,b]$ either.

Case 4. Without loss of generality, let a and b be the endpoints of the largest interval containing t such that $Q^*(t)$ is constant on (a,b). Now, since

$\nabla Q^*(t) \neq 0$ on a set of nonzero measure within $[a, b]$, it must be the case that there exists some $u \in [a, b]$ such that

$$\int_a^u \nabla Q^*(t)dt \neq 0.$$

If $\int_a^u \nabla Q^*(t)dt > 0$, then define $\xi^+(t) = -I\{t \in (a, u)\}$ (to be contd.)

Remark. More specifically, the supremum is attained by a distribution with density $p_\iota(x, y)$ where

$$p_\iota(x, y) = \begin{cases} g_\iota(y - x) & \text{for } x \geq y \\ g_\iota(1 + y - x) & \text{for } x < y \end{cases}$$

where

$$g_\iota(x) = \frac{d}{dx} G_\iota(x)$$

and G_ι is the inverse of Q_c.

In this case, letting $X_1, ..., X_k \sim \text{Unif}[0, 1]$, and $Y \sim \text{Unif}[0, 1]$ define $Z_i(y) = p(y|X_i)$. We have $\mathbf{E}(Z(y)) = 1$ and,

$$\mathrm{I}[p(x, y)] = \mathbf{E}(Z(Y) \log Z(Y))$$

while

$$\mathrm{ABA}_k[p(x, y)] = k^{-1}\mathbf{E}(\max_i Z_i(Y)).$$

Letting g_y be the density of $Z(y)$, we have

$$\mathrm{I}[p(x, y)] = \mathbf{E}(-H[g_Y])$$

and

$$\mathrm{ABA}_k[p(x, y)] = \mathbf{E}(\psi_k[g_Y])$$

where

$$H[g] = -\int g(x)x \log x dx$$

and

$$\psi_k[g] = \int xg(x)G(x)^{k-1}dx$$

for $G(x) = \int_0^x g(t)dt$. Additionally g_y satisfies the constraint $\int xg(x)dx = 1$ since $\mathbf{E}[Z(y)] = 1$.

Define the set $D = \{(\alpha, \beta)\}$ as the set of possible values of $(-H[g], \psi_k[g])$ taken over all distributions g supported on $[0, \infty)$ with $\int xg(x)dx = 1$. Next, let $\mathcal{C}(D)$ denote the convex hull of D. It follows that $(\mathrm{I}[p], \mathrm{ABA}_k[p]) \in \mathcal{C}(D)$ since the pair is obtained via a convex average of points $(-H[g_y], \psi_k[g])$.

Define the upper envelope of D as the curve

$$d_k(\alpha) = \sup\{\beta : (\alpha, \beta) \in D\}.$$

We make the claim (to be shown in the following section) that $d_k(\alpha)$ is convex in α. As a result, the upper envelope of D is also the upper envelope of $\mathcal{C}(D)$. This in turn implies that $C_k^{unif}(\iota) = d_k(\iota)$. We establish these results, along with a open-form expression for C_k^{unif}, in the following section.

3.1 Variational methods

Consider the quantile function $Q(t) = G^{-1}(t)$. $Q(t)$ must be a continuous function from $[0, 1]$ to $[0, \infty)$. We can rewrite the moment constraint $\mathbf{E}[g] = 1$ as

$$\int_0^1 Q(t)dt = 1.$$

Meanwhile, $\beta = \psi_k[g]$ takes the form

$$\beta = \int_0^1 Q(t)x^{k-1}dt.$$

and $\alpha = -H[g]$ takes the form

$$\alpha = \int_0^1 Q(t) \log Q(t)dt.$$

To find the upper envelope, it will be useful to write the Langrangian

$$\begin{aligned}\mathcal{L}[g] &= \lambda \int_0^1 Q(t)dt + \mu \int_0^1 Q(t)x^{k-1}dt + \lambda \int_0^1 Q(t) \log Q(t)dt \\ &= \int_0^1 Q(t)(\lambda + \mu x^{k-1} + \nu \log Q(t))dt.\end{aligned}$$

In order for a quantile function $Q(t)$ to be on the upper envelope, it must be a local maximum of $-H$ with respect to small perturbations. Therefore, consider the functional derivative

$$D[\xi] = \lim_{\epsilon \to 0} \frac{\mathcal{L}[g + \epsilon\xi] - \mathcal{L}[g]}{\epsilon}.$$

We have

$$D[\xi] = \int_0^1 \xi(t)(\lambda + \nu + \mu x^{k-1} + \nu \log Q(t))dt.$$

Now consider the following three cases:

- $Q(t)$ is strictly monotonic, i.e. $Q'(t) > 0$.
- $Q(t)$ is differentiable but not strongly monotonic:
- $Q(t)$ is not strongly monotonic: there exist intervals $A_i = [a_i, b_i)$ such that $Q(t)$ is constant on A_i, and isolated points t_i where $Q'(t_i) = 0$.

Strictly monotonic case. Because Q is defined on a closed interval, strict monotonicity further implies the property of *strong monotonicity* where $\inf_[0, 1]Q'(t) > 0$. Therefore, for any differentiable perturbation $\xi(t)$ with $\sup |\xi'(t)| < \infty$, and further imposing that $\xi(0) \geq 0$ in the case that $Q(0) = 0$, there exists some $\epsilon > 0$ such that $(Q + \epsilon\xi)(t)$ is still a valid quantile function. Therefore, in order for $Q(t)$ to be a local maximum, we must have

$$0 = \lambda + \nu + \mu x^{k-1} + \nu \log Q(t)$$

for $t \in [0, 1]$. This implies that

$$Q(t) = c_0 e^{-c_1 x^{k-1}}$$

for some $c_0, c_1 \geq 0$.

Other cases. (TODO) We have to show that these cannot be local maxima.

4 General case

We claim that the constants $C_k^{unif}(\iota)$ obtained for the special case also apply for the general case, i.e.

$$C_k(\iota) = C_k^{unif}(\iota).$$

We make use of the following Lemma:

Lemma. *Suppose X, Y, W, Z are continuous random variables, and that $W \perp Y|Z$, $Z \perp X|Y$, and $W \perp Z|(X, Y)$. Then,*

$$I[p(x, y)] = I[p((x, w), (y, z))]$$

and

$$ABA_k[p(x,y)] = ABA_k[p((x,w),(y,z))].$$

Proof. Due to conditional independence relationships, we have

$$p((x,w),(y,z)) = p(x,y)p(w|x)p(z|y).$$

It follows that

$$\begin{aligned}
\mathrm{I}[p((x,w),(y,z))] &= \int dxdwdydz\ p(x,y)p(w|x)p(z|w)\log\frac{p((x,w),(y,z))}{p(x,w)p(y,z)} \\
&= \int dxdwdydz\ p(x,y)p(w|x)p(z|w)\log\frac{p(x,y)p(w|x)p(z|y)}{p(x)p(y)p(w|x)p(z|y)} \\
&= \int dxdwdydz\ p(x,y)p(w|x)p(z|w)\log\frac{p(x,y)}{p(x)p(y)} \\
&= \int dxdy\ p(x,y)\log\frac{p(x,y)}{p(x)p(y)} = \mathrm{I}[p(x,y)].
\end{aligned}$$

Also,

$$\begin{aligned}
\mathrm{ABA}_k[p((x,w),(y,z))] &= \int\left[\prod_{i=1}^k p(x_i,w_i)dx_idw_i\right]\int dydz\ \ \max_i p(y,z|x_i,w_i). \\
&= \int\left[\prod_{i=1}^k p(x_i,w_i)dx_idw_i\right]\int dy\ \ \max_i p(y|x_i)\int dz\ p(z|y). \\
&= \int\left[\prod_{i=1}^k p(x_i)dx_i\right]\left[\prod_{i=1}^k\int dw_ip(w_i|x_i)\right]\int dy\ \ \max_i p(y|x_i) \\
&= \mathrm{ABA}_k[p(x,y)].
\end{aligned}$$

□

Next, we use the fact that for any $p(x,y)$ and $\epsilon > 0$, there exists a discrete distribution $p_\epsilon(\tilde{x},\tilde{y})$ such that

$$|\mathrm{I}[p(x,y)] - \mathrm{I}[p_\epsilon(\tilde{x},\tilde{y})]| < \epsilon,$$

where for discrete distributions, one defines

$$\mathrm{I}[p(x,y)] = \sum_x\sum_y p(x,y)\log\frac{p(x,y)}{p(x)p(y)}.$$

We require the additional condition that the marginals of the discrete distribution are close to uniform: that is, for some $\delta > 0$, we have

$$\sup_{x,x':p_\epsilon(x)>0 \text{ and } p_\epsilon(x')>0} \frac{p_\epsilon(x)}{p_\epsilon(x')} \leq 1 + \delta.$$

and likewise

$$\sup_{y,y':p_\epsilon(y)>0 \text{ and } p_\epsilon(y')>0} \frac{p_\epsilon(y)}{p_\epsilon(y')} \leq 1 + \delta.$$

To construct the discretization with the required properties, choose a regular rectangular grid Λ over the domain of $p(x, y)$ sufficiently fine so that partitioning X, Y into grid cells, we have

$$|\mathrm{I}[p(x, y)] - \mathrm{I}[\tilde{p}(\tilde{x}, \tilde{y})]| < \epsilon.$$

[NOTE: to be written more clearly] Next, define