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

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

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}.

2.1 Notation

$|\cdot|$ denotes set cardinality.

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 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, with $\inf A_i < \sup A_i$, 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 *Let $f(t)$ be a measurable function from $[a, b] \to \mathbb{R}$, where $a < b$. Then there exists sets $\mathcal{B}_0$ and $\mathcal{B}_1$, satisfying the following properties:*

- *$\mathcal{B} = \mathcal{B}_0 \cup \mathcal{B}_1$ is countable partition of $[a, b]$,*
- *$f(t)$ is constant on all $B \in \mathcal{B}_0$, but not constant on any proper super-interval $B' \supset B$, and*
- *$B \in \mathcal{B}_1$ contains no positive-length subinterval where $f(t)$ is constant.*

Lemma 3.4 *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

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

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 3.5 *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 consisting of open, closed, or half-open intervals. Let $\mathcal{H}^+$ be the collection of all partitions of A^+ consisting of such intervals. There exists a least refined partition $\mathcal{A}^+$ within $\mathcal{H}^+$. Define $\mathcal{A}^-$ analogously, and let

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

and enumerate the elements

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

We claim that the partitions $\mathcal{A}^+$ and $\mathcal{A}^-$ have the the property that for all $t \in A^{\pm}$, ther interval $I \in \mathcal{A}^{\pm}$ containing t has endpoints $l \leq u$ defined by

$$l = \inf_{x \in [a,b]} \{x : \mathrm{Sign}(h([x,t])) = \{\mathrm{Sign}(h(t))\}\}$$

and

$$u = \sup_{x \in a[,b]} \{x : \mathrm{Sign}(h([t,x])) = \{\mathrm{Sign}(h(t))\}\}.$$

We prove the claim for the partition $\mathcal{A}^+$. Take $t \in A^+$ and define l and u as above. It is clear that $(l,u) \in A^+$, and furthermore, there is no $l' < l$ and $u' > u$ such that $(l', x) \in A^+$ or $(x, u') \in A^+$ for any $x \in I$. Let $\mathcal{H}$ be any other partition of A^+. Some disjoint union of intervals $H_i \in \mathcal{H}$ necessarily covers I for $i = 1, ...,$ and we can further require that none of the H_i are disjoint with I. Since each H_i has nonempty intersection with I, and I is an interval, this implies that $\cup_i H_i$ is also an interval. Let $l'' \leq u''$ be the endpoints of $\cup_i H_i$ Since $I \subseteq \cup_i H_i$, we have $l'' \leq l \leq u \leq u''$. However, since also $I \in A^+$, we must have $l \leq l'' \leq u'' \leq u$. This implies that $l'' = l$ and $u'' = u$. Since $\cup_i H_i = I$, and this holds for any $I \in \mathcal{A}^+$, we conclude that $\mathcal{H}$ is a refinement of $\mathcal{A}^+$. The proof of the claim for $\mathcal{A}^-$ is similar.

It remains to show that there are not isolated points in $\mathcal{A}$, i.e. that for all $I \in \mathcal{A}$ with endpoints $l \leq u$, we have $l < u$. Take $I \in \mathcal{A}$ with endpoints $l \leq u$ and let $t = \frac{l+u}{2}$. By definition, we have $h(t) \neq 0$. Consider the two cases $h(t) > 0$ and $h(t) < 0$.

If $h(t) > 0$, then $t' = g^{-1}(h(t)) > t$, and for all $x \in [t, t']$ we have $h(x) > 0$. Therefore, it follows from definition that $[t, t'] \in I$, and since $l \leq t < t' \leq u$, this implies that $l < u$. The case $h(t) < 0$ is handled similarly. $\square$

Proof of Lemma 3.3. (This will appear in the appendix of the paper.) To construct the interval, define

$$l(t) = \inf\{x \in [0,1] : f([x,t]) = \{f(t)\}\}$$

$$u(t) = \sup\{x \in [0,1] : f([t,x]) = \{f(t)\}\},$$

Let B_0 be the set of all t such that $l(t) < u(t)$, and let B_1 be the set of all t such that $l(t) = t = u(t)$. For all $t \in B_0$, define

$$I(t) = (l(t), u(t)) \cup \{x \in \{l(t), u(t)\} : f(x) = f(t)\}.$$

Then we claim

$$\mathcal{B}_0 = \{I(t) : t \in B_0\}$$

is a countable partition of B_0. The claim follows since the members of $\mathcal{B}_0$ are disjoint intervals of nonzero length, and B_0 has finite length. It follows from definition that for any $B \in B_0$, that f is not constant on any proper superinterval $B' \supset B$.

Meanwhile, let $\mathcal{B}_1$ be a countable partition of B_1 into intervals.

Next, we show that for all $I \in \mathcal{B}_1$, I does not contain a subinterval I' of nonzero length such that f is constant on I'. Suppose to the contrary, we could find such an interval I and subinterval I'. Then for any $t \in I'$, we have $t \in B_0$. However, this implies that $t \notin B_1$, a contradiction.

Since $t \in [a,b]$ belongs to either B_0 or B_1, letting $\mathcal{B} = \mathcal{B}_0 \cup \mathcal{B}_1$ yields the desired partition of $[a,b]$. $\Box$.

Proof of Lemma 3.4. (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 $[0,\infty)$. Let $\mathcal{Q}$ denote the collection of all such quantile functions.

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

$$\mathcal{L}[Q + \xi] \approx \mathcal{L}[Q] + \int_0^1 \xi(t)(1 + \lambda + \lambda \log Q(t) + \nu t^{k-1})dt \tag{2}$$

for small ξ. Define

$$\nabla\mathcal{L}_{Q^*}(t) = 1 + \lambda + \lambda \log Q^*(t) + \nu t^{k-1}. \tag{3}$$

The function $\nabla\mathcal{L}_{Q^*}(t)$ is a *functional derivative* of the Lagrangian. Note that if we were able to show that $\nabla\mathcal{L}_{Q^*}(t) = 0$, this immediately yields

$$Q^*(t) = \exp[-\lambda^{-1} - 1 - \nu\lambda^{-1}t^{k-1}]. \tag{4}$$

At this point, we know that the right-hand side of (4) gives a stationary point of $\mathcal{L}$, but we cannot be sure that it gives the global minimzer. The reason is because the optimization occurs on a constrained space. We will show that (4) indeed gives the global minimizer Q^*, but we do so by showing that the set of points t where $\nabla\mathcal{L}_{Q^*}(t) \neq 0$ is of zero measure. Since sets of zero measure don't affect the integrals defining the optimization problem (1), we conclude there exists a global optimal solution with $\nabla\mathcal{L}_{Q^*}(t) = 0$ everywhere, which is therefore given explicitly by (4) for some $\lambda > 0$, $\nu < 0$.

The rest of the proof proceeds as follows. We will use Lemmas 3.2 and 3.3 to define a decomposition $A = D_0 \cup D_1 \cup D_2$, where D_2 is of measure zero. First, we show that assuming the existence of $t \in D_0$ yields a contradiction, and hence $D_0 = \emptyset$. Then, again using argument from contradiction we establish that $D_1 = \emptyset$. Finally, since D_2 is a set of zero measure, this allows us to conclude that the $Q^*(t) = 0$ on all but a set of zero measure.

We will now apply the Lemmas to obtain the necessary ingredients for constructing the sets D_i. Since $\nabla\mathcal{L}_{Q^*}(t)$ is a difference between an increasing function and a continuous stricly increasing function, we can apply Lemma 3.2 to conclude that there exists a countable partition $\mathcal{A}$ of the set $A : \{t \in [0,1] : \nabla\mathcal{L}_{Q^*}(t) \neq 0\}$ into intervals such that for all $J \in \mathcal{A}$, $|\mathrm{Sign}(\nabla Q^*(J))| = 1$ and $\inf J < \sup I$. Applying Lemma 3.3 we get a countable partition $\mathcal{B} = \mathcal{B}_0 \cup \mathcal{B}_1$ of $[0,1]$ so that each element $J \in \mathcal{B}_0$ is an interval such that $\nabla\mathcal{L}_{Q^*}(t)$ is constant on J, and furthermore is not properly contained in any interval with the same property, and each element $J \in \mathcal{B}_1$ is an interval, such that J contains no positive-length subinterval where $\nabla\mathcal{L}_{Q^*}(t)$ is constant. Also define B_i as the union of the sets in $\mathcal{B}_i$ for $i = 0, 1$.

Note that B_0 is necessarily a subset of A. That is because if $\nabla\mathcal{L}_{Q^*}(t) = 0$ on any interval J, then that $Q^*(t)$ is necessarily not constant on the interval.

We will construct a new countable partition of A, called $\mathcal{D}$. The partition $\mathcal{D}$ is constructed by taking the union of three families of intervals,

$$\mathcal{D} = \mathcal{D}_0 \cup \mathcal{D}_1 \cup \mathcal{D}_2.$$

Define D_i to be the union of intervals in $\mathcal{D}_i$ for $i = 0, 1, 2$.

Define $\mathcal{D}_0 = \mathcal{B}_0$, Define a countable partition $\mathcal{D}_1$ by

$$\mathcal{D}_1 = \{J \cap L : J \in \mathcal{A}, L \in \mathcal{B}_1, \text{ and } |L| > 1\},$$

in order words, $\mathcal{D}_1$ consists of positive-length intervals where $\nabla Q^*(t)$ is entirely positive or negative and is not constant. Define

$$\mathcal{D}_2 = \{J \in \mathcal{B}_1 : J \subset A \text{ and } |J| = 1\},$$

i.e. $\mathcal{D}_2$ consists of isolated points in A.

One verifies that $\mathcal{D}$ is indeed a partition of A by checking that $D_0 = B_0$, $D_1 \cup D_2 = B_1 \cap A$, so that $D_0 \cup D_2 \cup D_2 = A$: it is also easy to check that elements of $\mathcal{D}$ are disjoint. Furthermore, as we mentioned earlier, the set D_2 is indeed of zero measure, since it consists of countably many isolated points.

Now we will show that the existence of $t \in D_0$ implies a contradiction. Take $t \in D$ for $D \in \mathcal{D}_0$, and let $a = \inf D$ and $b = \sup D$. Define

$$\xi^+ = I\{t \in D\}(Q^*(b) - Q^*(t))$$

and

$$\xi^- = I\{t \in D\}(Q^*(a) - Q^*(t)).$$

Observe that $Q + \epsilon\xi^+ \in \mathcal{Q}$ and $Q + \epsilon\xi^- \in \mathcal{Q}$ for any $\epsilon \in [0, 1]$. Now, if $\nabla\mathcal{L}_{Q^*}(t)$ is strictly positive on D, 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 $\nabla\mathcal{L}_{Q^*}(t)$ cannot be strictly negative on D either. From this pertubation argument, we conclude that $\nabla\mathcal{L}_{Q^*}(t) = 0$. Since this argument applies for all $t \in D_0$, we conclude that $D_0 = \emptyset$: therefore, on the set $[0, 1] \setminus (D_1 \cup D_2)$, we have $\nabla\mathcal{L}_{Q^*}(t) = 0$.

The following observation is needed for the next stage of the proof. If we look at the function $Q^*(t)$, then up so sets of neglible measure, it is given by the expression (4) on the set $[0, 1] \setminus D_1$, and it is piecewise constant inbetween. But since (4) gives a strictly increasing function, and since Q^* is increasing, this implies that Q^* is discontinuous at the boundary of D_1.

Now we are prepared to show that $\nabla\mathcal{L}_{Q^*}(t) = 0$ for $t \in D_1$. Take $t \in D$ for $D \in \mathcal{D}_1$, and let $a = \inf D$ and $b = \sup D$. From the previous argument, there is a discontinuity at both a and b, so that $\lim_{u \to a^-} Q(u) < Q(t) < \lim_{u \to b^+} Q(u)$. Therefore, for any $\xi(t)$ which is increasing on D and zero elsewhere, there exists $\epsilon > 0$ such that $\nabla Q^* + \epsilon\xi \in \mathcal{Q}$. It remains to find such a perturbation ξ such that $\mathcal{L}[Q + \epsilon\xi] < \mathcal{L}[Q]$.

Also, since by definition $\nabla\mathcal{L}_{Q^*}(t)$ is constant on D, follows from(3) that ∇Q^* is strictly decreasing, and thus either

- Case 1: $\nabla \mathcal{L}_{Q^*}(t) \geq 0$ on D,
- Case 2: $\nabla \mathcal{L}_{Q^*}(t) \leq 0$ on D, or
- Case 3: $\nabla \mathcal{L}_{Q^*}(t) \geq 0$ for all $t \in D \cap [a, t_0]$ and $\nabla \mathcal{L}_{Q^*}(t) \leq 0$ for all $t \in D \cap [t_0, b]$.

Depending on the case, we construct a suitable perturbation ξ:

- Case 1: Construct $\xi(t) = -I\{t \in D\}$.
- Case 2: Construct $\xi(t) = I\{t \in D\}$
- Case 2: Construct

$$\xi(t) = \begin{cases} -1 & \text{for } t \in D \cap [a, t_0], \\ 0 & \text{otherwise.} \end{cases}$$

In all three cases, given the corresponding construction for $\xi(t)$ we get

$$\int_0^1 \xi(t) \nabla \mathcal{L}_{Q^*}(t) dt < 0.$$

Therefore, from (2), there exists some $\epsilon > 0$ such that $\mathcal{L}[Q + \epsilon\xi] < \mathcal{L}[Q]$, a contradiction. Again, since the contradiction applies for all $t \in D_1$, we conclude that $D_1 = \emptyset$.

By now we have established that a global optimum for (1) exists, and is given by (4) for some $\lambda > 0$, $\nu < 0$. It remains to determine the values of λ and ν.

Reparameterize $\alpha = \exp[-1 - \lambda^{-1}]$ and $\beta = -\nu\lambda t^{k-1}$. Therefore,

$$Q^*(t) = \alpha \exp[\beta t^{k-1}]$$

for $\alpha > 0$, $\beta > 0$. There is a one-to-one mapping from $(\alpha, \beta) \in (0, \infty)^2$ to $(\lambda, \nu) \in (0, \infty) \times (-\infty, 0)$.

Now, from the constraint

$$1 = E[Q^*] = \int_0^1 \alpha \exp[\beta t^{k-1}] dt.$$

we conclude that

$$\alpha = \frac{1}{\int_0^1 \exp[\beta t^{k-1}] dt.}$$

Therefore, we have reduced the set of possible solutions Q^* to a one-parameter family,

$$Q^*(t) = \frac{\exp[\beta t^{k-1}]}{Z(\beta)}.$$

where

$$Z(\beta) = \int_0^1 \exp[\beta t^{k-1}]dt.$$

Next, consider that

$$I[Q^*] = \int_0^1 Q^*(t) \log Q^*(t) = \frac{\beta}{Z(\beta)} \int_0^1 \exp[\beta t^{k-1}] t^{k-1} dt - \log Z(\beta).$$

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

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

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

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

and

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

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