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

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

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

$$ABA_k[p(x,y)] = \sup_{f} \Pr[f(X_1,...,X_k,Y) = Z]$$

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

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

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

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

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

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

To show this claim, write

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

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 $f(x_1,...,x_k,y)=\arg\max_z p(y|x_z)$ —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

$$ABA_{k}[p(x,y)] = \sup_{f} \Pr[f(X_{1},...,X_{k},Y) = Z]$$

$$= \frac{1}{k} \int p_{X}(x_{1}) \dots p_{X}(x_{k}) p(y|x_{f(x_{1},...,x_{k},y)}) dx_{1} \dots dx_{k} dy.$$

$$= \frac{1}{k} \int p_{X}(x_{1}) \dots p_{X}(x_{k}) \max_{i=1}^{k} p(y|x_{i}) dx_{1} \dots dx_{k} dy.$$

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 :

$$C_k(\iota) = \sup_{p \in \mathcal{P}: I[p(x,y)] \le \iota} ABA_k[p(x,y)].$$

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

$$ABA_k[p(x,y)] \le C_k(I[p(x,y)]).$$

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

Conversely we have

$$I[p(x,y)] \ge C_k^{-1}(ABA_k[p(x,y)])$$

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

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

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 Theory

In this section we determine the value of $C_k(\iota)$, leading to 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,

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

We obtain this result by first reducing the problem to the case of densities with uniform marginals, then doing the optimization over the reduced space.

3.1 Reduction

Let p(x, y) be a density supported on $\mathcal{X} \times \mathcal{Y}$, where \mathcal{X} is a subset of \mathbb{R}^{d_1} and \mathcal{Y} is a subset of \mathbb{R}^{d_2} , and such that p(x) is uniform on \mathcal{X} and p(y) is uniform on \mathcal{Y} .

Now let \mathcal{P}^{unif} denote the set of such distributions: in other words, \mathcal{P}^{unif} is the space of joint densities in Euclidean space with uniform marginals over the marginal supports. In this section, we prove that

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

thus reducing the problem of optimizing over the space of all densities to the problem of optimizing over densities with uniform marginals.

Also define $\mathcal{P}^{bounded}$ to be the space of all densities p(x,y) with finite-volume support. Since uniform distributions can only be defined over sets of finite volume, we have

$$\mathcal{P}^{unif} \subset \mathcal{P}^{bounded} \subset \mathcal{P}.$$

Therefore, it is necessary to first show that

$$\inf_{p \in \mathcal{P}: \mathbf{I}[p(x,y)] \leq \iota} \mathbf{ABA}_k[p(x,y)] = \inf_{p \in \mathcal{P}^{bounded}: \mathbf{I}[p(x,y)] \leq \iota} \mathbf{ABA}_k[p(x,y)].$$

This is accomplished via the following lemma.

Lemma 3.2 (Truncation). Let p(x,y) be a density on $\mathbb{R}^{d_x} \times \mathbb{R}^{d_y}$. For all $\epsilon > 0$, there exists a subset $\mathcal{X} \subset \mathbb{R}^{d_x}$ with finite volume with respect to d_x -dimensional Lesbegue measure, and a subset $\mathcal{Y} \subset \mathbb{R}^{d_y}$ with finite volume with respect to d_y -dimensional Lesbegue measure, such that defining

$$\tilde{p}(x,y) = \frac{I\{(x,y) \in \mathcal{X} \times \mathcal{Y}\}}{\int_{\mathcal{X} \times \mathcal{Y}} p(x,y) dx dy} p(x,y),$$

we have

$$|I[p] - I[\tilde{p}]| < \epsilon$$

and

$$|ABA_k[p] - ABA_k[\tilde{p}]| < \epsilon.$$

Proof. Recall the definition of the Shannon entropy H:

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

It is a well-known in information theory that

$$I[p(x,y)] = H[p(x)] + H[p(y)] - H[p(x,y)].$$

There exists a sequence $(\mathcal{X}_i, \mathcal{Y}_i)_{i=1}^{\infty}$ where $(\mathcal{X}_i)_{i=1}^{\infty}$ is an increasing sequence of finite-volume subsets of \mathbb{R}^{d_x} and $(\mathcal{Y}_i)_{i=1}^{\infty}$ is an increasing sequence of finite-volume subsets of \mathbb{R}^{d_y} , and $\lim_{i\to\infty} \mathcal{X}_i = \mathbb{R}^{d_x}$, $\lim_{i\to\infty} \mathcal{Y}_j$. Define

$$\tilde{p}_i(x,y) = \frac{I\{(x,y) \in \mathcal{X}_i \times \mathcal{Y}_i\}}{\int_{\mathcal{X}_i \times \mathcal{Y}_i} p(x,y) dx dy} p(x,y)$$

Note that \tilde{p}_i gives the conditional distribution of (X, Y) conditional on $(X, Y) \in \mathcal{X}_i \times \mathcal{Y}_i$. Furthermore, it is convenient to define $\tilde{p}_{\infty} = p$. We can find some i_1 , such that for all $i \geq i_1$, we have

$$\left| \int_{x \notin \mathcal{X}_i} p(x) \log p(x) dx \right| < \frac{\epsilon}{6}$$

$$\left| \int_{y \notin \mathcal{Y}_i} p(y) \log p(y) dy \right| < \frac{\epsilon}{6}$$

$$\left| \int_{(x,y) \notin \mathcal{X}_i \times \mathcal{Y}_i} p(x,y) \log p(x,y) dx dy \right| < \frac{\epsilon}{6}$$

and also such that

$$-\log\left[\int_{x,y\in\mathcal{X}_i\times\mathcal{Y}_i}p(x,y)dxdy\right]<\frac{\epsilon}{2}$$

Then, it follows that

$$|I[p] - I[\tilde{p}_i]| < \epsilon$$

for all $i \geq i_1$.

Now we turn to the analysis of average Bayes error. Let f_i denote the Bayes k-class classifier for $\tilde{p}_i(x,y)$ and f_{∞} the Bayes k-class classifier for p(x,y): recall that by definition,

$$ABA_k[\tilde{p}_i] = \Pr_{\tilde{p}_i}[f_i(X_1, ..., X_k, Y) = Z]$$

Define

$$\epsilon_i = \Pr_{p}[(X_1, ..., X_k, Y) \notin \mathcal{X}_i^k \times \mathcal{Y}_i];$$

by continuity of probability we have $\lim_{i} \epsilon_{i} \to 0$. We claim that

$$|ABA_k[\tilde{p}_i] - ABA_k[p]| \le \epsilon_i.$$

Given the claim, the proof is completed by finding $i > i_1$ such that $\epsilon_i < \epsilon$, and defining $\mathcal{X} = \mathcal{X}_i$, $\mathcal{Y} = \mathcal{Y}_i$.

Consider using f_i to obtain a classification rule for p(x, y): define

$$\tilde{f}_i = \begin{cases} f_i(x_1, ..., x_k, y) & \text{when } (x_1, ..., x_k, y) \in \mathcal{X}_i^k \times \mathcal{Y} \\ 0 & \text{otherwise.} \end{cases}$$

We have

$$ABA_{k}[p] = \sup_{f} \Pr_{p}[f(X_{1}, ..., X_{k}, Y) = Z]$$

$$\geq$$

$$= (1 - \epsilon_{i}) \Pr_{p}[f_{i}(X_{1}, ..., X_{k}, Y) = Z | (X_{1}, ..., X_{k}, Y) \in \mathcal{X}_{i}^{k} \times \mathcal{Y}_{i}]$$

$$+ \epsilon_{i} \Pr_{p}[f_{i}(X_{1}, ..., X_{k}, Y) = Z | (X_{1}, ..., X_{k}, Y) \notin \mathcal{X}_{i}^{k} \times \mathcal{Y}_{i}]$$

$$= (1 - \epsilon_{i}) \Pr_{\tilde{p}}[f_{i}(X_{1}, ..., X_{k}, Y) = Z] + \epsilon_{i}0$$

$$= (1 - \epsilon_{i}) ABA_{k}[\tilde{p}_{i}] \geq ABA_{k}[\tilde{p}_{i}] - \epsilon_{i}.$$

In other words, when \tilde{p}_i is close to p, the Bayes classification rule for \tilde{p}_i obtains close to the Bayes rate when the data is generated under p.

Now consider the reverse scenario of using f_p to perform classification under \tilde{p}_i . This is equivalent to generating data under p(x, y), performing classification using f, then only evaluating classification accuracy conditional on $(X_1, ..., X_k, Y) \in \mathcal{X}_i^k \times \mathcal{Y}_i$. Therefore,

$$ABA_{k}[\tilde{p}_{i}] = \sup_{f} \Pr_{\tilde{p}_{i}}[f(X_{1}, ..., X_{k}, Y) = Z]$$

$$\geq \Pr_{\tilde{p}_{i}}[f_{p}(X_{1}, ..., X_{k}, Y) = Z]$$

$$= \Pr_{p}[f_{p}(X_{1}, ..., X_{k}, Y) = Z | (X_{1}, ..., X_{k}, Y) \in \mathcal{X}_{i}^{k} \times \mathcal{Y}_{i}]$$

$$= \frac{1}{1 - \epsilon_{i}} \Pr_{p}[I\{(X_{1}, ..., X_{k}, Y) \in \mathcal{X}_{i}^{k} \times \mathcal{Y}_{i}\} \text{ and } f_{p}(X_{1}, ..., X_{k}, Y) = Z]$$

$$\geq \frac{1}{1 - \epsilon_{i}} \left(1 - \Pr_{p}[I\{(X_{1}, ..., X_{k}, Y) \notin \mathcal{X}_{i}^{k} \times \mathcal{Y}_{i}\}] - \Pr_{p}[f_{p}(X_{1}, ..., X_{k}, Y) \notin Z]\right]$$

$$= \frac{ABA_{k}[p] - \epsilon_{i}}{1 - \epsilon_{i}} \geq ABA_{k}[p] - \epsilon_{i}.$$

In other words, when \tilde{p}_i is close to p, the Bayes classification rule for p obtains close to the Bayes rate when the data is generated under \tilde{p}_i .

Combining the two directions gives $|ABA_k[\tilde{p}_i] - ABA_k[p]| \le \epsilon_i$, as claimed.

One can go from bounded-volume sets to uniform distributions by adding auxiliary variables. To illustrate the intution, consider a density p(x) on a

set of bounded volume, \mathcal{X} . Introduce a variable W such that conditional on X = x, we have w uniform on [0, p(x)]. It follows that the joint density p(x, w) = 1 and is supported on a set $\mathcal{X}' = \mathcal{X} \times [0, \infty]$. Furthermore, \mathcal{X}' is of bounded volume (in fact, of volume 1) since

$$\int_{\mathcal{X}'} dx = \int_{\mathcal{X}'} p(x, w) dx = 1.$$

Therefore, to accomplish the reduction from \mathcal{P} to \mathcal{P}^{unif} , we start with a density $p(x,y) \in \mathcal{P}$, and using Lemma 3.2, find a suitable finite-volume truncation $\tilde{p}(x,y)$. Finally, we introduce auxiliary variables w and z so that the expanded joint distribution p(x,w,y,z) has uniform marginals p(x,w) and p(y,z). However, we still need to check that the introduction of auxiliary variables preserves the mutual information and average Bayes error; this is the content of the next lemma.

Lemma 3.3 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,

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

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

$$I[p((x,w),(y,z))] = \int dx dw dy dz \ p(x,y)p(w|x)p(z|w) \log \frac{p((x,w),(y,z))}{p(x,w)p(y,z)}$$

$$= \int dx dw dy dz \ p(x,y)p(w|x)p(z|w) \log \frac{p(x,y)p(w|x)p(z|y)}{p(x)p(y)p(w|x)p(z|y)}$$

$$= \int dx dw dy dz \ p(x,y)p(w|x)p(z|w) \log \frac{p(x,y)}{p(x)p(y)}$$

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

Also,

$$ABA_{k}[p((x, w), (y, z))] = \int \left[\prod_{i=1}^{k} p(x_{i}, w_{i}) dx_{i} dw_{i} \right] \int dy dz \max_{i} p(y, z | x_{i}, w_{i}).$$

$$= \int \left[\prod_{i=1}^{k} p(x_{i}, w_{i}) dx_{i} dw_{i} \right] \int dy \max_{i} p(y | x_{i}) \int dz \ p(z | y).$$

$$= \int \left[\prod_{i=1}^{k} p(x_{i}) dx_{i} \right] \left[\prod_{i=1}^{k} \int dw_{i} p(w_{i} | x_{i}) \right] \int dy \max_{i} p(y | x_{i})$$

$$= ABA_{k}[p(x, y)].$$

Combining these lemmas gives the needed reduction, given by the following theorem.

Theorem 3.4 (Reduction.)

$$\inf_{p \in \mathcal{P}: I[p(x,y)] \le \iota} ABA_k[p(x,y)] = \inf_{p \in \mathcal{P}^{unif}: I[p(x,y)] \le \iota} ABA_k[p(x,y)].$$

The proof is trivial given the previous two lemmas.

3.2 Optimization

Having reduced the problem to an optimization over \mathcal{P}^{unif} , in this section we use variational calculus to find the global optimum to the optimization problem

$$\text{maximize}_{p \in \mathcal{P}^{unif}: \mathbf{I}[p(x,y)] \le \iota} ABA_k[p(x,y)]$$

The proof depends on the following lemmas.

Lemma 3.5 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 3.6 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 superinterval $B' \supset B$, and
- $B \in \mathcal{B}_1$ contains no positive-length subinterval where f(t) is constant.

Lemma 3.7 Define an exponential family on [0,1] by the density function

$$q_{\beta}(t) = \exp[\beta t^{k-1} - \log Z(\beta)]$$

where

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

Then, the negative entropy

$$I(\beta) = \int_0^1 q_{\beta}(t) \log q_{\beta}(t) dt$$

is decreasing in β on the interval $(-\infty, 0]$. and increasing on the interval $[0, \infty)$.

Furthermore, for any $\iota \in (0, \infty)$, there exist two solutions to $I(\beta) = \iota$: one positive and one negative.

Lemma 3.8 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 3.9 The map

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

is concave in $\iota > 0$.

Proof of Lemma 3.5. (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 property that for all $t \in A^{\pm}$, ther interval $I \in \mathcal{A}^{\pm}$ containing t has endpoints $l \leq u$ defined by

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

and

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

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 $l \le t < t' \le u$, this implies that l < u. The case h(t) < 0 is handled similarly. \square

Proof of Lemma 3.6. (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]. \square .

Proof of Lemma 3.7.

Define $\beta(\mu)$ as the solution to

$$\mu = \int_0^1 t q_{\beta}(t) dt.$$

By [Wainwright and Jordan 2008], the function $\beta(\mu)$ is well-defined. Furthermore, since the sufficient statistic t^{k-1} is increasing in t, it follows that $\beta(\mu)$ is increasing.

Define the negative entropy as a function of μ ,

$$N(\mu) = \int_0^1 q_{\beta(\mu)}(t) \log q_{\beta(\mu)}(t) dt.$$

By Theorem 3.4 of [Wainwright and Jordan 2008], $N(\mu)$ is convex in μ . We claim that the derivative of $N(\mu) = 0$ at $\mu = \frac{1}{2}$. This implies that $N(\mu)$ is decreasing in μ for $\mu \leq \frac{1}{2}$ and increasing for $\mu \geq \frac{1}{2}$. Since $I(\beta(\mu)) = N(\mu)$, β is increasing in μ , and $\beta(\frac{1}{2}) = 0$, this implies that $I(\beta)$ is decreasing in β for $\beta \leq 0$ and increasing for $\beta \geq 0$.

We will now prove the claim. Write

$$\left. \frac{d}{d\mu} N(\mu) \right|_{\mu=1/2} = \frac{d}{d\beta} I(\beta(\mu)) \left| \frac{d\beta}{\beta=0} \frac{d\beta}{d\mu} \right|_{\mu=1/2}.$$

We have

$$\frac{d}{d\beta}I(\beta) = \beta \int q_{\beta}t^{k-1}dt - \log Z(\beta).$$

Meanwhile, Z(0) = 1 so $\log Z(0) = 0$. Therefore,

$$\left. \frac{d}{d\beta} I(\beta) \right|_{\beta=0} = 0.$$

This implies that $\frac{d}{d\mu}N(\mu)|_{\mu=1/2}=0$, as needed.

For the final statement of the lemma, note that I(0) = 0 since q_0 is the uniform distribution. Meanwhile, since q_{β} tends to a point mass as either $\beta \to \infty$ or $\beta \to -\infty$, we have

$$\lim_{\beta \to \infty} I(\beta) = \lim_{\beta \to -\infty} I(\beta) = \infty.$$

And, as we can check that $I(\beta)$ is continuous in β , this means that

$$I((-\infty, 0]) = I([0, \infty)) = [0, \infty)$$

by the mean-value theorem. Combining this fact with the monotonicity of $I(\beta)$ restricted to either the positive and negative half-line yields the fact that for any $\iota > 0$, there exists $\beta_1 < 0 < \beta_2$ such that $I(\beta_1) = I(\beta_2) = \iota$. \square .

Proof of Lemma 3.8. (This will appear in the appendix of the paper.)

Consider the quantile function $Q(t) = \inf_{x \in [0,1]} : G((-\infty, x]) \ge t$. 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

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

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

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

and

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

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

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

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

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

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

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

The global minimizer Q^* is also necessarily a stationary point: that is, for any perturbation function $\xi:[0,1]\to\mathbb{R}$ such that $Q^*+\xi\in\mathcal{Q}$, we have $\mathcal{L}[Q^*]\leq\mathcal{L}[Q^*+\xi]$. For sufficiently small ξ , we have

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

Define

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

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

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

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 $\lambda \in \mathbb{R}$, $\nu \geq 0$.

We will need the following result: that for $\iota > 0$, any solution to (1) satisfies $\phi_k[Q] < 1$. This follows from the fact that

$$E[Q] - \phi_k[Q] = \int_0^1 (1 - t^{k-1})Q(t)dt,$$

where the term $(1-t^{k-1})$ is negative, except for the one point t=1. Therefore, in order for $\phi_k[Q]=1=E[Q]$, we must have Q(t)=0 for t<1. However, this yields a contradiction since Q(t)=0 for t<1 implies that E[Q]=0, a violation of the hard constraint E[Q]=1.

Let us establish that $\nu > 0$: in other words, the constraint $I[Q] = \iota$ is tight. Suppose to the contrary, that for some $\iota > 0$, the global optimum Q^* minimizes a Lagrangian with $\nu = 0$. Let $\phi^* = \phi_k[Q^*] < 1$. However, if we define $Q_{\kappa}(t) = I\{t \geq 1 - \frac{1}{\kappa}\}\kappa$, we have $E[Q_{\kappa}] = 1$, and also for some sufficiently large $\kappa > 0$, $\phi_k[Q_{\kappa}] > \phi^*$. But since the Lagrangian lacks a term corresponding to I[Q], we conclude that $\mathcal{L}[Q_{\kappa}] < \mathcal{L}[Q^*]$, a contradiction.

The rest of the proof proceeds as follows. We will use Lemmas 3.5 and 3.6 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 strictly increasing function, we can apply Lemma 3.5 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 3.6 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 $\lambda \in \mathbb{R}$, $\nu > 0$. It remains to determine the values of λ and ν .

Reparameterize $\alpha = \exp[-1 - \lambda \nu^{-1}]$ and $\beta = \nu^{-1}$. 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 $(\lambda, \nu) \in \mathbb{R} \times (0, \infty)$.

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, note that

$$I[Q^*] = \int_0^1 Q^*(t) \log Q^*(t) = \beta \mu_{\beta} - \log Z(\beta),$$

as a function of β , is completely characterized by Lemma 3.7. Let us define c_i as the unique positive solution to the equation

$$c_{\iota}\mu_{c_{\iota}} - \log Z(c_{\iota}) = \iota$$

given by Lemma 3.7. We therefore have

$$Q^*(t) = \frac{\exp[c_t t^{k-1}]}{\int_0^1 \exp[c_t t^{k-1}]},$$

as needed. \square

Proof of Lemma 3.9. It is equivalent to show that the inverse function

$$C_k^{-1}(p) = \inf_{G: E[G]=1, \phi_k[G]=p} I[G]$$

is convex. Let $p_1, p_2 \in [0, 1]$. From lemma 3.8, we can find measures G_1, G_2 on $[0, \infty)$ which minimize $I[G_i]$ subject to $E[G_i] = 1$ and $\phi_k[G_i] = p_i$. Define the measure

$$H = \frac{G_1 + G_2}{2}.$$

Since ϕ_k is a linear functional,

$$\phi_k[H] = \frac{\phi_k[G_1] + \phi_k[G_2]}{2} = \frac{p_1 + p_2}{2}.$$

But since I is a convex functional,

$$I[H] \le \frac{I[G_1] + I[G_2]}{2}.$$

Therefore,

$$C_k^{-1}\left(\frac{p_1+p_2}{2}\right) \le I[H] = \frac{I[G_1]+I[G_2]}{2} = \frac{C_k^{-1}(p_1)+C_k^{-1}(p_2)}{2}.$$

 \Box .

Proof of theorem 3.1

Using Theorem 3.4, we have

$$C_k(\iota) = \inf_{p \in \mathcal{P}^{unif}: \mathbb{I}[p(x,y)] \le \iota} ABA_k[p(x,y)].$$

Define $f(\iota) = \int_0^1 Q_{c_{\iota}}(t) t^{k-1} dt$: our goal is to establish that $C_k(\iota) = f(\iota)$. Note that $f(\iota)$ is the same function which appears in Lemma 3.9 and the same bound as established in Lemma 3.8.

Define the density $p_{\iota}(x,y)$ where

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

where

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

and G_{ι} is the inverse of Q_c .

One can verify that $I[p_{\iota}] = \iota$, and

$$ABA_k[p] = \int_0^1 Q_{c_i}(t)t^{k-1}dt.$$

This establishes that

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

It remains to show that for all $p \in \mathcal{P}^{unif}$ with $I[p] \leq \iota$, that $ABA_k[p] \leq ABA_k[p_{\iota}]$.

Take $p \in \mathcal{P}^{unif}$ such that $I[p] \leq \iota$. 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,

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

while

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

Letting G_y be the distribution of Z(y), we have

$$E[G_y] = 1$$

$$I[p(x, y)] = \mathbf{E}(I[G_Y])$$

$$ABA_k[p(x, y)] = \mathbf{E}(\psi_k[G_Y])$$

where the expectation is taken over $Y \sim \text{Unif}[0,1]$ and where E[G], I[G], and $\psi_k[G]$ are defined as in Lemma 3.8.

Define the random variable $J = I[G_Y]$. We have

$$ABA_{k}[p(x,y)] = \mathbf{E}(\psi_{k}[G_{Y}])$$

$$= \int_{0}^{1} \psi_{k}[G_{y}] dy$$

$$\leq \int_{0}^{1} \left(\sup_{G:I[G] \leq I[G_{y}]} \psi_{k}[G] \right) dy$$

$$= \int_{0}^{1} f(I[G_{y}]) dy = \mathbf{E}[f(J)].$$

Now, since f is concave by Lemma 3.9, we can apply Jensen's inequality to conclude that

$$ABA_k[p(x,y)] = \mathbf{E}[f(J)] \le f(\mathbf{E}[J]) = f(\iota),$$

which completes the proof. \square

Appendix

3.3 Computation

Noting that Q_{β} in theorem 3.1 defines an exponential family on [0, 1], we obtain the following result:

$$C_k(\iota) = \sup_{\beta: \mathcal{I}^{(k)}(\beta) = \iota} ABA^{(k)}(\beta)$$

where

$$I^{(k)}(\beta) = \beta \dot{\Lambda}^{(k)}(\beta) - \Lambda^{(k)}(\beta)$$

and

$$ABA^{(k)}(\beta) = \dot{(}\Lambda)^{(k)}(\beta)$$

for

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

Therefore, computing $C_k(\iota)$ depends in turn on computing $\Lambda^{(k)}(\beta)$ and its first derivative.

The following result provides a rapidly converging power series for $\Lambda^{(k)}(\beta)$ and also a limiting result which facilitates large-k approximation.

Theorem 3.10

$$\Lambda^{(k)}(\beta) = \log \sum_{j=0}^{\infty} \frac{\beta^j}{j!(j + \frac{1}{k-1})} - \log(k-1)$$

and therefore,

$$\lim_{k \to \infty} (k-1)(\exp(\Lambda^{(k)}) - 1) = W(\beta),$$

where

$$W(\beta) = \sum_{j=1}^{\infty} \frac{\beta^j}{j!j}.$$

Proof. Write

$$(k-1)(e^{\Lambda^{(k)}(\beta)} - 1) = (k-1)(\int_0^1 \exp(\beta t^{k-1})dt - 1)$$

$$= (k-1)\left(\int_0^1 \sum_{j=0}^\infty \frac{\beta^j t^{j(k-1)}}{j!}dt - 1\right)$$

$$= (k-1)\left(\sum_{j=0}^\infty \int_0^1 \frac{\beta^j t^{j(k-1)}}{j!}dt - 1\right)$$

$$= (k-1)\left(\sum_{j=0}^\infty \frac{\beta^j}{j!(j(k-1)+1)}dt - 1\right)$$

$$= \left(\sum_{j=0}^\infty \frac{\beta^j}{j!(j+\frac{1}{k-1})}dt - (k-1)\right)$$

$$= \sum_{j=1}^\infty \frac{\beta^j}{j!(j+\frac{1}{k-1})}dt.$$

Taking the limit as $k \to \infty$ yields the stated formula for $W(\beta)$. \square