What does classification tell us about the brain? Statistical inference through machine learning

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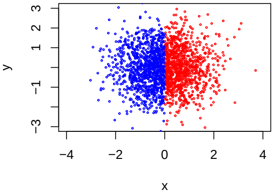
(Joint work with Yuval Benjamini.)

Dependence, distance, and information



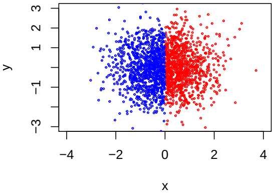
- X is independent of Y:

$$X \perp Y$$

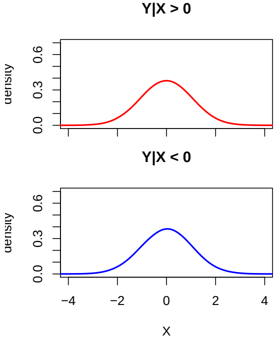
- X and Y have no mutual information:

$$I(X;Y) = 0$$

Dependence, distance, and information



Classifying Sign(X) from Y



- X is independent of Y:

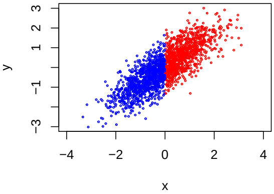
$$X \perp Y$$

- X and Y have no mutual information:

$$I(X;Y) = 0$$

$KL(Y|X > 0, Y|X < 0) = 0.$
Bayes accuracy $= 0.5$.

Dependence, distance, and information



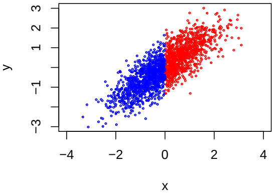
- X is dependent of Y:

$$\text{Cor}(X, Y) = 0.8.$$

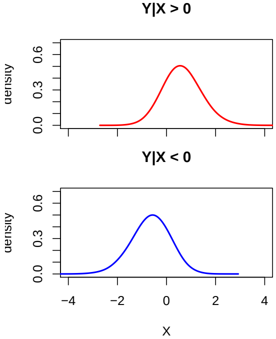
- X and Y have mutual information:

$$I(X; Y) = 0.51.$$

Dependence, distance, and information



Classifying Sign(X) from Y



- X is dependent of Y:

$$\mathrm{Cor}(X, Y) = 0.5.$$

- X and Y have mutual information:

$$I(X; Y) = 0.51.$$

$$KL(Y|X > 0, Y|X < 0) = 1.64$$

Bayes accuracy $= 0.795$.

Bayes accuracy

- Discrete $Y \in \{1, ..., k\}$, continuous or discrete X.
- A classifier is a function f mapping x to a label in $\{1, .., k\}$
- Generalization accuracy of the classifier:

$$\text{GA}(f) = \Pr[Y = f(x)]$$

- Bayes accuracy:

$$\text{BA} = \sup_f \Pr[Y = f(x)] = \Pr[Y = \text{argmax}_{i=1} p(X|Y = i)]$$

- Since random guessing is correct with probability $1/k$,

$$\text{BA} \in [1/k, 1]$$

(if Y is uniformly distributed)

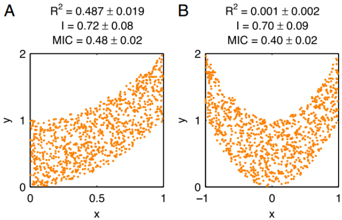
Mutual information

- Invented by Claude Shannon; central to *information theory*.
- Given (X, Y) with joint density $p(x, y)$,

$$I(X;Y) = \int p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dxdy$$

where $p(x)$ and $p(y)$ are marginal densities.

Mutual information



- $I(X;Y) \in [0,\infty]$. (0 if $X \perp Y$, ∞ if $X = Y$ and X continuous.)
- Symmetry: $I(X;Y) = I(Y;X)$.
- Data-processing inequality

$$I(X;Y) \geq I(\phi(X);\psi(Y))$$

  equality for ϕ, ψ bijections
- Additivity. If $(X_1, Y_1) \perp (X_2, Y_2)$, then

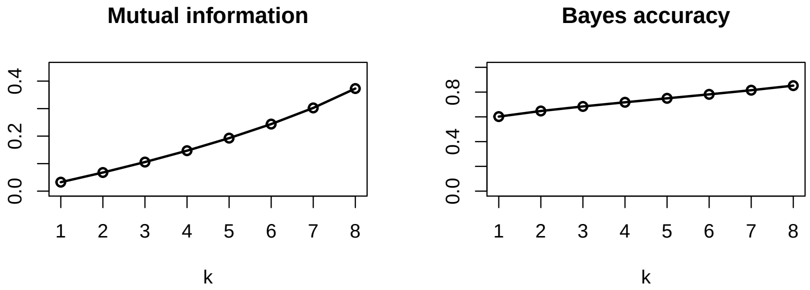
$$I((X_1, X_2);(Y_1, Y2)) = I(X_1; Y_1) + I(X_2; Y_2).$$

Image credit Kinney et al. 2014.

Informativity of predictor sets

Consider predicting binary Y with:

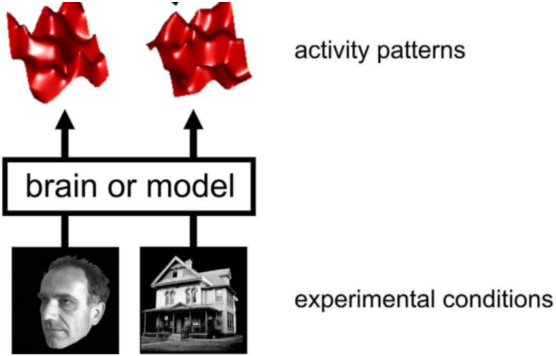
- X_1 only
- X_1 and X_2
- $X_1, \ldots, X_k$



Mutual information vs Bayes accuracy

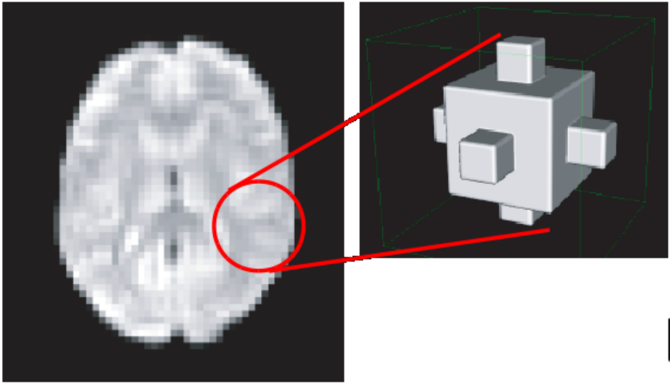
- Both are measures of "informativity".
- Due to its properties, mutual information is easier to interpret.
- Both are intractable to estimate in high dimensions.
- However, Bayes accuracy has a tractable *lower bound*: the generalization error of *any* classifier.

Studying the neural code



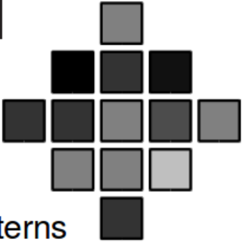
Present the subject with visual stimuli, pictures of faces and houses.
Record the subject's brain activity in the fMRI scanner.

Searchlight analysis



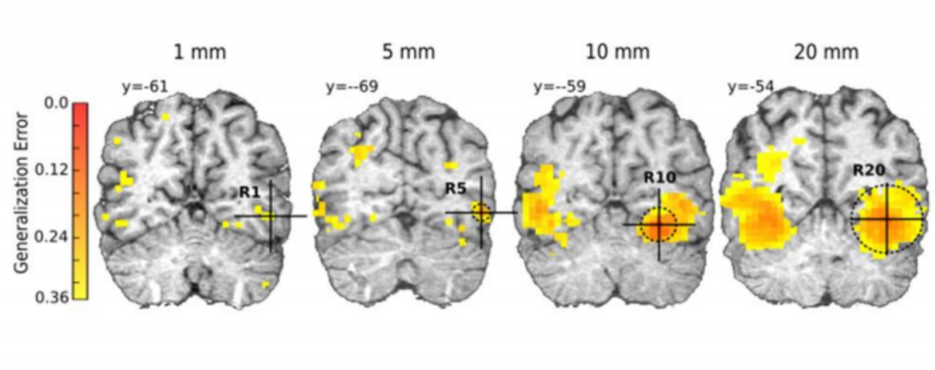
Pull out a local neighbourhood

BOLD image



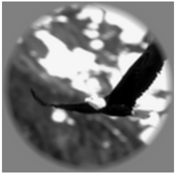
Look at the patterns in that neighbourhood

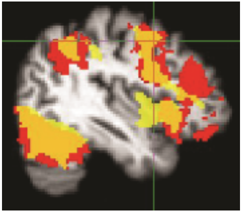
Searchlight analysis



Produces a map of "informative" regions of the brain (as measured by generalization accuracy).

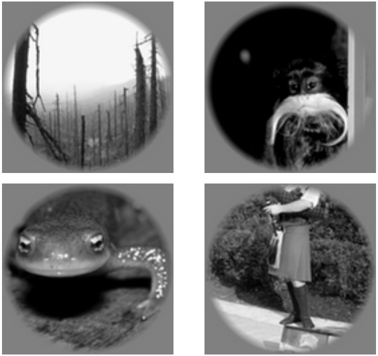
Fixed classification task

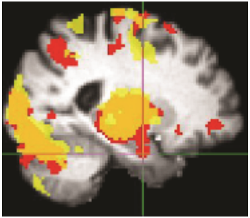




- Experimenter chooses k stimuli.
- Generalization accuracy depends on size of training set, classifier, and choice of stimuli.

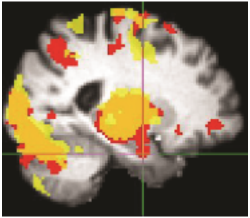
Fixed classification task





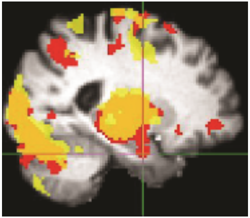
- Different stimuli sets not only lead to different generalization accuracy maps, but also different *Bayes accuracy*.
- Results are incomparable, even in the large-sample limit.

Generalizing beyond the design



Scientists are not innately interested in the Bayes accuracy of a *particular* stimuli set, which is often chosen arbitrarily...

Generalizing beyond the design



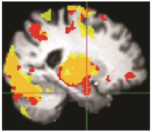
But it would be more interesting to be able to make inferences from the data about a *larger* class of stimuli...

Randomized classification

1. Population of stimuli $p(x)$

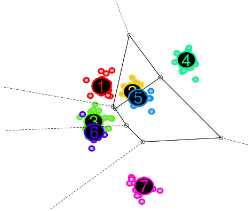
2. Subsample k stimuli

3. Data

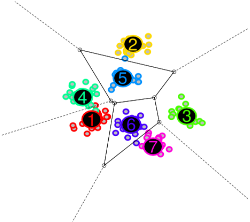


Randomized classification: gaussian example

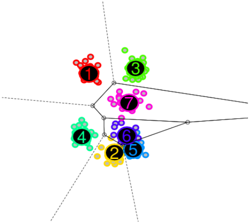
Experiment 1



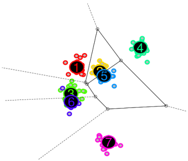
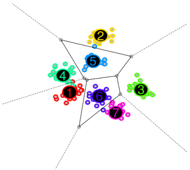
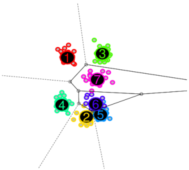
Experiment 2



Experiment 3



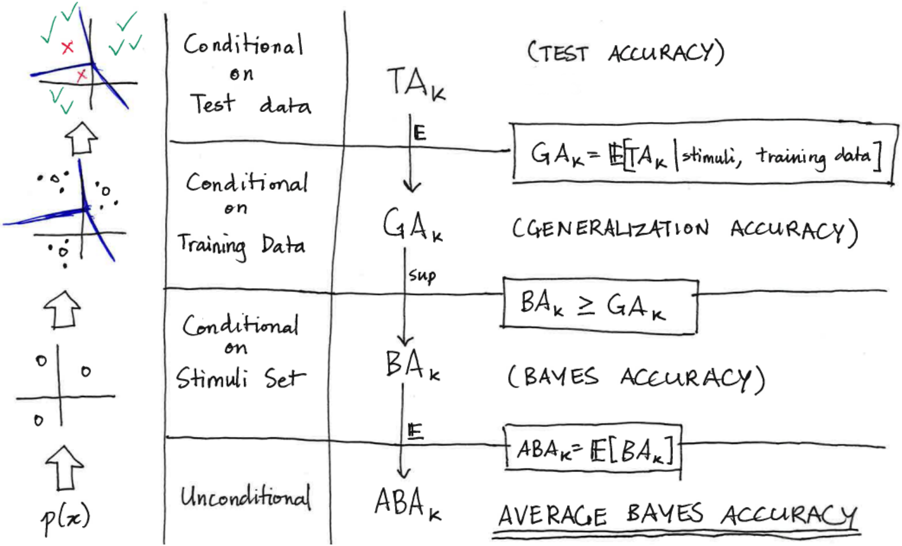
Randomized classification: gaussian example

	Experiment 1	Experiment 2	Experiment 3
			
Bayes accuracy	0.55	0.65	0.52

- Bayes accuracy depends on the stimuli drawn.
- Therefore, define k-class *average Bayes error* as the expected Bayes error for $X_1, .., X_k \overset{iid}{\sim} p(x)$.

$$\text{ABA}_k = \mathbf{E}[BA(X_1, ..., X_k)]$$

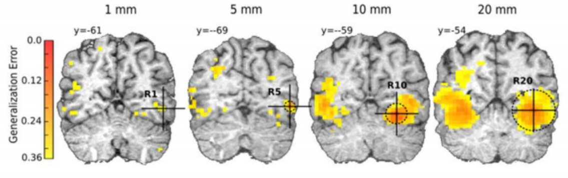
Average Bayes accuracy



Outline of the talk

Suppose we have data from *randomized classification*

1. Can we infer k-class average Bayes error?
2. Can we infer mutual information?



Section 2

Inference of average Bayes accuracy

Inferring average Bayes accuracy

- We cannot observe either ABA_k, or even BA_k.
- However, we can obtain a *lower confidence bound* for BA_k, since the generalization accuracy is an *underestimate* of BA_k
- But we actually want a lower confidence bound for ABA_k!

Concentration of Bayes accuracy

Recall that

$$\mathrm{ABA}_k = \mathbf{E}[\mathrm{BA}_k]$$

Converting a lower confidence bound (LCB) for BA_k to an LCB on ABA_k boils down to the following problem:

What is the variability of BA_k?

An identity

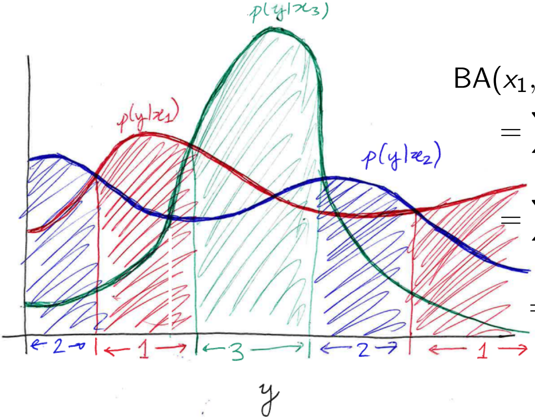
- It is a well-known result from Bayesian inference that the optimal classifier f is defined as

$$f(y) = \text{argmax}_{i=1}^{k} p(y|x_i),$$

  since the prior class probabilities are uniform.
- Therefore,

$$\begin{aligned} \text{BA}(x_1, ..., x_k) &= \Pr[\text{argmax}_{i=1}^{k} p(y|x_i) = Z | x_1, ..., x_k] \\ &= \frac{1}{k} \int \max_{i=1}^{k} p(y|x_i) dy. \end{aligned}$$

Intuition behind identity



$$\mathrm{BA}(x_1, x_2, x_3)$$
$$= \sum_i \Pr[x_i] \Pr_{Y \sim p(y|x_i)}[Y \in \text{zone } i]$$
$$= \sum_i \frac{1}{k} \text{Area under curve } i \text{ in zone } i$$
$$= \frac{1}{k} \text{Area under } \max_{i=1}^{k} p(y|x_i)$$

Efron-Stein lemma

- We have
$$\mathrm{ABA}_k = \mathbf{E}[\mathrm{BA}(X_1, ..., X_k)]$$
where the expectation is over the independent sampling of $X_1, ..., X_k$ from $p(x)$.
- According to the Efron-Stein lemma,
$$\mathrm{Var}[\mathrm{BA}(X_1, ..., X_k)] \leq \sum_{i=1}^{k} \mathbf{E}[\mathrm{Var}[\mathrm{BA}|X_1, ..., X_{i-1}, X_{i+1}, ..., X_k]].$$
which is the same as
$$\mathrm{Var}[\mathrm{BA}(X_1, ..., X_k)] \leq k\mathbf{E}[\mathrm{Var}[\mathrm{BA}|X_1, ..., X_{k-1}]].$$
- The term $\mathrm{Var}[\mathrm{BA}|X_1, ..., X_{k-1}]$ is the variance of $\mathrm{BA}(X_1, ..., X_k)$ conditional on fixing the first $k-1$ curves $p(y|x_1), ..., p(y|x_{k-1})$ and allowing the final curve $p(y|X_k)$ to vary randomly.

Efron-Stein lemma

- $$\mathrm{Var}[\mathrm{BA}(X_1, ..., X_k)] \leq k\mathbf{E}[\mathrm{Var}[BA|X_1, ..., X_{k-1}]].$$
- Note the following trivial results
$$-p(y|x_k) + \max_{i=1}^{k} p(y|x_i) \leq \max_{i=1}^{k-1} p(y|x_i) \leq \max_{i=1}^{k} p(y|x_i)$$
- This implies
$$\mathrm{BA}(X_1, ..., X_k) - \frac{1}{k} \leq \frac{k-1}{k}\mathrm{BA}(X_1, ..., X_{k-1}) \leq \mathrm{BA}(X_1, ..., X_k).$$
i.e. conditional on $(X_1, ..., X_{k-1})$, BA_k is supported on an interval of size $1/k$.
- Therefore,
$$\mathrm{Var}[\mathrm{BA}|X_1, ..., X_{k-1}] \leq \frac{1}{4k^2}$$
since $\frac{1}{4c^2}$ is the maximal variance for any r.v. with support of length c.

Variance bound

Therefore, Efron-Stein bound gives

$$\mathrm{sd}[\mathrm{BA}_k] \leq \frac{1}{2\sqrt{k}}$$

Compare this with empirical results (searching for worst-case distributions):

k	2	3	4	5	6	7	8
$\frac{1}{2\sqrt{k}}$	0.353	0.289	0.250	0.223	0.204	0.189	0.177
Worst-case sd	0.25	0.194	0.167	0.150	0.136	0.126	0.118

Improving the variance bound?

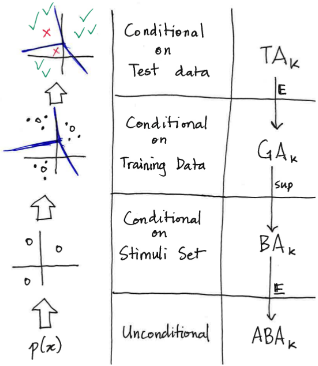
- All of the worst-case distributions found so far have the following simple form:
$$\mathcal{Y} = \mathcal{X} = \{1, ..., d\} \text{ for some } d$$
$$p(y|x) = \frac{1}{d} I\{x = y\}$$
Can we prove this rigorously?
- Recalling that
$$\text{BA}(X_1, ..., X_k) - \frac{1}{k} \leq \frac{k-1}{k}\text{BA}(X_1, ..., X_{k-1}) \leq \text{BA}(X_1, ..., X_k).$$
it is worth noting that distributions of this type actually concentrate on the two endpoints of the bound, thus in some sense "maximizing" the variance.

Section 3

Inferring mutual information

Outline

- Step 1: Apply machine learning to obtain *test accuracy* TA_k
- Step 2: Infer ABA_k from TA_k
- Step 3: Obtain a lower bound on $I(X;Y)$ from ABA_k!



We already know how to do steps 1 and 2; now we discuss step 3.

Related work

- Classically, *Fano's inequality* obtains a lower bound for mutual information from *Bayes accuracy*. (We do the same, but for *average Bayes error*).
- Treves (1997) proposes using the *confusion matrix* obtained from classification to estimate mutual information. This has been a popular approach; see Quiroga (2009).
- Gastpar et al (2010) develop *nonparametric* estimators of mutual information for the randomized classification setup (but does not involve using supervised learning.)

Comparison of ABA and I

Average Bayes accuracy $\text{ABA}_k[p(x,y)]$ and mutual information $\text{I}[p(x,y)]$ are both *functionals* of $p(x,y)$.

$$\text{ABA}_k[p(x,y)] = \frac{1}{k}\int p_X(x_1)\dots p_X(x_k) \max_{i=1}^{k} p(y|x_i) dx_1 \dots dx_k dy.$$

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

Natural questions

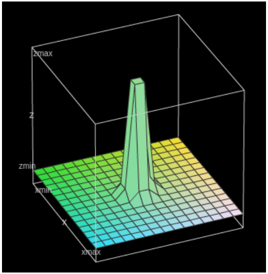
- Does ABA_k close to 1 imply I large?
- Does ABA_k close to $1/k$ imply I close to 0?
- Does I large imply ABA_k close to 1?
- Does I close to 0 imply ABA_k close to $1/k$?

Does I close to 0 imply ABA_k close to $1/k$?

Answer is yes, since $\text{I}[p(x, y)] = 0$ implies that X is independent of Y. And when $X \perp Y$, the best classifier does not better than random guessing.

Does I large imply ABA_k close to 1?

Answer is **no**... per the following counterexample.



$$X \in [0,1], \;\; Y \in [0,1]$$

$$p(x,y) \propto (1-\alpha) + \alpha \left(\frac{e^{-\frac{x^2+y^2}{2\sigma^2}}}{2\pi\sigma^2} \right)$$

$$\mathrm{I}[p(x,y)] \approx \alpha(\frac{1}{2}\log\frac{1}{\sigma^2} - 1 - \log(2\pi))$$

Taking $\alpha \to 0$ and $\sigma^2 \leq e^{-\frac{1}{\alpha^2}}$, we get

$$\mathrm{I}[p(x,y)] \to \infty, \;\; \text{ABA}_k[p(x,y)] \to \frac{1}{k}.$$

This also answers "*Does ABA_k close to $1/k$ imply I close to 0?*" (Also no.)

Natural questions

- Does ABA_k close to $1/k$ imply I close to 0? **No**. (counterexample)
- Does I large imply ABA_k close to 1? **No**. (counterexample)
- Does I close to 0 imply ABA_k close to $1/k$? **Yes**.

The only remaining question is:

Does ABA_k close to 1 imply I large?

The answer is yes and provides the desired lower bound. In fact,

$$\text{ABA}_k \to 1$$

implies

$$\text{I}[p(x,y)] \to \infty.$$

Problem formulation

Take $\iota > 0$, and fix $k \in \{2, 3, ...\}$. Let $p(x, y)$ be a joint density (where (X, Y) could be random vectors of any dimensionality.) Supposing

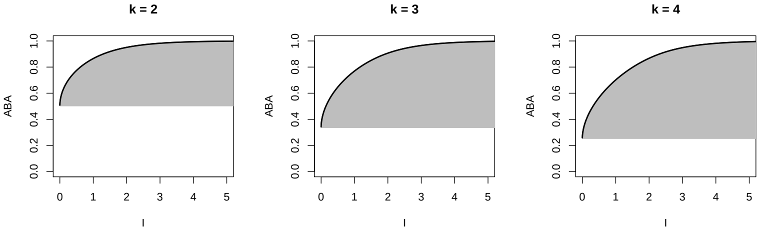
$$\mathrm{I}[p(x, y)] \leq \iota,$$

then can we find an upper bound on $\mathrm{ABA}_k[p(x, y)]$?
In other words, can we compute the value of

$$C_k(\iota) = \sup_{p(x,y):\mathrm{I}[p(x,y)]<\iota} \mathrm{ABA}_k[p(x, y)]?$$

Preview

Yes we can, and this is what the resulting function $C_k(\iota)$ looks like:



As information increases, the maximal average Bayes accuracy goes to 1. We find these curves using *variational calculus*.

Reduced Problem

Consider a special class of densities with the following properties:

- $p(x, y)$ is on the unit square
- The marginal distributions of x and y are both uniform
- The conditional distributions $p(x|y)$ are just "shifted" copies of a common density, $q(x)$, on $[0, 1]$

$$p(x|y) = q(x - y + I\{x < y\})$$

- Furthermore, $q(x)$ is increasing in x.

We claim (but will not show) that this special class of densities achieves the maximal average Bayes error. Therefore, it suffices to search over this special class of densities to compute $C_k(\iota)$.

Simplified formulae

The information and average Bayes error can be written in terms of $q(x)$.

$$\mathrm{I}[p(x,y)] = \int_0^1 q(x) \log q(x) dx$$

$$\mathrm{ABA}_k[p(x,y)] = \int_{[0,1]^k} \max_{i=1}^{k} q(x_i) dx_1 \cdots dx_k$$

Simplified formulae

Overload the notation and "redefine" information and average Bayes error as functionals of $q(x)$.

$$\mathrm{I}[q(x)] \overset{def}{=} \int_0^1 q(x) \log q(x) dx$$

$$\mathrm{ABA}_k[q(x)] \overset{def}{=} \frac{1}{k} \int_{[0,1]^k} \max_{i=1}^{k} q(x_i) dx_1 \cdots dx_k$$

Simplified formulae

We can simplify the expression for ABA_k even more.
Observe that since $q(x)$ is increasing,

$$\max_{i=1}^{k} q(x_i) = q\left(\max_{i=1}^{k} x_i\right)$$

Therefore,

$$\begin{aligned}\text{ABA}_k[q(x)] &= k^{-1}\int_{[0,1]^k} \max_{i=1}^{k} q(x_i)dx_1\cdots dx_k \\ &= k^{-1}\int_{[0,1]^k} q\left(\max_{i=1}^{k} x_i\right) dx_1\cdots dx_k \\ &= k^{-1}\mathbf{E}\left[q\left(\max_{i=1}^{k} X_i\right)\right] = k^{-1}\mathbf{E}[q(M)]\end{aligned}$$

where $X_1,\ldots,X_k \overset{iid}{\sim} \text{Unif}[0,1]$ and $M = \max_{i=1}^{k} X_i$.

Simplified formulae

Recall that the max of k iid uniforms has density

$$f(m) = km^{k-1}.$$

Therefore,

$$\text{ABA}_k[q(x)] = k^{-1}\mathbf{E}[q(M)] = \int_0^1 q(t)t^{k-1}dt.$$

Optimization problem

We now pose the question: how do we find $q(x)$ which maximizes $\text{ABA}_k[q(x)]$ subject to $\text{I}[q(x)] \leq \iota$?

- *Domain of the optimization*: Recall that $q(x)$ satisfies $q(x) \geq 0$, $\int_0^1 q(x)dx = 1$, and is increasing in x. Let $\mathcal{Q}$ denote the space of functions on $[0,1] \to [0,\infty)$ which are increasing in x.
- *Constraints*: We have two remaining constraints, $\text{I}[q(x)] \leq \iota$ and $\int_0^1 q(x)dx = 1$.

Hence the problem is

$$\text{maximize}_{q(x)\in\mathcal{Q}}\ \text{ABA}_k[q(x)] \text{ subject to } \int_0^1 q(x)dx = 1 \text{ and } \text{I}[q(x)] \leq \iota.$$

Optimization problem

$$\text{maximize}_{q(x)\in\mathcal{Q}} \ \text{ABA}_k[q(x)] \text{ subject to } \int_0^1 q(x)dx = 1 \text{ and } \mathrm{I}[q(x)] \leq \iota.$$

- Does a solution exist? *Yes*, because the space of measures with density $q(x)$ satisfying $\mathrm{I}[q(x)] \leq \iota$ is tight, and both the constraints and objective are continuous wrt to the topology of weak convergence.
- Given a solution $q^*(x)$ exists, there exist Lagrange multipliers $\lambda \in \mathbb{R}$ and $\nu > 0$ such that q^* minimizes

$$\begin{aligned}\mathcal{L}[q(x)] &= -\text{ABA}_k[q(x)] + \lambda \int_0^1 q(x)dx + \nu \mathrm{I}[q(x)] \\ &= \int_0^1 (-t^{k-1} + \lambda + \nu \log q(x))q(x)dx.\end{aligned}$$

Functional derivatives

- Functional derivatives are essential to variational calculus.
- Let $\mathcal{F}$ be a *Hilbert space* of functions with domain $\mathcal{X}$ and range $\mathbb{R}$.
- Suppose F is a functional which maps functions f to the real line. Then the functional derivative $\nabla F[f]$ at f is a function in the space $\mathcal{F}$ such that

$$\lim_{\epsilon \to 0} \frac{F(f + \epsilon\xi) - F(f)}{\epsilon} = \int_{\mathcal{X}} \nabla F[f](x)\xi(x)dx.$$

for all $\xi \in \mathcal{F}$.

Functional derivatives

- Taylor explansions are a useful trick for computing functional derivatives
- We can compute the functional derivative of $\mathcal{L}[q(x)]$ by writing

$$\begin{aligned}
&\mathcal{L}[q(x) + \epsilon\xi(x)] \\
&\quad = \int_0^1 (-t^{k-1} + \lambda + \nu \log(q(x) + \epsilon\xi(x)))(q(x) + \epsilon\xi(x))dx. \\
&\quad \approx \int (q(x)+\epsilon\xi(x))(-t^{k-1} + \lambda + \nu\{\log q(x) + \frac{\epsilon\xi(x)}{q(x)}\})dx \\
&\quad \approx \mathcal{L}[q(x)] + \int_0^1 (-t^{k-1} + \lambda + \nu(1 + \log q(x))\epsilon\xi(x)dx.
\end{aligned}$$

- Hence

$$\nabla\mathcal{L}[q](x) = -t^{k-1} + \lambda + \nu(1 + \log q(x))$$

Variational magic!

Suppose we set the functional derivative to 0,

$$0 = \nabla \mathcal{L}[q](t) = -t^{k-1} + \lambda + \nu + \nu \log q(t).$$

Then we conclude that the optimal $q^*(t)$ takes the form

$$q^*(t) = \alpha e^{\beta t^{k-1}}$$

for some $\alpha > 0$, $\beta > 0$.
From the constraint $\int q(t)dt = 1$, we get

$$q_\beta(t) = \frac{e^{\beta t^{k-1}}}{\int e^{\beta t^{k-1}} dt}.$$

Technical sidenote

For the optimal $q(t)$, how do we know $\nabla \mathcal{L}[q](t) = 0$?

- Since $\mathcal{Q}$ has a monotonicity constraint, we cannot simply take for granted that
$$\nabla \mathcal{L}[q^*](t) = 0$$
- However, we can show that assuming
$$\nabla \mathcal{L}[q^*](t) \neq 0$$
on a set of positive measure results in a contradiction.
- The contradiction is achieved by constructing a suitable perturbation ξ which is "localized" around a region where $\mathcal{L}[q^*](t) \neq 0$, such that $q^* + \epsilon\xi \in \mathcal{Q}$ and also so that $\int \xi(t) \nabla \mathcal{L}[q^*](t) dt < 0$. This implies that for ϵ sufficiently small, $\mathcal{L}[q^* + \epsilon\xi] < \mathcal{L}[q^*]$–a contradiction, since we assumed that q^* was optimal.

Result

Theorem. For any $\iota > 0$, there exists $\beta_\iota \geq 0$ such that defining

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

we have

$$\int_0^1 q_{\beta_\iota}(t) \log q_{\beta_\iota}(t) dt = \iota.$$

Then,

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