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

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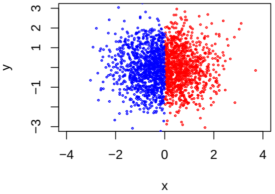
(Joint work with Yuval Benjamini.)

Dependence, distance, and information

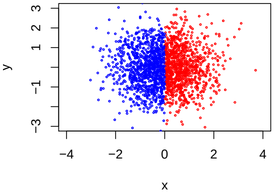


- X is independent of Y:

$$X \perp Y$$

- X and Y have no mutual information:

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



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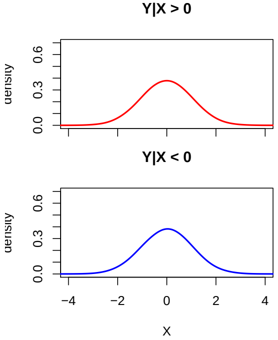
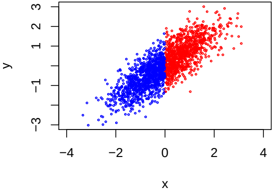
Classifying Sign(X) from Y



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

Bayes accuracy $= 0.5$.

Dependence, distance, and information

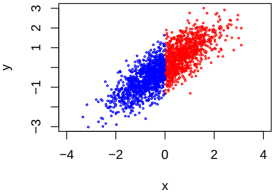


- X is dependent of Y:

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

- X and Y have mutual information:

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



- X is dependent of Y:

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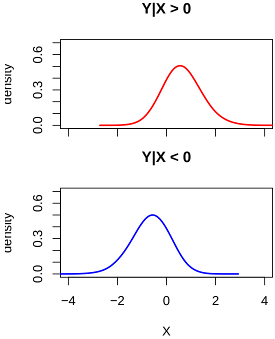
Classifying Sign(X) from Y



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

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 $1/k$,

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

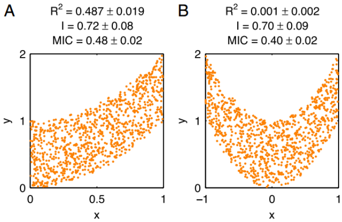
(if Y is uniformly distributed)

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.



- $I(X;Y) \in [0, \infty]$. (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

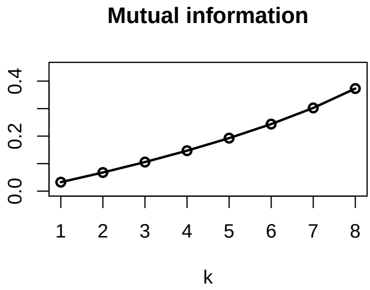
$$I((X_1, X_2); (Y_1, Y2)) = I(X_1; Y_1) + I(X_2; Y_2).$$

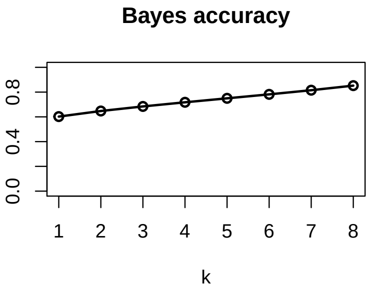
Image credit Kinney et al. 2014.

Informativity of predictor sets

Consider predicting binary Y with:

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

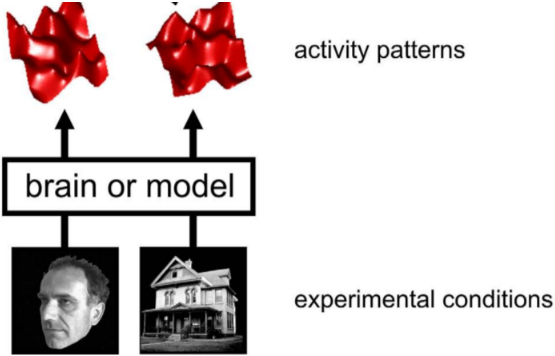




Mutual information vs Bayes accuracy

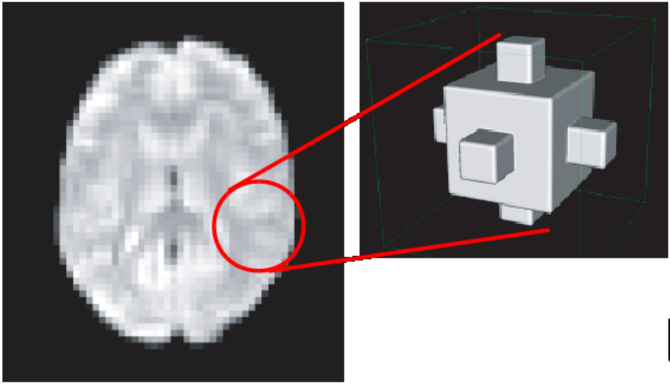
- Both are measures of “informativity”.
- Due to its properties, mutual information is easier to interpret.
- Both are intractable to estimate in high dimensions.
- However, Bayes accuracy has a tractable *lower bound*: the generalization error of *any* classifier.

Studying the neural code



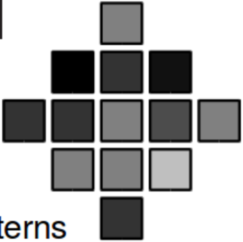
Present the subject with visual stimuli, pictures of faces and houses.
Record the subject's brain activity in the fMRI scanner.

Searchlight analysis



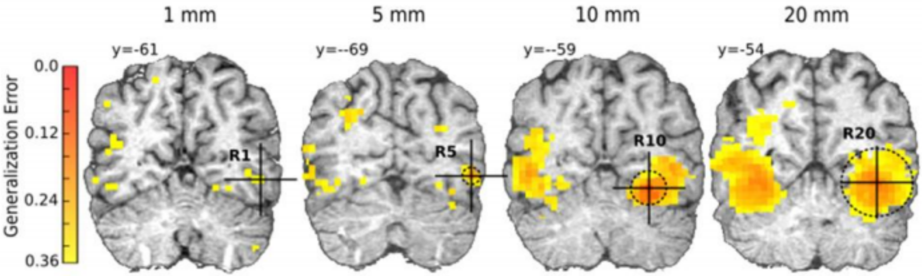
BOLD image

Pull out a local neighbourhood



Look at the patterns in that neighbourhood

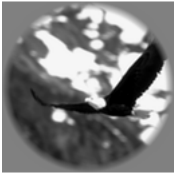
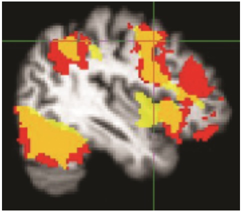
Searchlight analysis



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

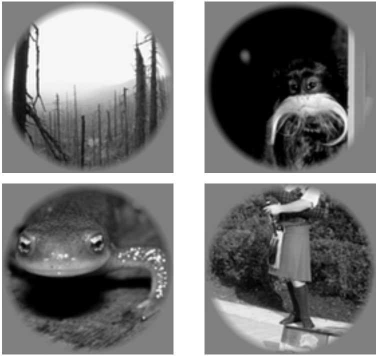
Fixed classification task

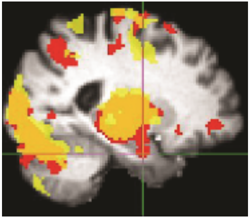


- Experimenter chooses k stimuli.
- Generalization accuracy depends on size of training set, classifier, and choice of stimuli.

Fixed classification task



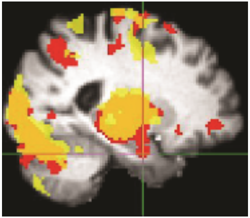


- Different stimuli sets not only lead to different generalization accuracy maps, but also different *Bayes accuracy*.
- Results are incomparable, even in the large-sample limit.

Generalizing beyond the design

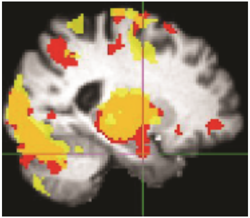






Scientists are not innately interested in the Bayes accuracy of a *particular* stimuli set, which is often chosen arbitrarily...

Generalizing beyond the design



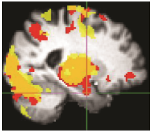
But it would be more interesting to be able to make inferences from the data about a *larger* class of stimuli...

Randomized classification

1. Population of stimuli $p(x)$

2. Subsample k stimuli

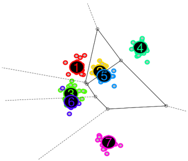
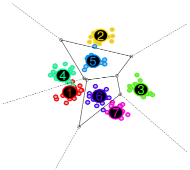
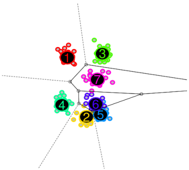
3. Data



4. Train a classifier

5. Estimate generalization accuracy (which is lower bound for the *random* Bayes accuracy BA_k)

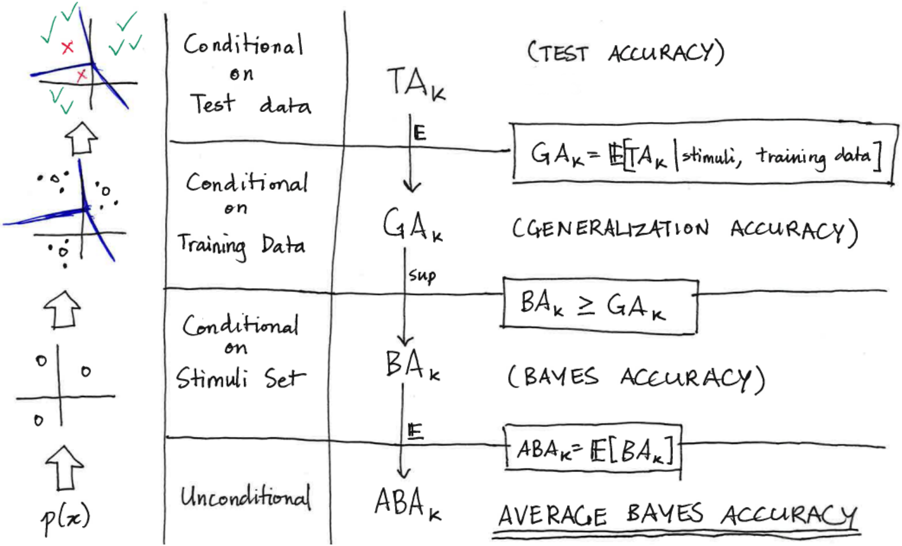
Average Bayes error

	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



Two measures of informativity: ABA and mutual information

Both are:

- measures of informativity between X and Y
- invariant to bijective transformations of either X or Y
- defined with reference to a *population* of stimuli and either a single subject or population of subjects

Comparison of ABA and mutual information

ABA_k advantages:

- intuitive to understand "classification performance".
- easy to average over a *population* of subjects.
- closer to what you can measure: (generalization accuracy).

ABA_k disadvantages:

- Not symmetric with respect to X and Y. Have to choose one as predictor and one as response.
- Dependent on k, the number of classes.
- Problem of *saturation*. If k is too large, ABA_k gets close to chance accuracy. If k is too large, ABA_k gets close to 1.

Comparison of ABA and mutual information

Mutual information advantages:

- already has a tradition of usage in neuroscience.
- symmetric between X and Y: X is equally informative of Y as Y is of X.
- doesn't depend on k, the number of stimuli.
- additional theoretical properties like independent additivity.

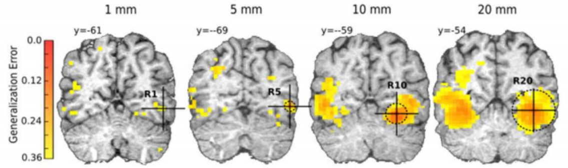
Mutual information disadvantages:

- not robust: $I(X;Y)$ becomes unbounded if $p(x,y)$ contains singularities.
- does it make sense to take the average mutual information across subjects?

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

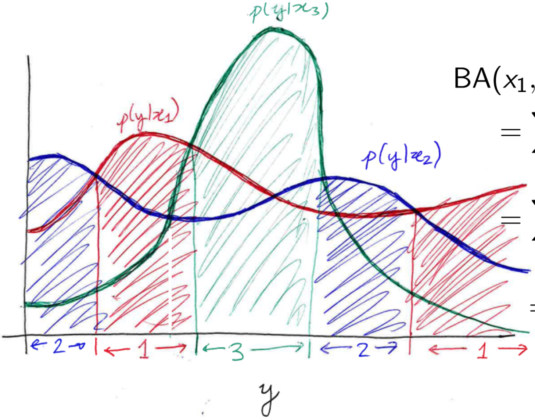
$$f(y) = \text{argmax}_{i=1}^k p(y|x_i),$$

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



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

Variance bound

From the Efron-Stein lemma, we get

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

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

Intuition for variance bound

Write

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

so that

$$\text{BA}(x_1, ..., x_k) = \Pr[f(y, X_1, ..., X_k) = Z|X_1 = x_1, ..., X_k = x_k].$$

Intuition for variance bound

We expect the variance to be order $1/k$, because the Bayes accuracy is an average of individual class accuracies

$$\text{BA}_k(X_1, ..., X_k) = \frac{1}{k}\sum_{i=1}^k \Pr[f(X_1, X_2, ..., X_k, y) = Z|Z = i]$$

The ith term,

$$\Pr[f(X_1, X_2, ..., X_k, y) = Z|Z = i]$$

is "almost" independent of the jth term when k is large. Hence, since BA_k is an average of k "almost-indpendent" terms, it should have variance $\approx \frac{1}{k}$.

Improving the variance bound?

- All of the worst-case distributions take the form

$$\mathcal{Y} = \mathcal{X} = \{1, ..., d\} \text{ for some } d$$

$$p(y|x) = \frac{1}{d} I\{x = y\}$$

- Sampling k items from d with replacement; BA_k is the number of unique items divided by k.
- According to Birthday paradox,

$$\text{ABA}_k \approx (1 - e^{-d/k})$$

  and

$$\text{Var}(\text{BA}_k) \approx \frac{1}{d} e^{-d/k} (1 - e^{-d/k})$$

- "Discreteness" of the distribution seems to maximize variance?
- If we could prove that this is indeed the worst case, then we have a better constant for variance bound.

Recap: inferring average Bayes error

1. *Experimental design*: draw k stimuli $X_1, ..., X_k$ iid from $p(x)$. Then collect data (X_i, Y_i^j).
2. *Supervised learning*: train a classifier and obtain a test accuracy TA_k.
3. *Generalization accuracy*: if n_{test} is the size of the test set,

$$\underline{\text{GA}_k} = \text{TA}_k - \frac{z_{\alpha/2}\sqrt{\text{TA}_k(1 - \text{TA}_k)}}{\sqrt{n_{test}}}$$

   is a lower confidence bound for GA_k
4. *Bayes accuracy*:

$$\underline{\text{BA}_k} = \underline{\text{GA}_k}$$

   is a lower confidence bound for BA_k
5. *Average Bayes accuracy*

$$\underline{\text{ABA}_k} = \underline{\text{BA}_k} - \frac{1}{2\sqrt{\alpha k}}$$

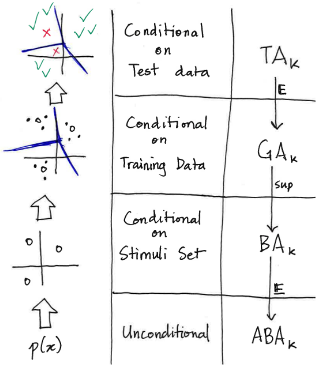
   is a lower confidence bound for ABA_k.

Section 3

Inferring mutual information

Outline

- Step 1: Apply machine learning to obtain *test accuracy* TA_k.
- Step 2: Obtain lower confidence bound $\underline{\mathrm{ABA}}_k$.
- Step 3: Obtain a lower confidence bound on $I(X; Y)$ from $\underline{\mathrm{ABA}}_k$.



We just discussed 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

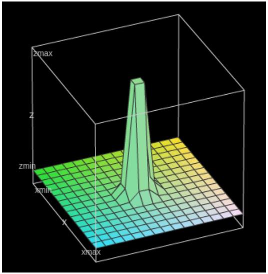
- Does ABA_k close to 1 imply I large?
- Does ABA_k close to $1/k$ imply I close to 0?
- Does I large imply ABA_k close to 1?
- Does I close to 0 imply ABA_k close to $1/k$?

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

Answer is yes, since $\mathrm{I}[p(x, y)] = 0$ 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.



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

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

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

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

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

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

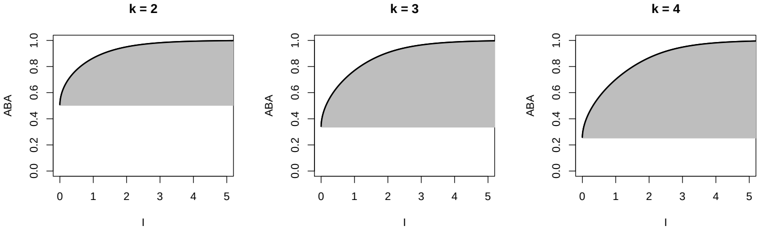
$$\mathrm{I}[p(x, y)] \leq \iota,$$

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

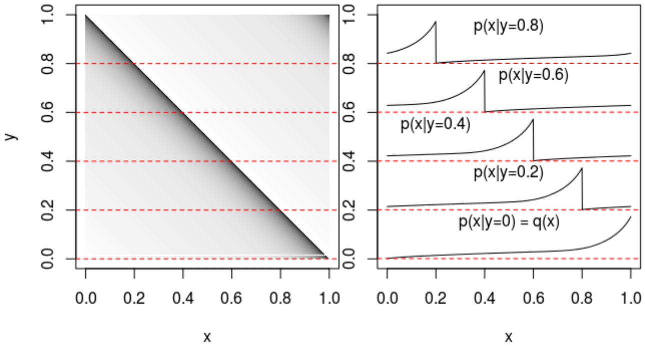
Yes we can, and this is what the resulting function $C_k(\iota)$ looks like:



As information increases, the maximal average Bayes accuracy goes to 1.

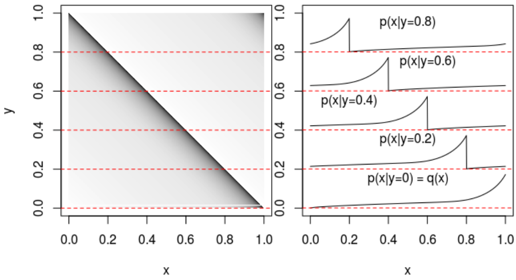
Reduced Problem

Rather than show the whole proof, we consider a simplified problem to illustrate the methods.



Actually, the simplified problem is equivalent to the full problem and we get the same answer (but this is non-trivial).

Reduced Problem



- $p(x, y)$ on unit square with uniform marginals.
- 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.

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

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

- Does a solution exist? *Yes*, because the space of measures with density $q(x)$ satisfying $\text{I}[q(x)] \leq \iota$ 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

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

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

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

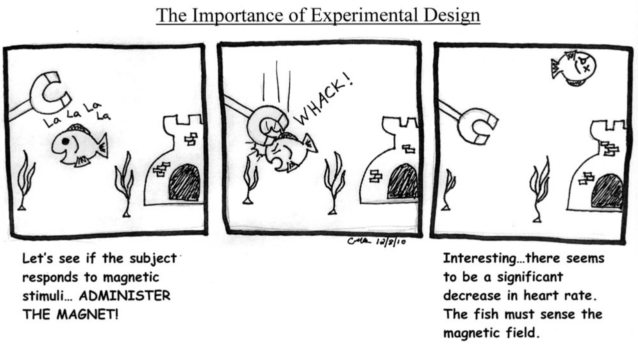
we have

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

Then,

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

The end



(credit C. Ambrosino)