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

Charles Zheng

Stanford University

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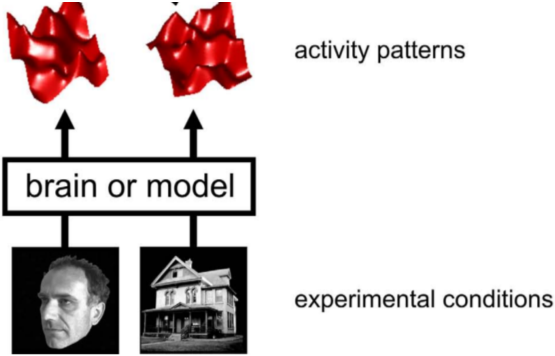
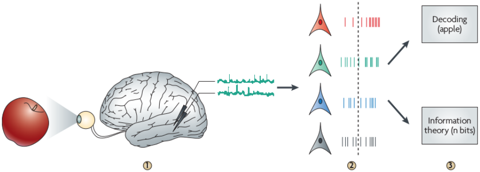
(Joint work with Yuval Benjamini.)

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.

Studying the neural code: data

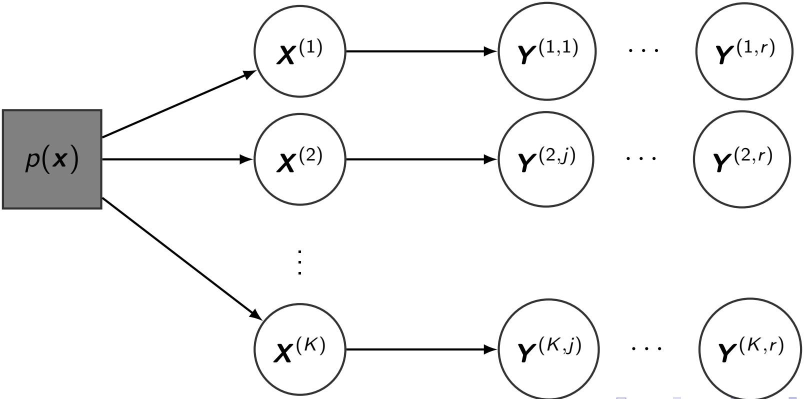


- Let $\mathcal{X}$ define a class of stimuli (faces, objects, sounds.)
- Stimulus $\boldsymbol{X} = (X_1, \ldots, X_p)$, where X_i are features (e.g. pixels.)
- Present $\boldsymbol{X}$ to the subject, record the subject's brain activity using EEG, MEG, fMRI, or calcium imaging.
- Recorded response $\boldsymbol{Y} = (Y_1, \ldots, Y_q)$, where Y_i are single-cell responses, or recorded activities in different brain region.

Image credits: Quiroga et al. (2009).

Experimental design

- How to make inferences about the population of stimuli in $\mathcal{X}$ using finitely many examples?
- *Randomization.* Select $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(K)}$ randomly from some distribution $p(\boldsymbol{x})$ (e.g. an image database). Record r responses from each stimulus.



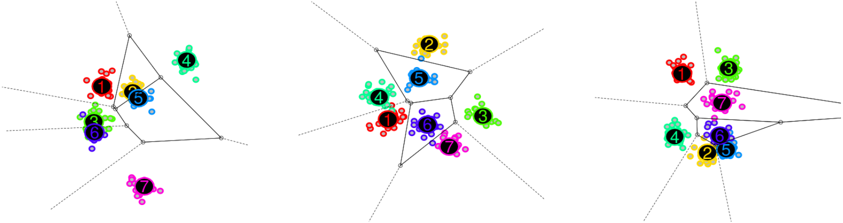
Analyzing the data using machine learning

- Now we have data consisting of (stimulus, reponse) pairs.
- Can we classify the response using the stimulus? What is the confusion matrix?

Gaussian example

To help think about these problems, consider a concrete example:

- Let $\boldsymbol{X} \sim N(0, I_d)$ and $\boldsymbol{Y}|\boldsymbol{X} \sim N(\boldsymbol{X}, \sigma^2 I_d)$.
- We draw stimuli $\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(K)} \sim N(0, I_d)$ i.i.d.
- For each stimulus $\boldsymbol{x}^{(i)}$, we draw observations $\boldsymbol{y}^{(i,j)} = \boldsymbol{x}^{(i)} + \epsilon^{(i,j)}$, where $\epsilon^{(i,j)} \sim N(0, \sigma^2 I_d)$.



Motivation for my research

Ultimately, the goal of these experiments is to understand the dependence between X (stimulus) and Y (the brain response).
Possible goals for statistical methodology (which currently don't exist):

1. What can be inferred from the classification accuracy?
2. Can we predict what the result (classification accuracy) would be in a similar (but possibly larger or smaller) experiment?
3. Can we *summarize* the total information content contained in Y about X?
4. Can we *decompose* the total information contained in Y about X? (Something like a nonlinear ANOVA decomposition?)

Motivation 1: What can be inferred from the classification accuracy?

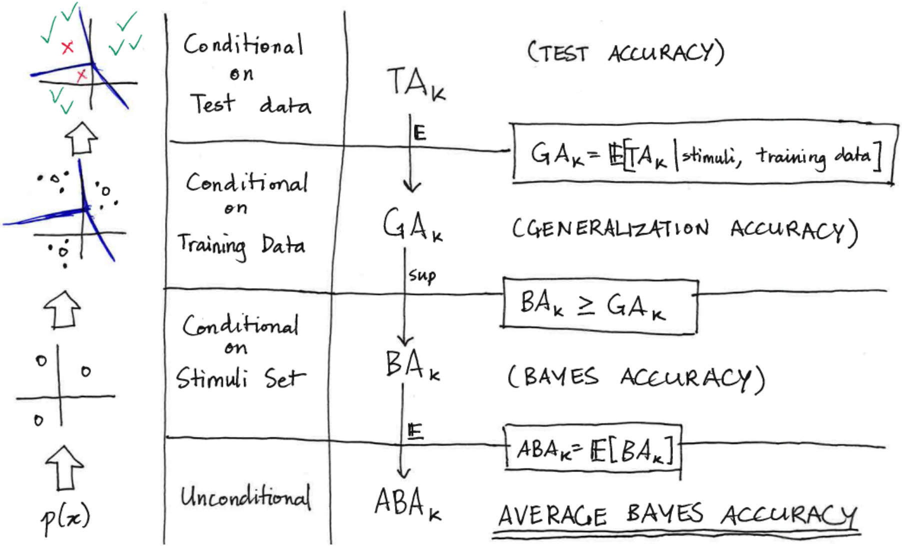
- The achieved classification accuracy is an estimate of *generalization accuracy*...
- which in turn lower bounds on the generalization error of the best classifier, the *Bayes accuracy*.
- But the Bayes accuracy varies depending on the stimuli set $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(K)}$!

$$\text{BA}(X_1, ..., X_k)$$

Define *average Bayes accuracy* as the expected Bayes accuracy

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

where expectation is taken over sampling $X_1, .., X_k$ from $p(x)$.



Conditional on Test data
TA_K
(TEST ACCURACY)
E
$GA_K = \mathbb{E}[TA_K \mid \text{stimuli, training data}]$
Conditional on Training Data
GA_K
(GENERALIZATION ACCURACY)
sup
$BA_K \geq GA_K$
Conditional on Stimuli Set
BA_K
(BAYES ACCURACY)
$\mathbb{E}$
$ABA_K = \mathbb{E}[BA_K]$
Unconditional
ABA_K
AVERAGE BAYES ACCURACY
$p(x)$

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

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

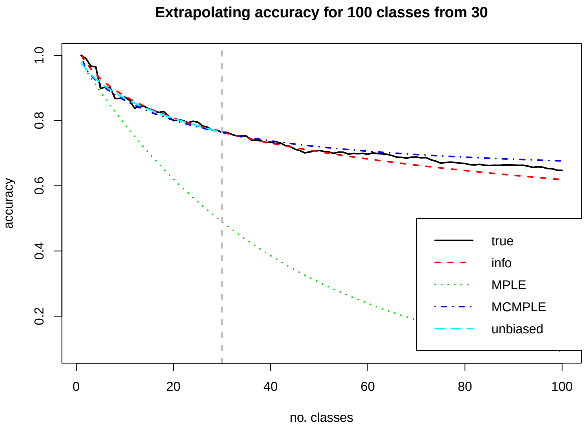
Converting a LCB for BA_k to an LCB on ABA_k boils down to the following problem:

What is the variability of BA_k?

We will discuss this later in the talk!

Motivation 2: Generalizing to similar designs

Define ABA_k as the average Bayes accuracy for k classes.
Can we predict ABA_{100} given data from 30 classes? See Z., Achanta and Benjamini (2016).



Motivation 3 and 4: Quantifying and decomposing information

Can we summarize the total information content contained in Y about X?
Can we decompose the total information contained in Y about X?

The answer is yes, and the solution was provided by Claude Shannon. *Mutual information* measures the information contained in Y about X (or vice versa) in a nonlinear way.

Mutual information

Section 2

Variability of Bayes accuracy

Definitions

- Suppose (X, Y) have a joint density $p(x, y)$,
- The Bayes accuracy is a function of the stimuli set $x_1, ..., x_k$,

$$\text{BA}(x_1, ..., x_k)$$

- Draw $Z \sim \{1, ..., k\}$, and draw $Y \sim p(y|x_z)$.
- Let f (the *classifier*) that associates a label $\{1, ..., k\}$ to each possible value of y:

$$f : \mathcal{Y} \to \{1, ..., k\}$$

- Define

$$\text{BA}(x_1, ..., x_k) = \sup_f \Pr[f(Y) = Z | x_1, ..., x_k]$$

where the probability is over the joint distribution (Y, Z) defined above. Notice we condition on the particular stimuli set $x_1, ..., x_k$.

An identity

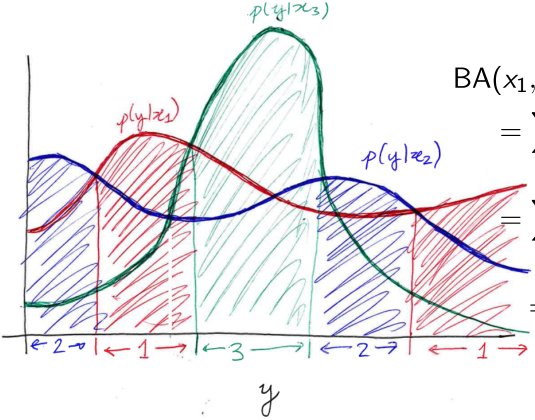
- It is a well-known result from Bayesian inference that the optimal classifier f is defined as

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

  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



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

Efron-Stein lemma

- We have

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

  where the expectation is over the independent sampling of $X_1, ..., X_k$ from $p(x)$.

- According to the Efron-Stein lemma,

$$\text{Var}[\text{BA}(X_1, ..., X_k)] \leq \sum_{i=1}^{k} \mathbf{E}[\text{Var}[\text{BA}|X_1, ..., X_{i-1}, X_{i+1}, ..., X_k]].$$

  which is the same as

$$\text{Var}[\text{BA}(X_1, ..., X_k)] \leq k\mathbf{E}[\text{Var}[\text{BA}|X_1, ..., X_{k-1}]].$$

- The term $\text{Var}[\text{BA}|X_1, ..., X_{k-1}]$ is the variance of $\text{BA}(X_1, ..., X_k)$ 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

- $$\text{Var}[\text{BA}(X_1, ..., X_k)] \leq k\mathbf{E}[\text{Var}[BA|X_1, ..., X_{k-1}]].$$
- 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
$$\text{BA}(X_1, ..., X_k) - \frac{1}{k} \leq \frac{k-1}{k}\text{BA}(X_1, ..., X_{k-1}) \leq \text{BA}(X_1, ..., X_k).$$
i.e. conditional on $(X_1, ..., X_{k-1})$, BA_k is supported on an interval of size $1/k$.
- Therefore,
$$\text{Var}[\text{BA}|X_1, ..., X_{k-1}] \leq \frac{1}{4k^2}$$
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

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

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
$$\mathrm{BA}(X_1, ..., X_k) - \frac{1}{k} \leq \frac{k-1}{k}\mathrm{BA}(X_1, ..., X_{k-1}) \leq \mathrm{BA}(X_1, ..., X_k).$$
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

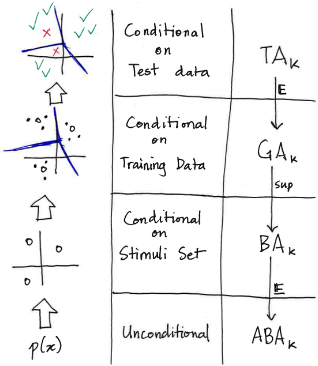
Inferring mutual information from classification accuracy

Outline

- We observe (X, Y) pairs from the random-stimulus repeated-sampling design.
- Goal is to infer $I(X; Y)$, also written $\mathrm{I}[p(x, y)]$.

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.

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

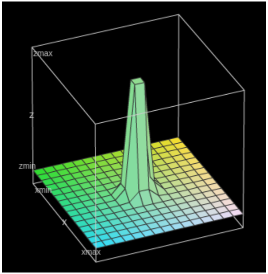
- Does ABA_k close to 1 imply I large?
- Does ABA_k close to $1/k$ imply I close to 0?
- Does I large imply ABA_k close to 1?
- Does I close to 0 imply ABA_k close to $1/k$?

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

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

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 bound

$$\mathrm{ABA}_k[p(x, y)]?$$

In other words, does there exist a constant

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

Step 1: Reduction

Let $\mathcal{P}^{unif}$ be the class of densities $p(x, y)$ on the unit square, with uniform marginals

$$p(x) = 1, \quad p(y) = 1.$$

We can show that if $C_k(\iota)$ exists, then we need only to search through distributions in $\mathcal{P}^{unif}$ to compute it:

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

We omit the proof.

Step 1: Reduction

Reduction simplifies the formulas. For $p(x, y) \in \mathcal{P}^{unif}$,

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

and

$$\mathrm{ABA}_k[p(x, y)] = \frac{1}{k} \int \max_{i=1}^{k} p(x_i, y) dx_1 \cdots dx_k dy.$$

Step 2: Conditioning

Due to uniform marginals $p(x, y) = p(x|y) = p(y|x)$. Therefore,

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

and

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

Step 2: Conditioning

Write both functionals as an nested integral, with the outer integration over y

$$\mathrm{I}[p(x,y)] = \int \left[\int p(x|y) \log p(x|y) dx \right] dy,$$

and

$$\mathrm{ABA}_k[p(x,y)] = \int \left[\frac{1}{k} \int \max_{i=1}^{k} p(x_i|y) dx_1 \cdots dx_k \right] dy.$$

Notice that in both cases, the inner integral is a functional of $p(x|y)$.

Step 2: Conditioning

Name the functionals, as *conditional information*

$$\mathrm{I}[p(x,y)] = \int \underbrace{\left[\int p(x|y) \log p(x|y) dx\right]}_{\mathrm{CI}[p(x|y)]} dy,$$

and *conditional accuracy*

$$\mathrm{ABA}_k[p(x,y)] = \int \underbrace{\left[\int \frac{1}{k} \max_{i=1}^{k} p(x_i|y) dx_1 \cdots dx_k\right]}_{\mathrm{CA}_k[p(x|y)]} dy.$$

Step 2: conditioning

Conditional information and conditional accuracies are functionals of one-dimensional densities.

$$\text{CI}[q(x)] = \int q(x) \log q(x) dx,$$

$$\text{CA}_k[q(x)] = \frac{1}{k} \int \max_{i=1}^{k} q(x_i) dx_1 \cdots dx_k.$$

And, we have

$$\text{I}[p(x,y)] = \int \text{CI}[p(x|y)] dy = \mathbf{E}[\text{CI}[p(x|Y)]],$$

and

$$\text{ABA}_k[p(x,y)] = \int \text{CA}_k[p(x|y)] dy = \mathbf{E}[\text{CA}_k[p(x|Y)]].$$

for $Y \sim \text{Unif}[0,1]$.

Step 3: convexity

- Given $p(x, y) \in \mathcal{P}^{unif}$, define a map $\phi : [0, 1] \to \mathbb{R}^2$ by

$$\phi(y) = (\text{CI}[p(x|y)], \text{CA}_k[p(x|y)]).$$

  We are mapping observations y to their associated conditional information and accuracy.

- Consider the image of ϕ:

$$\text{Im}(\phi) = \{(\text{CI}[p(x|y)], \text{CA}_k[p(x|y)]) : y \in [0, 1]\}$$

- We have $(\text{I}[p(x, y)], \text{ABA}_k[p(x, y)]) = \mathbf{E}[\phi(y)]$.
- Therefore,

$$(\text{I}[p(x, y)], \text{ABA}_k[p(x, y)]) \in \mathcal{C}(\text{Im}(\phi)),$$

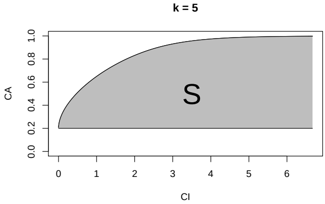
  the convex hull of the image of ϕ.

Step 3: convexity

- Let $\mathcal{P}^1$ denote the set of all densities $q(x)$ on $[0, 1]$. Define the set S as
$$S : \{(\mathrm{CI}[q(x)], \mathrm{CA}_k[q(x)]) : q \in \mathcal{P}^1\}$$
- Since all conditional densities $p(x|y) \in \mathcal{P}^1$, we have
$$\mathrm{Im}(\phi) \subset S,$$
and therefore
$$\mathcal{C}(\mathrm{Im}(\phi)) \subset \mathcal{C}(S).$$
- Therefore,
$$(\mathrm{I}[p(x, y)], \mathrm{ABA}_k[p(x, y)]) \in \mathcal{C}(S).$$

Skipping ahead

It turns out that for any $k \in \{2, 3, ...\}$, that the set S is already convex, so $\mathcal{C}(S) = S$.



The *upper envelope* of S can be viewed as a function of ι (the conditional information). In fact, this is exactly the lower bound we are seeking.

$$C_k(\iota) = \max\{\beta : (\iota, \beta) \in S\} = \sup_{q(x) \in \mathcal{P}^1 : \mathrm{CI}[q(x)] = \iota} \mathrm{CA}_k[q(x)].$$

Step 4: Compute the upper envelope

We can prove that

$$C_k(\iota) = \sup_{q(x) \in \mathcal{P}^1 : \mathrm{CI}[q(x)] = \iota} \mathrm{CA}_k[q(x)].$$

Therefore, it remains to solve the optimization problem

$$\text{maximize}_{q(x) \in \mathcal{P}^1}\ \mathrm{CA}_k[q(x)] \text{ subject to } \mathrm{CI}[q(x)] = \iota.$$

This is accomplished using *calculus of variations*.

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 $\text{CI}[q(x)]$ by writing

$$\begin{aligned}
\text{CI}[q(x) + \epsilon\xi(x)] &= \int (q(x) + \epsilon\xi(x)) \log(q(x) + \epsilon\xi(x)) dx \\
&\approx \int (q(x) + \epsilon\xi(x))(\log q(x) + \frac{\epsilon\xi(x)}{q(x)}) dx \\
&\approx \text{CI}[q(x)] + \int q(x)\frac{\epsilon\xi(x)}{q(x)} + \epsilon\xi(x) \log q(x) dx
\end{aligned}$$

- Hence

$$\nabla \text{CI}[q](x) = 1 + \log q(x).$$

Functional derivatives

- Unfortunately, the functional derivative of CA_k is not easy to work with...

$$\text{CA}_k[q(x) + \epsilon\xi(x)] = \int \max_{i=1}^{k}(q(x_i) + \epsilon\xi(x_i))dx_1 \cdots dx_k = ??$$

- This will pose an obstacle to applying variational methods, so we use a *reparameterization trick*

Reparameterization trick

- For any $q(x) \in \mathcal{P}^1$, define a corresponding function $Q : [0, 1] \to [0, \infty)$ as follows:
- If $q(x)$ is already monotonic, then $Q(x) = q(x)$.
- Otherwise, $Q(t)$ "sorts" $q(x)$,

$$Q(t) = sup\{u : \int I\{q(x) \leq u\}dx \leq t\}.$$

Reparameterization trick

- We call $Q(t)$ the *quantile function* corresponding to $q(x)$ since $Q(t)$ is a monotonically increasing function from $[0, 1]$ to $[0, \infty)$.
- We have $\int_0^1 Q(t)dt = 1$, since $\int_0^1 q(t)dt = 1$.
- We can rewrite the functionals CI and CA_k in terms of Q

$$\text{CI}[Q(t)] = \int_0^1 Q(t) \log Q(t) dt.$$

This is basically the same formula as $\text{CA}[q(x)]$.

- What is more surprising,

$$\text{CA}_k[Q(t)] = \int_0^1 Q(t) t^{k-1} dt.$$

This allows us to obtain a simple expression for the functional derivative $\nabla \text{CA}_k[Q]$!

How does it work?

- We will show that

$$\mathrm{CA}_k[q(x)] = \frac{1}{k}\int \max_{i=1}^{k} q(x_i)dx_1\cdots dx_k = \int_0^1 Q(t)t^{k-1}dt = \mathrm{CA}_k[Q(t)].$$

- Given $q(x) \in \mathcal{P}^1$, define an *order function* $\sigma(t)$ such that σ is a piecewise differentiable bijection from $[0,1]$ to $[0,1]$, and so that

$$\int I\{\sigma(t) < u\}dt = u$$

  for all $u \in [0,1]$, and with the property that

$$q(\sigma(t)) < q(\sigma(t')).$$

  if and only if

$$t < t'.$$

- One can check that $Q(t) = q(\sigma(t))$ for any function σ satisfying these properties.

How does it work?

- Due to change-of-variables formula, defining

$$T = \sigma^{-1}(X),$$

  we have $T \sim \text{Unif}[0, 1]$.
- If $x_i = \sigma(t_i)$ for $i = 1, \ldots, k$, then

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

How does it work?

- Combining the two results,

$$\mathrm{CA}_k[q(x)] = \frac{1}{k}\int \max_{i=1}^{k} q(x_i) dx_1 \cdots dx_k$$
$$= \frac{1}{k}\int \max_{i=1}^{k} q(\sigma(\max_{i=1}^{k} t_i)) dt_1 \cdots dt_k.$$

- Note that the above integral can be written as

$$\mathrm{CA}_k[q(x)] = \frac{1}{k}\mathbf{E}[q(\sigma(\max_{i=1}^{k} T_i))]$$

for T_i independently $\mathrm{Unif}[0,1]$.

How does it work?

- Hence, letting $M = \max_{i=1}^{k} T_i$, the density of M is

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

and we get

$$\begin{aligned} \mathrm{CA}_k[q(x)] &= \frac{1}{k}\mathbf{E}[q(\sigma(M))] \\ &= \frac{1}{k}\mathbf{E}[\max_{i=1}^{k} Q(M)] \\ &= \int_0^1 Q(m)m^{k-1}dm = \mathrm{CA}_k[Q] \end{aligned}$$

as needed.

Step 4: Compute the upper envelope

Let $\mathcal{Q}$ denote the space of quantile functions

$$\mathcal{Q} = \{Q(t) : [0,1] \to [0,\infty) \text{ and } Q(t) \text{ increasing } \}.$$

We now have the reparameterized problem

$$\text{maximize}_{Q(t)\in\mathcal{Q}} \ \mathrm{CA}_k[Q(t)] \text{ subject to } \mathrm{CI}[Q(t)] = \iota \text{ and } \mathrm{E}[Q(t)] = 1$$

where note that additional constraint

$$\mathrm{E}[Q(t)] \stackrel{def}{=} \int_0^1 Q(t)dt = 1.$$

Step 4: Compute the upper envelope

Switch to Langrangian form

$$\text{minimize}_{Q(t)\in\mathcal{Q}}\ \mathcal{L}[Q(t)]$$

where

$$\mathcal{L}[Q(t)] = -\text{CA}_k[Q(t)] + \nu\text{CI}[Q(t)] + \lambda\text{E}[Q(t)]$$

for some $\nu > 0$, $\lambda \in \mathbb{R}$.
Then we can compute the functional derivative,

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

Step 5: 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 $Q(t)$ takes the form

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

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

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

As we vary $\beta \in [0, \infty)$, the points $(\mathrm{CI}[Q_\beta(t)], \mathrm{CA}[Q_\beta(t)])$ trace out the upper envelope!

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,

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

Technical sidenote

But wait a second... can we simply assume that

1. There even exists a $Q(t) \in \mathcal{Q}$ that attains the supremum?
2. That given such a $Q(t)$ exists, that the functional derivative is equal to zero?

Indeed, some technical arguments are needed for both points.

Technical sidenote

Does there exists a $Q(t) \in \mathcal{Q}$ that attains the constrained supremum?

- First define $\mathcal{Q}'$ as the space of distributions with $\mathrm{E}[Q(t)] \leq 1$.
- If we view it as a family of probability measures, the family is tight.
- Therefore it is closed with respect to weak convergence
- Noting that CA_k and CI are continuous with respect to weak convergence, this establishes that there does exist $Q^*(t)$ which attains the constrained supremum

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.