

# How many neurons does it take to classify a lightbulb?

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(Joint work with Yuval Benjamini.)

## *Introduction*

- Review of information theory.
- Study of neural coding.

## *Related work*

- Estimating mutual information between stimulus and response.
- Can we use machine learning methods to estimate MI?

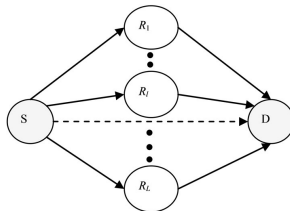
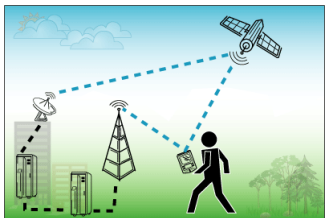
## *Theory*

- Gaussian example.
- Low-SNR universality.

## *Results*

# Information theory

The high performance and reliability of modern communications system is made possible by information theory, founded by Shannon in 1948.



A information-processing network can be analyzed in terms of interactions between its components (which are viewed as random variables.)

Image credit CartouCHe, Aziz et al. 2011.

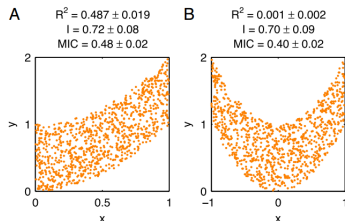
# Entropy and mutual information

$X$  and  $Y$  have joint density  $p(x, y)$  with respect to  $\mu$ .

Quantity	Definition	Linear analogue
Entropy	$H(X) = - \int (\log p(x)) p(x) \mu_X(dx)$	$\text{Var}(X)$
Conditional entropy	$H(X Y) = \mathbf{E}[H(X Y)]$	$\mathbf{E}[\text{Var}(X Y)]$
Mutual information	$I(X; Y) = H(X) - H(X Y)$	$\text{Cor}^2(X, Y)$

The above definition includes both *differential* entropy and *discrete* entropy.  
Information theorists tend to use log base 2, we will use natural logs in this talk.

# Properties of mutual information



- $I(X; Y) \in [0, \infty]$ . (0 if  $X \perp Y$ ,  $\infty$  if  $X = Y$  and  $X$  continuous.)
- Symmetry:  $I(X; Y) = I(Y; X)$ .
- Bijection-invariant:  $I(\phi(X); \psi(Y)) = I(\psi(Y); \phi(X))$ .
- Additivity. If  $(X_1, Y_1) \perp (X_2, Y_2)$ , then

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

- Relation to KL divergence:

$$\mathbb{D}(p(x, y) || p(x)p(y)) = I(X; Y).$$

# Relationship between mutual information and classification

- Suppose  $X$  and  $Y$  are discrete random variables, and  $X$  is uniformly distributed over its support.
- Classify  $X$  given  $Y$ . The optimal rule is to guess

$$\hat{X} = \operatorname{argmax}_x p(Y|X = x).$$

- Bayes error:

$$p_e = \Pr[X \neq \hat{X}].$$

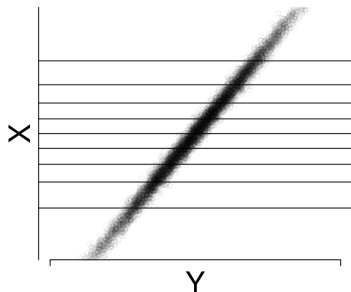
- Fano's inequality:

$$I(X; Y) \geq (1 - p_e) \ln K - \text{const.}$$

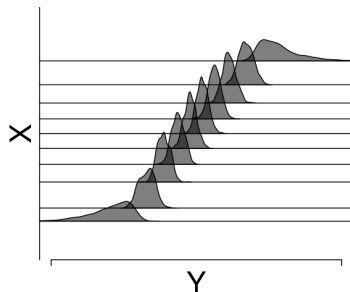
where  $K$  is the size of the support of  $X$ .

# Nice interpretation of $I(X; Y)$ for continuous rvs

- If we bin the continuous  $X$  into  $K \approx e^{I(X; Y)}$  equal-probability bins, we can reliably guess the bin given  $Y$ .
- Heuristic is more accurate if  $I(X; Y)$  is large, due to Shannon's noisy channel theorem.



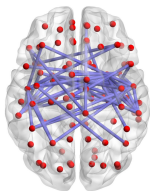
$$I(X; Y) = 2.3038$$



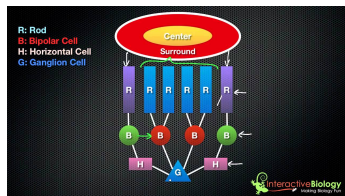
$$\ln 10 = 2.3025$$

# Motivation: the neural code

The brain is the *most complex* information processing system we know!



Neural network inferred from data.  
(Hong et al.)



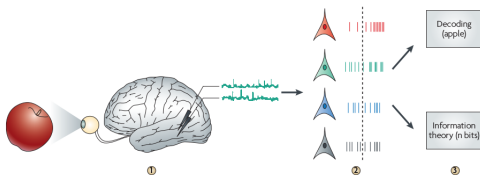
Organization of human retina

How do neurons encode, process, and decode sensory information?

Image credit: Hong et al., Interactive Biology



# Studying the neural code: data



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

Image credits: Quiroga et al. (2009).

# Problem statement

Given stimulus-response data  $(\mathbf{X}, \mathbf{Y})$ , can we estimate the mutual information  $I(\mathbf{X}; \mathbf{Y})$ ?

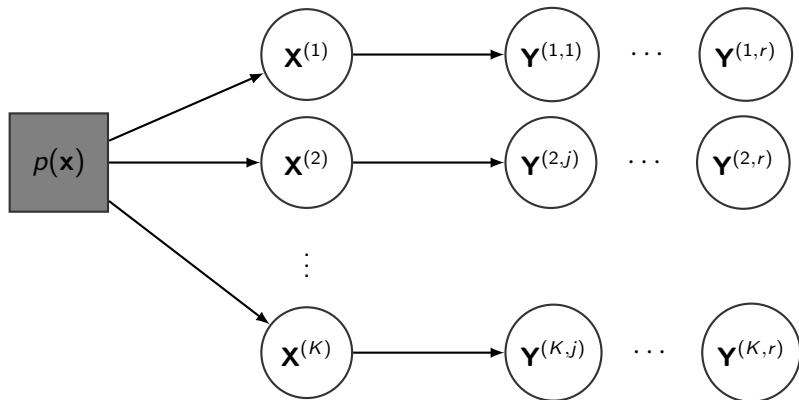
*Why do we care?*

- Selecting the correct model for neural encoding.
- Assessing the *efficiency* of the neural code.
- Measuring the *redundancy* of a population of neurons

$$r' = \frac{\sum_{i=1}^q I(\mathbf{X}; Y_i) - I(\mathbf{X}; \mathbf{Y})}{\sum_{i=1}^q I(\mathbf{X}; Y_i)}.$$

# Experimental design

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



# Can we learn $I(\mathbf{X}; \mathbf{Y})$ from such data?

Answer: yes.

- We have  $I(\mathbf{X}; \mathbf{Y}) = H(\mathbf{Y}) - H(\mathbf{Y}|\mathbf{X})$ .
- We can estimate  $H(\mathbf{Y})$  from the data
- We can estimate  $H(\mathbf{Y}|\mathbf{x}^{(i)})$  from the data, and define

$$\hat{H}(\mathbf{Y}|\mathbf{X}) = \frac{1}{K} \sum_{i=1}^K \hat{H}(\mathbf{Y}|\mathbf{x}^{(i)})$$

- As  $K$  and  $r$  both tend to infinity,

$$\hat{I}(\mathbf{X}; \mathbf{Y}) = \hat{H}(\mathbf{Y}) - \hat{H}(\mathbf{Y}|\mathbf{X})$$

is consistent for  $I(\mathbf{X}; \mathbf{Y})$ .

# Limitations with the 'naive' approach

Naive estimator:

$$\hat{l}(\mathbf{X}; \mathbf{Y}) = \hat{H}(\mathbf{Y}) - \frac{1}{K} \sum_{i=1}^K \hat{H}(\mathbf{Y} | \mathbf{x}^{(i)})$$

- If  $K$  is small, the naive estimator may be quite biased, even for low-dimensional problems. Gastpar et al. (2010) introduced an *antropic correction* to deal with the small- $K$  bias.
- Difficult to estimate differential entropies  $H(\mathbf{Y})$ ,  $H(\mathbf{Y} | \mathbf{x}^{(i)})$  in high dimensions. Best rates are  $O(1/\sqrt{n})$  for  $d \leq 3$  dimensions. Convergence rates for  $d > 3$  unknown!

# Can we use machine learning to deal with dimensionality?

- Supervised learning becomes an extremely common approach for dealing with high-dimensional data, for numerous reasons!
- Perhaps we can use supervised learning to estimate  $I(\mathbf{X}; \mathbf{Y})$  as well.

*Procedure.*

- Fix  $r_{train} < r$ . Let  $r_{test} = r - r_{train}$ .
- Use  $\{(\mathbf{x}^{(i)}, \mathbf{y}^{(i,j)}) : i = 1, \dots, K, j = 1, \dots, r_{train}\}$  as training data to learn a classifier  $\hat{\mathbf{x}}$ .
- Compute the confusion matrix, normalized so that each row adds to  $1/K$ :

$$C(i, j) = \frac{1}{K^2 r_{test}} \sum_{i=1}^K \sum_{j=1}^K \sum_{\ell=r_{train}+1}^r I(\hat{\mathbf{x}}(\mathbf{y}^{(i,\ell)}) = \mathbf{x}^{(j)}).$$

Normalized this way,  $C(i, j)$  gives the empirical joint distribution

$$C(i, j) = \hat{\text{Pr}}[\mathbf{X} = \mathbf{x}^{(i)}, \hat{\mathbf{X}} = \mathbf{x}^{(j)}].$$

# Can we use machine learning to deal with dimensionality?

- Treves et al. (1997) suggest computing the mutual information from the confusion matrix, i.e.

$$\hat{I}(\mathbf{X}; \mathbf{Y}) \approx \sum_{i=1}^K \sum_{j=1}^K C(i, j) \ln \left( \frac{C(i, j)}{\left( \sum_{\ell=1}^K C(i, \ell) \right) \left( \sum_{\ell=1}^K C(j, \ell) \right)} \right)$$

- Quiroga (2009) review the applications of this approach, and note sources of bias or “information loss.”

# Why use supervised learning to estimate $I(\mathbf{X}; \mathbf{Y})$ ?

- Successful supervised learning exploits structure in the data, which *nonparametric methods ignore*.
- Using supervised learning to estimate mutual information can be viewed as *using prior information* to improve the estimate of  $I(\mathbf{X}; \mathbf{Y})$ .
- So while the general problem of information estimation is nearly impossible in high dimensions, the problem might become tractable if we can exploit known structure in the problem!



# Interesting connection to machine learning literature

While we are considering

supervised learning  $\rightarrow$  estimate mutual information,

a vast literature exists on applications of mutual information (as the 'infomax criterion') for feature selection, training objectives, i.e.

estimate mutual information  $\rightarrow$  supervised learning.

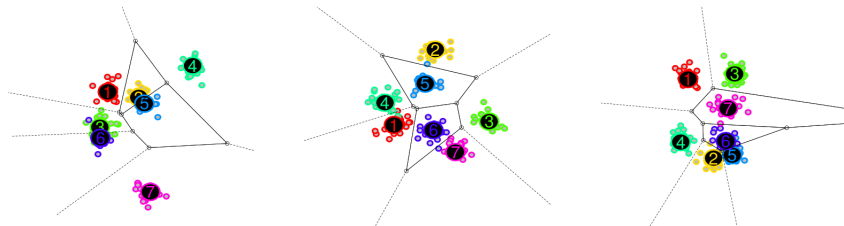
- How much could we potentially gain in estimating  $I(\mathbf{X}; \mathbf{Y})$  by using supervised learning, compared to nonparametric approaches?
- Is the Bayes confusion matrix sufficient for consistently estimating  $I(\mathbf{X}; \mathbf{Y})$ ?
- Is the Bayes error sufficient for consistently estimating  $I(\mathbf{X}; \mathbf{Y})$ ?
- In practice, we cannot obtain the Bayes error due to:
  - Model misspecification.
  - Finite training data to fit the model (even if correctly specified).
  - Finite test data to estimate the generalization error.

How sensitive is our estimator to these issues?

# Gaussian example

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

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



# Gaussian example

The mutual information is given by

$$I(\mathbf{X}; \mathbf{Y}) = \frac{d}{2} \log\left(1 + \frac{1}{\sigma^2}\right).$$

The Bayes rule takes the form

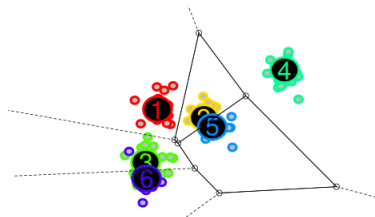
$$\hat{\mathbf{X}}(\mathbf{Y}) = \operatorname{argmax}_{\mathbf{x}^i} \underbrace{-\frac{1}{2\sigma^2} \|\mathbf{Y} - \mathbf{x}\|^2}_{Z_i}.$$

*Notation:* Without loss of generality, assume  $\mathbf{Y}$  belongs to the centroid  $\mathbf{x}^{(K)}$ . Then write  $\mathbf{x}^* = \mathbf{x}^{(K)}$  and  $Z_* = Z_K$ .

The average Bayes error can be written

$$\text{ABE} = \Pr[Z_* < \max_{i=1}^{K-1} Z_i].$$

# Gaussian example: Average Bayes error



- Conditional on the centroid locations  $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(K)}$ , the Bayes misclassification error can be computed by integrating  $p$ -dimensional Gaussian density over Voronoi polytopes.
- This is pretty much intractable in high dimensions!
- The average Bayes error (ABE) is an average of an intractable quantity. Luckily, *taking averages makes the problem tractable*.

# Gaussian example: Average Bayes risk

- To make the problem even easier, we use another time-honored technique: the central limit theorem.
- Letting  $d \rightarrow \infty$ , the scores

$$Z_i = -\frac{1}{2\sigma^2} \|\mathbf{Y} - \mathbf{x}\|^2 = -\frac{1}{2\sigma^2} \sum_{i=1}^d \|Y_i - x_i\|^2$$

have a jointly multivariate distribution in the limit:

$$\begin{bmatrix} Z_* \\ Z_1 \\ \vdots \\ Z_{K-1} \end{bmatrix} \xrightarrow{d} N \left( \begin{bmatrix} -\frac{d}{2} \\ -\frac{d}{2} - \frac{d}{\sigma^2} \\ \vdots \\ -\frac{d}{2} - \frac{d}{\sigma^2} \end{bmatrix}, \begin{bmatrix} \frac{d}{2} & \frac{d}{2} & \cdots & \frac{d}{2} \\ \frac{d}{2} + \frac{2d}{\sigma^2} & \frac{d}{2} + \frac{2d}{\sigma^2} & \cdots & \frac{d}{2} + \frac{2d}{\sigma^2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{d}{2} & \frac{d}{2} + \frac{2d}{\sigma^2} & \cdots & \frac{d}{2} + \frac{2d}{\sigma^2} \end{bmatrix} \right).$$

# Gaussian example: Average Bayes risk

Assume  $(Z_*, Z_1, \dots, Z_{K-1})$  have a normal distribution with the given moments.

We can compute

$$\text{ABE} = \Pr[Z_* < \max_{i=1}^{K-1} Z_i]$$

by writing

$$Z_i = \frac{\text{Cov}(Z_*, Z_i)}{\text{Var}(Z_*)} (Z_* - \mathbf{E}Z_*) + \sqrt{\text{Var}(Z_i) - \frac{\text{Cov}(Z_*, Z_i)^2}{\text{Var}(Z_*)}} W_i,$$

where  $W_i$  are i.i.d. standard normal.

This yields

$$\Pr[Z_* < \max_{i=1}^{K-1} Z_i] = \Pr[N(\mu, \nu^2) < \max_{i=1}^{K-1} W_i]$$

where

$$\mu = \frac{\mathbf{E}[Z_* - Z_i]}{\sqrt{\frac{1}{2}\text{Var}(Z_i - Z_j)}}, \quad \nu^2 = \frac{\text{Cov}(Z_* - Z_i, Z_* - Z_j)}{\frac{1}{2}\text{Var}(Z_i - Z_j)}$$

for  $i \neq j \neq K$ .

# Gaussian example: Average Bayes risk

Finally, we get

$$\text{ABE} = \Pr[Z_* < \max_{i=1}^{K-1} Z_i] \rightarrow f_K\left(\frac{\sqrt{d}}{\sigma}\right)$$

where

$$f_K(\mu) = 1 - \int_{-\infty}^{\infty} \phi(z - \mu)(1 - \Phi(z))^{K-1} dz.$$



# Gaussian example: Average Bayes risk

Recall that

$$I(\mathbf{X}; \mathbf{Y}) = \frac{d}{2} \log\left(1 + \frac{1}{\sigma^2}\right),$$

while

$$\text{ABE} = f_K(\sqrt{d}/\sigma).$$

Hence ABE is not a function of  $I(\mathbf{X}; \mathbf{Y})$ !

# Gaussian example: Low SNR limit

However, what if we consider a limit where the noise level  $\sigma^2$  increases with  $d$ ?

Fix some  $\sigma_1^2 > 0$ , and let  $\sigma_d^2 = d\sigma_1^2$ .

Then when  $d$  is large,

$$I(\mathbf{X}; \mathbf{Y}) = \frac{d}{2} \log\left(1 + \frac{1}{d\sigma_1^2}\right) \approx \frac{d}{2} \frac{1}{d\sigma_1^2} = \frac{1}{2\sigma_1^2}.$$

We get

$$\text{ABE} = f_k(\sqrt{2I(\mathbf{X}; \mathbf{Y})})$$

in the limit!

# Low SNR limit: generalization

In a sequence of gaussian models of increasing dimensionality with

$$\lim_{d \rightarrow \infty} I(\mathbf{X}; \mathbf{Y}) \rightarrow \iota < 0,$$

we get an exact relationship between the limiting mutual information and the average Bayes error,

$$\text{ABE} = f_K(\sqrt{2\iota}).$$

**This limiting relationship holds more generally!**

# Exponential family sequence model

The Gaussian sequence is a special case of the following class of models. Let  $b_X(x)$  and  $b_Y(y)$  be probability densities and  $u(x, y)$  be an arbitrary smooth function. Let

$$b_\theta(x, y) = \frac{b_X(x)b_Y(y) \exp[\theta u(x, y)]}{\int b_X(x)b_Y(y) \exp[\theta u(x, y)] dx dy}.$$

A corresponding *exponential family sequence model* is a sequence of joint probability distributions  $p_d(\mathbf{x}, \mathbf{y})$  given by

$$p_d(\mathbf{x}, \mathbf{y}) = \prod_{i=1}^d b_{\theta_d}(x_i, y_i)$$

such that

$$\lim_{d \rightarrow \infty} d\theta_d = c < \infty.$$

For instance, choosing  $b_X(x) = b_Y(y) = \phi(x)$  and  $u(x, y) = xy$  yields the Gaussian sequence model (up to marginal scaling.)

**Theorem.** *Given an exponential family sequence model  $p_d(\mathbf{x}, \mathbf{y})$ , for random variates  $(\mathbf{X}^{[d]}, \mathbf{Y}^{[d]}) \sim p_d(\mathbf{X}, \mathbf{Y})$ , we have*

$$\lim_{d \rightarrow \infty} I(\mathbf{X}^{[d]}, \mathbf{Y}^{[d]}) = \iota < \infty$$

*for some constant  $\iota < \infty$ ; and the limiting  $K$ -class average Bayes error is given by*

$$\lim_{d \rightarrow \infty} ABE = f_K(\sqrt{2\iota}).$$

# The low-SNR estimator of $I(\mathbf{X}; \mathbf{Y})$

We are willing to bet that the relationship

$$\text{ABE} \approx f_K(\sqrt{2\iota})$$

holds in much greater generality than we managed to prove—namely, whenever  $I(\mathbf{X}; \mathbf{Y}) \ll p$ , and the scores  $Z_i$  are approximately jointly multivariate normal.

Based on these assumptions, our proposed estimator for mutual information is

$$\hat{I}_{ls}(\mathbf{X}; \mathbf{Y}) = \frac{1}{2} f_K^{-1}(\widehat{\text{ABE}})^2$$

where  $\widehat{\text{ABE}}$  is the test error of the classifier. (The subscript *ls* stands for low-SNR.)

- Cover and Thomas. Elements of information theory.
- Muirhead. Aspects of multivariate statistical theory.
- van der Vaart. Asymptotic statistics.