

Outline of Stimulus Identification Project

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1 Introduction

Neuroscientists have developed an extensive theory of how simple phenomena (e.g. wind direction, arm reaching angle) are encoded by single neurons, and presumably decoded by higher cognitive functions. However, much remains to be understood about how complex phenomena (e.g. visual stimuli) are encoded or decoded.

In particular, how much information about the stimulus is captured by the various subsystems of the brain, or discarded? Taking vision as an example, we know that information from the retina is passed up successive layers of visual subsystems (V1, V2, ...), and presumably information is lost as each layer successively filters the signal recieved from the previous layer.

One might also ask about the redundancy of the information encoded by different neurons. Presumably each and every neuron is not unique, but can be grouped with similar, nearby neurons, so that the entire group can be understood as a homogenous population of neurons. In that case, one would expect that the information contained by a subsample of neurons tends to plateau as one includes more and more 'redundant' neurons in the subsample.

These two questions can both be posed in the framework of information theory. In principle, we have the tools to answer these kinds of questions. We can infer the connective structure of neural circuits in living brains, and infer their patterns of neuron activation using a variety of imaging modalities, including EEG, MEG, fMRI, and calcium imaging.

However, even after the data has been collected, there exists an inferential barrier between the data and the information theoretic conclusions we might wish to make. First of all, in order to quantify the information content of a neural system, we would ideally know the encoding scheme. However, usually

the encoding scheme has to be hypothesized, and then fit to the data. And even if we had the correct encoding scheme, we still can only estimate the information content due randomness inherent in our experimental design, measurement devices, and the neuronal dynamics themselves.

This inferential barrier has classically been ignored in classical studies of encoding and decoding, for good reason. When the stimulus is relatively simple, such as wind direction, we can often discover the correct model based on intuition, and estimate its parameters in data to a high reliability. Therefore our error in estimating the information in a population of neurons might be fairly accurate.

However, the limitations of this naive approach have been recognized for more complex, multivariate phenomena. As noted by Quiroga and Panzeri,

... decoding algorithms may fail to decode stimuli owing to a high-dimensional response space... In such circumstances it may therefore be dangerous to rule out a candidate neuronal code only because it gives a near-chance performance with a given decoding algorithm.

To give a concrete example of why it might be difficult to estimate an encoding scheme from data, we introduce our motivating example of natural image identification (Kay 2008). Here the stimulus s is a grayscale image with 128×128 pixels. Suppose for the sake of illustration that one was able to measure neural activations directly. Then, one might suppose that the firing rate of the i th neuron as a function of the stimulus is some linear function of the pixels,

$$r_i(s) = \langle a_i, s \rangle$$

One might further assume that a_i belongs to a family of Gabor filters, parameterized by a location x_i , orientation θ_i , frequency f_i , and scale τ_i . Given that each neuron only has five parameters, this might be relatively easy. However, in fact we do not have the means to measure individual neurons, but rather voxels v_i which are some time-and-space average version of the neural activity. Hence we might model each voxel as

$$v_i(s) = \langle b_i, s \rangle$$

where now b_i is a mixture of many Gabor filters. The complexity of each voxel limits the accuracy to which we can recover its encoding parameters, even supposing we have an accurate model of encoding.

As statisticians, we can develop methodology which account for the uncertainty in estimation. Such methodology can be used for the purpose of evaluating candidate encoding schemes, and inferring the information content of neuronal populations. Depending on the quality of the measurements and the sample size, the uncertainty may be too great to draw any conclusions. In that case, statistics is at the very least informative of the difficulty of the problem, or the need to acquire more data or use different modalities.

In the next sections, we narrow our scope to a specific hypothetical model of stimulus encoding, which motivates our statistical approach for inferring the information content of a population of neurons. Section 2 introduces the measure of information we employ, Section 3 discusses methods to estimate the encoding and decoding schemes, and Section 4 proposes methodology for inferring information content given a candidate encoding scheme, which accounts for statistical uncertainty.

2 Quantifying Information

2.1 Mutual Information and Fisher Information

The information content of a neural system has traditionally been understood as the mutual information between the population of neural responses, X , and the stimulus, S : that is, the information encoded by X is

$$I(S; X) = H(S) - H(S|X)$$

where H is entropy.

Gatspar et al. (2010) give a good overview of the main applications of MI (mutual information) in neuroscience. First, MI is used to compare different models of encoding. An encoding model decomposes the relationship between S and X by

$$X = f(S) + E$$

where f is an encoding map, and E is noise which is totally uninformative of the stimulus (for example, variation in spike counts due to the variance of the Poisson distribution). In that case, $I(S; X) = I(f(S); X)$. Now, given two or more encoding models given by candidate encoding maps f_1 , f_2 , etc, one can estimate a mutual information score for each model given by $MI_i = I(f_i(S); X)$. A high value of MI_i is interpreted as evidence of

the accuracy of f_i as a model of the neural system, and therefore be used to argue that the neural system is sensitive to certain stimulus features (e.g. Gabor filters for images.)

One can just as well test the validity of decoding maps $g(X)$ by postulating that $MI(S; X) = MI(S; g(X))$, where g maps responses X to stimulus features S . This approach is used to study the nature of the neural code X , i.e., to determine whether information about S is contained in spike timings, or the correlations between neurons. As before, a high MI for a candidate decoding map g is interpreted as evidence of the accuracy of g , and can be used to argue of the significance (or lack thereof) of spike timings and correlations.

Thirdly, MI can be used to study the distributed nature of the neural code. It is well-known that many stimuli are encoded in a population fashion: neurons have non-identical response patterns to stimuli, hence the population of neurons collectively encode more information than any single neuron. A more detailed understanding of the diversity of response patterns, or the redundancy of the population, can be gained by comparing the MI of subsystems of various sizes and spatial structures with the entire system.

We now mention yet another potential application of MI: validation of the scope and resolution of various imaging modalities. An ideal imaging modality would capture the activity of every single neuron in the population of encoding neurons. However, available technology and ethical considerations limit the scope and resolution of the measurements we can make of the population in question. Most modalities involve averaging over populations of neurons (EEG, fMRI). Functional MRI measures hemodynamic activity as a proxy for neural activation, hence yielding at best a temporal and spatial average of neural activity. Calcium imaging can potentially capture the activity of individual neurons, but may not be able to measure the entire population of interest. For any given modality, details in the measurement process and data processing further impact the quality of the measurements.

Supposing that X denotes the neural activity in question, while Y denotes the measurements actually obtained (hence we never observe X directly), one can use MI to measure the quality of the measurements Y , via $I(S; Y)$. Due to the data-processing inequality (and the natural assumption that Y is conditionally independent of S given X), we have $I(S; Y) \leq I(S; X)$, with $I(S; Y)$ approaching $I(S; X)$ as the scope and resolution of the measurements Y improve. One interesting question, for example, is if Y_1 denotes calcium imaging measurements and Y_2 fMRI measurements of the same brain volume

(e.g. the visual system), how much do $I(S; Y_1)$ and $I(S; Y_2)$ differ. If $I(S; Y_1)$ is much greater, this lends support to the value of the increased resolution of calcium imaging.

In any of the above applications, it becomes necessary to *estimate* quantities of the form $I(S; X)$ (where now we take S and X to more generally denote functions or measurements of the stimulus and responses, respectively) from empirical data. Empirical estimation of mutual information is a challenging theoretical problem, and much work remains to be done to develop the relevant theory.

Mutual information is most commonly used when the stimulus and response are both low-dimensional. When the response is high-dimensional, Fisher information becomes more commonly used (Yarrow et al. 2012). The reason for this is that mutual information become difficult to estimate for a high-dimensional response.

What is the both the response and the stimulus are high-dimensional: for example, when the stimulus consists of natural images and the response consists of visual system populations? Here, estimation becomes problematic, but we also point out another issue: *ill-conditioning*. Let us consider a toy model where stimulus and response are multivariate gaussian, and related by

$$X = SB + E$$

where B is a coefficient matrix and E is multivariate gaussian noise. Given such a model, the information (either MI or FI) between S and X is a function of B and Σ_E . We claim that the Fisher information and Mutual information are both ill-conditioned in the sense that small perturbations to B and Σ_E result in huge difference in the resulting measure of information. This does not match our scientific intuition, in that an approximate understanding of B and Σ_E should suffice.

2.2 An alternative approach

The shortcomings of mutual information and Fisher information in high-dimensional stimulus and response spaces make it appealing to look for yet another measure of information. The measure of information should be intuitively interpretable: it should be useful for the four goals of testing encoding models, testing decoding models, measuring the efficiency or redundancy of the neural code, and quantifying the quality of measurements obtained from

various modalities. At the same time, it should be feasible to reliably estimate the quantity from empirical data.

We propose basing the measure of information on *the ability to discriminate between distinct stimuli*. That is, in order to measure the information content of some neuronal system \vec{r} , we need to specify some *discrimination test*, and supply a *discriminator* which uses information in \vec{r} to answer the discrimination test. Examples of discrimination tests are:

- I obtain \vec{r}_1 from s_1 and \vec{r}_2 from s_2 . Are s_1 and s_2 the same stimulus? (*Hypothesis testing*)
- I obtain \vec{r} from one of $\{s_1, \dots, s_k\}$. Which stimulus did I chose? (*Classification*)

An individual discrimination test provides little information about the information capacity of a system \vec{r} . However, a large collection of such tests might be more informative; and, indeed, in the discrete setting an exact correspondence can be made between the mutual information of \vec{r} and some measure of its average performance over a collection of tests.

In general, though, there are infinitely many possible measures of information based on different kinds of discrimination tests. As a start, we might look for a measure of information which does not involve a procedure that is too complicated or arbitrary, in terms of choosing discrimination tests. To give some good and bad examples:

- Fixing some *particular* stimuli s_1, \dots, s_K and defining the information content in terms of classification performance on that set. Too arbitrary: why did you choose those stimuli in particular?
- (Packing) Choosing a probability ϵ , and declaring a set s_1, \dots, s_k as *separable* if given any s_i, s_j in the set, one can distinguish between s_i and s_j with probability $1 - \epsilon$ or better. Then defining the information content as the log of the largest k for which there exists a separable set of that size. Too complicated: given that the actual value of K might be millions or billions, there is no way to actually validate this measure experimentally.
- (Random classification) Defining some probability distribution π over stimuli, and then defining the information content in terms of *average* classification performance on a set s_1, \dots, s_k drawn randomly from π .

Another reason to motivate a notion of information based on classification is that researchers in multivoxel pattern analysis already intuitively interpret classification performance as a measure of information; formalizing this intuition would therefore open a new perspective on existing results.

To narrow down what we might consider an ideal measure of information, we can turn to the properties of Shannon information as a guideline. Shannon information has nice properties for describing the information content of a combined system in terms of the information of its subsystems. Given that many of our motivating scientific questions involve understanding the redundancy of neuronal subsystems, these are highly desirable properties for our application. These properties are:

1. Given a random vector $\vec{r}^{(1)}$ and an independent random vector $\vec{r}^{(2)}$, the joint entropy is the sum of the individual entropies,

$$H(r^{(1)}, r^{(2)}) = H(r^{(1)}) + H(r^{(2)})$$

2. Given non-independent random vectors, the joint entropy is the sum of individual entropies minus the mutual information,

$$H(r^{(1)}, r^{(2)}) = H(r^{(1)}) + H(r^{(2)}) - I(r^{(1)}, r^{(2)})$$

The measure of information, H , has a desirable additive property, while the mutual information I provides a measure of redundancy.

In fact, the *packing* definition of information comes close to satisfying property 1, other than the fact that the probability threshold ϵ has to be adjusted. That is,

$$P_{\epsilon'}(r^{(1)}, r^{(2)}) = P_{\epsilon}(r^{(1)}) + P_{\epsilon}(r^{(2)})$$

where ϵ' might be different from ϵ . To intuitively see why this is, the packing number P is the log number of balls which can be ‘packed’ into the response space R . If e^{P_1} response balls can be packed in R_1 , and e^{P_2} balls can be packed into R_2 , then by taking products of balls in R_1 and R_2 , $e^{P_1+P_2}$ balls can be packed into $R_1 \times R_2$. This is exact if we happened to be talking about lattices of hypercubes, but it is approximately correct for general metrics.

Since the packing definition of information is impractical to measure, requiring some estimate of all k choose 2 discrimination tests, we might hope that this nice property of packing could be obtained by using random

classification. In fact, we can recover this property if we consider a range of test sizes k , which is quite feasible to do in practice. But if we are willing to make some distributional assumptions on \vec{r} , we can go even further and eliminate the arbitrary choice of ϵ . This is the subject of the next subsection.

2.3 Summarizing performance in random classification

Consider a large set of neurons, r_1, \dots, r_m . Each neuron $r_i(s)$ is the sum of a signal term $h_i(s)$ and a noise term, ϵ_i . Let us assume that for random stimuli S drawn from distribution $S \sim \pi$, we have

$$(h_1(S), \dots, h_m(S)) \sim N(0, \Sigma_H)$$

and

$$(\epsilon_1, \dots, \epsilon_m) \sim N(0, \Sigma_\epsilon).$$

hence $\vec{r} \sim N(0, \Sigma_H + \Sigma_\epsilon)$.

Now consider a random classification problem, s_1, \dots, s_K drawn from π . Let $\mu_i = h(s_i)$.

Let j^* be the random label drawn uniformly from $\{1, \dots, N\}$. Then the classification rule is to estimate

$$\hat{j} = \operatorname{argmin}_{j \in \{1, \dots, K\}} \|\vec{r} - \mu_j\|_{\Sigma_\epsilon}^2$$

The classification is correct in the event that $\|\vec{r} - \mu_j\|_{\Sigma_\epsilon}^2 < \|\vec{r} - \mu_{j^*}\|_{\Sigma_\epsilon}^2$ for all $j \neq j^*$. The average misclassification is a function $\text{MC}(\Sigma_H, \Sigma_\epsilon, K)$. By transformation of variables, we see that

$$\text{MC}(\Sigma_H, \Sigma_\epsilon, K) = \text{MC}(\Sigma_\epsilon^{-1/2} \Sigma_H \Sigma_\epsilon^{-1/2}, I, K)$$

so we might as well only consider $\Sigma_\epsilon = I$.

Now our goal is to find a summary statistic $\mathcal{I}(\Sigma_\epsilon, \Sigma_H)$ for the misclassification curve $\text{MC}(\Sigma_\epsilon, \Sigma_H, \cdot)$ as K varies. Ideally the curve $\text{MC}(\Sigma_H, I, K)$ versus K only depends on a one-dimensional function of Σ_H , hence yielding a perfect summary.

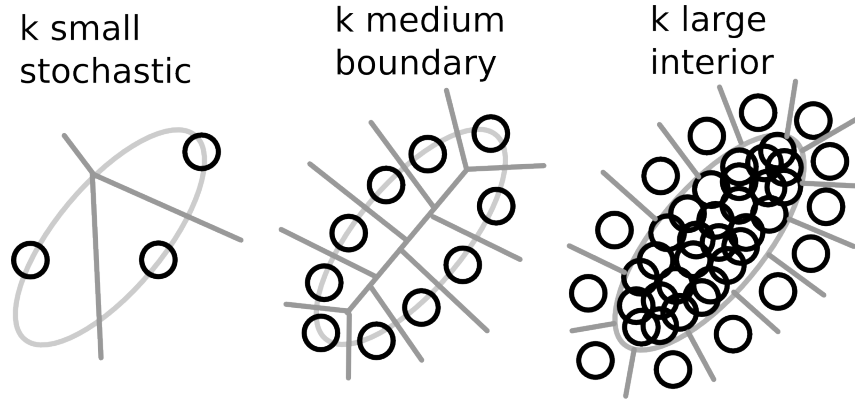
TODO: See if a good summary \mathcal{I} can be found, or if more than one summary statistic is needed.

Ideas. Approximations for MC can be found depending on K :

- K small, “stochastic” regime. Difficult to approximate because of variability in spacing.

- K medium, “boundary” regime. Concentration of measure: most centroids lie close to the level surface with Mahalanobis distance m . Therefore it’s basically a uniform distribution on an ellipsoid, and shouldn’t depend too much on Σ_h beyond the surface area of the ellipsoid.
- K large, “interior” regime. Most centroids are inside the convex hull, and hence have very high misclassification rates. Most observations \vec{r} are classified into the small minority of the centroids lying on the boundary. The boundary itself is very well behaved: it is a level surface of mahalanobis distance $\log(2K)$.

In the K large regime misclassification rate is necessarily quite high, so arguably the case of most interest (K medium) is also the most nicely behaved. See figure 1:



2.4 Relation to information theory

Somehow the above can be related to mutual information

$$I(\vec{h}, \vec{r}) \propto \ln(\Sigma_H) - \ln(\Sigma_H(\Sigma_H + \Sigma_\epsilon)^{-1}\Sigma_H)$$

2.5 Information theory facts

Suppose

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim \mathcal{N}\left(0, \begin{pmatrix} \Sigma_X & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_Y \end{pmatrix}\right)$$

Then, the mutual information between X and Y is

$$I(X; Y) = -\frac{1}{2} \log \det[\Sigma_X^{-1/2}(\Sigma_{XY}\Sigma_Y^{-1}\Sigma_{YX})\Sigma_X^{-1/2}]$$

while the Fisher information, treating X as the parameter and Y as the data, is

$$J = \Sigma_X^{-1}(\Sigma_{XY}\Sigma_{Y|X}^{-1}\Sigma_{YX})\Sigma_X^{-1}$$

where

$$\Sigma_{Y|X} = \text{Cov}(Y|X) = \Sigma_Y - \Sigma_{YX}\Sigma_X^{-1}\Sigma_{XY}$$

Notice the similarity between J and the argument of \det in the mutual information.

2.6 Robustness

We wish to apply the methods derived using the preceding Gaussian theory to non-Gaussian case: how well does it generalize?

2.7 Instability

Due to natural selection, the brain is optimized to selectively process the information from the outside world. Compared to the totality of information captured by the senses, only a small fraction may be relevant to survival. In more quantitative terms, sensory information may be extremely high-dimensional, but the useful portion of that information takes the form of a lower-dimensional summary.

Hence, if S is high-dimensional, but the relevant information takes the form of a low-dimensional summary $L = h(S)$, then we have $I(S; X) = I(L; X)$. Such a dimension-reduction assumption may be crucial to obtaining tractable estimates of $I(S; X)$.

We argue, however, that instability issues limit the possibility of using MI or FI in this fashion. For the sake of illustration, suppose we consider linear summaries $L = SA$, where A is a coefficient matrix. For instance, L may be the first k principal components of S . However, now note that estimation of the principal components (or even the number of components) is highly noisy. Hence... [argue that if L is estimated as first principal components, $I(L; X)$ will be highly variable for MI or FI.]

3 Estimating Encoding Parameters

3.1 Previous Work

Consider a parametric model

$$Y \sim F_\theta(X)$$

Such a *forward model* gives the distribution of the response conditional on the stimuli features.

The *maximum likelihood* (ML) principle can be invoked to identify the stimuli $i \in S$ “most likely” to have produced y^* . Let $x_i : i \in S$ denote features of the test stimuli, and identify y^*

$$i^* = \operatorname{argmax}_i \ell_\theta(y^* | x_i)$$

Example. We take the following as a representative approach, combining features of [1] and [2]:

- Assume the normal multivariate linear model

$$Y \sim N(XB, \Sigma_E), \text{ where } B \in \mathbb{R}^{q \times p}$$

- Estimate B using elastic net [4]
- Estimate Σ_E using off-diagonal shrinkage of sample covariance matrix of residuals
- The ML rule takes the form

$$i^* = \operatorname{argmin}_i (x_i^T \hat{B} - y^*)^T \hat{\Sigma}_E^{-1} (x_i^T \hat{B} - y^*) \quad (1)$$

3.2 Empirical Bayes Approach

- *Idea:* Unlike ML, the Bayes rule surely optimizes the “correct” objective function. Can we approximate the Bayes rule?
- *Empirical Bayes:* use the data to estimate the covariances Σ_B and Σ_E , then compute posterior distribution of B
- Assume coefficients of B independent; diagonals of Σ_B can be estimated using any estimate of signal strength, e.g. *Eigenprism* [3].

- Decision rule similiar to (1) but with “added noise” due to uncertainty of B .

$$\min(x_i^T B - y^*)^T (\text{Cov}(x_i^T B) + \hat{\Sigma}_E)^{-1} (x_i^T B - y^*)$$

- Analogous to LDA vs QDA

3.3 Covariance Estimation

Both ML approach and EB approach depend on estimates of the covariance of Y . We might assume a “Kronecker” model where $\text{Cov}(Y) = \Sigma_v \times \Sigma_t$ where Σ_v is the covariance of voxels (for a fixed time point) and Σ_t is the autocovariance of a given voxel.

New approaches to estimating covariance Σ_v might incorporate spatial information about voxel location, or functional information.

3.4 Computation

Suppose we have a $n \times p_Y$ response matrix Y and a $n \times p_X$ covariate matrix X . We have the model

$$Y = XB + E$$

where B is a $p_X \times p_Y$ coefficient matrix and E is a matrix of noise. Write

$$E = \begin{pmatrix} e_1^T \\ e_2^T \\ \dots \\ e_n^T \end{pmatrix}$$

Assume the rows of E are independent, and each row is distributed

$$e_i \sim N(0, \Sigma_e)$$

Let us assume a prior distribution on the coefficients,

$$B_{ij} \sim N(0, \sigma_{B,j}^2)$$

and where B_{ij} are independent. Note that each column $j = 1, \dots, p_Y$ has a different prior coviarance $\sigma_{B,j}^2$. This reflects our prior knowledge that some column of Y may have more signal than other columns.

Bayes’ rule gives us the posterior mean and covariance of the coefficients B_{ij} . First, we introduce the vectorized notation \vec{B} to denote the $p_X p_Y \times 1$

vector obtained by stacking the columns of B , and similarly \vec{Y} to denote the $p_Y n \times 1$ vector obtained by stacking the columns of Y . Also recall the definition of Kronecker product,

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \dots \\ a_{21}B & a_{22}B & \dots \\ \dots & \dots & \dots \end{pmatrix}$$

Also define

$$\Omega_e = \Sigma_e^{-1}$$

$$\Omega_b = \text{diag} \left(\frac{1}{\sigma_{b,1}^2}, \dots, \frac{1}{\sigma_{b,p_Y}^2} \right)$$

The posterior mean and covariance are given as follows.

$$\mathbb{E}[\vec{B}|Y] = (\Omega_e \otimes X^T X + \Omega_b \otimes I_{p_X})^{-1} ((I \otimes X)^T (\Omega_e \otimes I) \vec{y})$$

$$\text{Cov}(\vec{B}|Y) = (\Omega_e \otimes X^T X + \Omega_b \otimes I_{p_X})^{-1}$$

Given a new observation $y_* = B^T x_* + e_*$, where y_* and x_* are column vectors, the posterior predictive distribution is

$$\mathbb{E}[y_*|Y] = (I_{p_Y} \otimes x_*^T) \mathbb{E}[\vec{B}|Y]$$

$$\text{Cov}[y_*|Y] = (I_{p_Y} \otimes x_*^T) \text{Cov}(\vec{B}|Y) (I_{p_Y} \otimes x_*) + \Sigma_e$$

In the following, we assume that $p_X > n$.

Naively, computing the posterior covariance takes $O(p_X^3 p_Y^3)$ operations and computing the posterior mean takes $O(p_X^2 p_Y^2)$ operations.

However, by diagonalizing the covariance matrix and taking advantage of the properties of Kronecker products, we can make the computation much more efficient.

Using simultaneous diagonalization, find V_e, D_e such that

$$\Omega_e = V_e D_e V_e^T$$

and

$$\Omega_b = V_e V_e^T$$

Note that V_e is not orthogonal. The procedure for finding V_e, D_e is well-known and also given in the code.

Furthermore, define

$$\tilde{X} = \begin{pmatrix} X \\ 0 \end{pmatrix}$$

so that \tilde{X} is an $p_X \times p_X$ matrix. Then take the SVD

$$\tilde{X} = U_X D_X V_X^T$$

so that D_X and V_X are both $p_X \times p_X$. We have

$$V_X V_X^T = V_X V_X^T = I_{p_X}$$

and

$$V_X D_X^2 V_X^T = X^T X.$$

Now we can rewrite the expression

$$\begin{aligned} \text{Cov}(\vec{B}|Y) &= (\Omega_e \otimes X^T X + \Omega_b \otimes I_{p_X})^{-1} \\ &= ((V_e D_e V_e^T) \otimes (V_X D_X^2 V_X^T) + (V_e V_e^T) \otimes (V_X V_X^T))^{-1} \\ &= [(V_e \otimes V_X)(D_e \otimes D_X^2 + I_{p_X p_Y})(V_e^T \otimes V_X^T)]^{-1} \\ &= (V_e^{-1} \otimes V_X^T)^T (D_e \otimes D_X^2 + I_{p_X p_Y})^{-1} (V_e^{-1} \otimes V_X^T) \end{aligned}$$

In this form the expression is much easier to compute since

- Only a diagonal matrix needs be inverted, and yields a diagonal matrix
- Multiplying the transpose of a Kronecker product with a diagonal with itself is easy to compute.

To see the second point, consider computing the product

$$C = (A \otimes B)^T D (A \otimes B)$$

where A is $a_1 \times a_2$, B is $b_1 \times b_2$, and D is diagonal with

$$D = \begin{pmatrix} D_1 & 0 & 0 & 0 & \dots \\ 0 & D_2 & 0 & 0 & \dots \\ 0 & 0 & D_3 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

such that each D_1, \dots, D_{a_1} is $b_1 \times b_1$.

For $i, j = 1, \dots, a_2$, let $C_{[ij]}$ denote $b_2 \times b_2$ blocks such that

$$C = \begin{pmatrix} C_{[11]} & C_{[12]} & \dots \\ C_{[21]} & C_{[22]} & \dots \\ \dots & \dots & \dots \end{pmatrix}$$

Now we can write

$$C_{[ij]} = \sum_{k=1}^{a_1} a_{ki} a_{kj} B^T D_k B = \left(\sum_{k=1}^{a_1} a_{ki} a_{kj} B^T D_k B \right) = B^T \left(\sum_{k=1}^{a_1} a_{ki} a_{kj} D_k \right) B.$$

The second-to-last and last equality present two alternative methods to compute $C_{[ij]}$.

- Using the second-to-last equality, one precomputes each of the matrices $B^T D_i B$, which takes $O(b_2^2 b_1 a_1)$ operations. To compute each block, it takes $O(b_2^2 a_1)$ operations. Hence, to compute C takes $O(a_1 a_2^2 b_2^2)$.
- Using the last equality, for each block one takes $O(a_1 b_1)$ operations to compute the weighted sum of D_1, \dots, D_{a_1} , and then $O(b_2^2 b_1)$ to multiply on the left with B^T and on the right with B .

Therefore, we see that it takes $O(a_2^2 b_2^2 b_1)$ operations to compute C .

Choosing the best of the two methods, the cost to compute C is $O(a_2^2 b_2^2 \min(a_1, b_1))$. Applying to our problem, we see that the cost to evaluate the posterior covariance using this method is $O(p_Y^2 p_X^2 \min(p_X, p_Y))$, which is a saves a factor of $\max(p_Y, p_X)$ compared to the naive approach.

4 Inferring Information Content

4.1 Finite Sample Effect

Changing slightly the notation, let $\text{MC}(\vec{r}, K, n)$ denote the misclassification when classifying K random classes, given a training set of size n . Our definition of information is computed from $\text{MC}(\vec{r}, K, \infty)$: the misclassification curves assuming a *known* encoding rule. However, in practice, we only know $\text{MC}(\vec{r}, K, n)$ for finite n .

4.2 Learning Curves

The question is whether one can estimate $MC(\vec{r}, K, \infty)$ based on knowing $MC(\vec{r}, K, n)$ for various $n \leq N$, where N is the total number of observations available.

Cortes et al propose the following method to model the training and test error as a function of n , the training set size:

$$\begin{aligned} \text{Err}_{\text{train}} &= a - \frac{b}{n^\beta} \\ \text{Err}_{\text{test}} &= a + \frac{c}{n^\alpha} \end{aligned}$$

where a , b , c , α and β are to be determined empirically.

GOAL: Extend this type of empirical model to also incorporate K , the number of test classes, and justify somehow.

4.3 Two-class problem

Suppose $\mu_1, \mu_2 \sim N(0, \Sigma)$, and $Y_i \sim N(\mu_i, I)$. What is the misclassification rate, i.e.

$$MC(\Sigma, 2) = \Pr[||Y_1 - \mu_1||^2 > ||Y_1 - \mu_2||^2]$$

Without loss of generality, assume $\Sigma = \text{diag}(\lambda_1, \dots, \lambda_d)$. Let $X = Y_1 - \mu_1$ and $D = \mu_1 - \mu_2$. Then $X \sim N(0, I)$ and $D \sim N(0, 2\Sigma)$, where X and D are independent, and we have

$$\begin{aligned} MC(\Sigma, 2) &= \Pr[||X||^2 > ||X + D||^2] \\ &= \Pr \left[\sum_{i=1}^d X_i^2 > \sum_{i=1}^d (X_i + D_i)^2 \right] \\ &= \Pr \left[-2 \sum_{i=1}^d D_i X_i > \sum_{i=1}^d D_i^2 \right] \\ &= \mathbf{E} \left[\Pr \left[-2 \sum_{i=1}^d D_i X_i > \sum_{i=1}^d D_i^2 \right] | D \right] \end{aligned}$$

where we have conditioned on D . Let $S = \sum_{i=1}^d D_i^2$. Then conditional on D , we have $\sum_{i=1}^d D_i X_i \sim N(0, S)$, meaning that

$$\Pr \left[-2 \sum_{i=1}^d D_i X_i > \sum_{i=1}^d D_i^2 \middle| D \right] = \Pr[N(0, 4S) > S | D] = 1 - \Phi(\sqrt{S/4})$$

hence

$$MC(\Sigma, 2) = 1 - \mathbf{E}\Phi(\sqrt{S}/2)$$

4.4 High-dimensional asymptotics

Here we consider the limit $MC(\Sigma_d, k)$, for a sequence Σ_d with the appropriate limit properties.

Theorem. There exists a function $m(c, k)$ for $c > 0$, and $k \in \{1, 2, \dots\}$, such that

$$m(c, k) = \lim_{d \rightarrow \infty} MC(\Sigma_d, k)$$

for all sequences of covariance matrices such that

$$\lim_{d \rightarrow \infty} \text{tr} \Sigma_d = c$$

and also

$$\lim_{d \rightarrow \infty} \text{tr} \Sigma_d^2 = 0$$

Proof. Note that for $\mu \sim N(0, \Sigma)$, we have

$$\mathbf{E}||\mu||^2 = \text{tr} \Sigma$$

and

$$\text{Var}||\mu||^2 = 2\text{tr} \Sigma^2$$

Hence, the fact that $\text{tr} \Sigma_d \rightarrow c$ and $\text{tr} \Sigma_d^2 \rightarrow 0$ imply that for arbitrary $\epsilon > 0$, we can find d sufficiently large such that with probability greater than $1 - \epsilon$,

$$\max_{1 \leq i \leq j \leq k} \langle \mu_i, \mu_j \rangle < \epsilon$$

and

$$\max_{1 \leq i \leq k} ||\mu_i||^2 - c < \epsilon$$

for $\mu_1, \dots, \mu_k \sim N(0, \Sigma_d)$. Let A denote the event in which both inequalities hold.

In the event A ,

$$\mu_i = \sqrt{c}e_i + O(\epsilon)$$

given an appropriate orthonormal basis e_1, \dots, e_k .

Similar to before, we have

$$MC(\Sigma_d, k) = \Pr[||\mu_1 - Y_1||^2 > \min_i ||\mu_i - Y_1||^2]$$

where $Y_1 \sim N(\mu_1, I)$.

Let us write

$$Y_1 - \mu_1 = \sum_i Z_i e_i,$$

and in the event A , we have

$$Y_1 - \mu_i = \sum_i Z_i e_i + \sqrt{c}e_1 - \sqrt{c}e_i + O(\epsilon)$$

It follows that

$$\begin{aligned} MC(\Sigma_d, k) &= \Pr[||\mu_1 - Y_1||^2 > \min_i ||\mu_i - Y_1||^2] \\ &= \Pr[A] \Pr[||\mu_1 - Y_1||^2 > \min_i ||\mu_i - Y_1||^2 | A] \\ &\quad + \Pr[A^c] \Pr[||\mu_1 - Y_1||^2 > \min_i ||\mu_i - Y_1||^2 | A^c] \\ &= \Pr[||\mu_1 - Y_1||^2 > \min_i ||\mu_i - Y_1||^2 | A] + O(\epsilon) \\ &= \Pr[2\sqrt{c}Z_1 > \min_i 2\sqrt{c}Z_i + 2c + O(\epsilon)] + O(\epsilon) \\ &= \Pr[\min_i (Z_i + O(\epsilon)) < Z_1 - \sqrt{c}] + O(\epsilon) \end{aligned}$$

noting that the function $\Pr[\min_i (Z_i + \xi_i) < Z_1 - \sqrt{c}]$ is continuous and jointly differentiable with respect to ξ_i at $\xi = 0$,

$$\begin{aligned} &= \Pr[\min_i Z_i < Z_1 - \sqrt{c}] + O(\epsilon) \\ &= 1 - \int_{\mathbb{R}} \Phi(\sqrt{c} - z)^{k-1} d\Phi(z) + O(\epsilon) \end{aligned}$$

Hence in the limit,

$$\lim_{d \rightarrow \infty} MC(\Sigma_d, k) = 1 - \int_{\mathbb{R}} \Phi(\sqrt{c} - z)^{k-1} d\Phi(z)$$

4.5 High-SNR limit

Rather than fixing the number of classes K and increasing the dimension, we could also derive a limit by fixing the dimensionality and increasing both the signal covariance Σ and the number of classes K . The difference between the high-SNR limit and the high-dimensional limit is that the dimensionality of the space will influence the asymptotics.

Recall that we define $MC(\Sigma, k)$ by the misclassification given that that joint distribution of a class center μ and a member of the class Y is

$$\begin{pmatrix} \mu \\ Y \end{pmatrix} \sim N \left(0, \begin{pmatrix} \Sigma & \Sigma \\ \Sigma & \Sigma + I \end{pmatrix} \right)$$

In the high-SNR limit, it is notationally more convenient to consider an different parameterization. Defining $\Omega = \Sigma^{-1}$, one can compute $MC(\Sigma, K)$ as the misclassification rate of the model where

$$\begin{pmatrix} \mu \\ Y \end{pmatrix} \sim N \left(0, \begin{pmatrix} I & I \\ I & I + \Omega \end{pmatrix} \right)$$

Let $k = K - 1$. To compute the misclassification rate, we draw from the joint distribution of $(\mu^*, Y, \mu_1, \dots, \mu_k)$ where $\mu^*, \mu_1, \dots, \mu_k \sim N(0, I)$ and $Y \sim N(\mu^*, \Omega)$, and then compute

$$MC(\Sigma, K) = \Pr[\min_{i=1}^k \|Y - \mu_i\|_{\Sigma}^2 < \|Y - \mu^*\|_{\Sigma}^2]$$

under the specified joint distribution, where

$$\|x\|_{\Sigma}^2 = x^T \Sigma x = x^T \Omega^{-1} x.$$

We sample in the following way. First, draw $Y \sim N(0, I + \Omega)$. Then draw $\mu^* \sim N((I + \Omega)^{-1}Y, I - (I + \Omega)^{-1})$ and $\mu_1, \dots, \mu_k \sim N(0, I)$. Conditioning on $Y = y$, $Y - \mu^*$ is independent of $Y - \mu_1, \dots, Y - \mu_k$: defining $A = I - (I + \Omega)^{-1}$, we have

$$\begin{pmatrix} y - \mu^* \\ y - \mu_1 \\ \vdots \\ y - \mu_k \end{pmatrix} \sim N \left(\begin{pmatrix} Ay \\ y \\ \dots \\ y \end{pmatrix}, \begin{pmatrix} A & 0 & \dots & 0 \\ 0 & I & \dots & 0 \\ 0 & \vdots & \dots & 0 \\ 0 & 0 & \dots & I \end{pmatrix} \right)$$

Thus, we are computing

$$MC(\Sigma, K) = \mathbf{E}_Y[\Pr[\min_{i=1}^k \|y + Z_i\|_{\Sigma}^2 < \|Ay + A^{1/2}Z^*\|_{\Sigma}^2 | Y = y]]$$

where Z^*, Z_1, \dots, Z_k are iid $N(0, I)$.

To prepare for such a result, we approximate the distribution of M when Σ and y are large. The p th quantile of M is the $1 - (1 - p)^{1/k}$ th quantile of $\|y + Z_i\|^2$. For large Σ , we can approximate

$$\Pr[\|y + Z_i\|_\Sigma^2 < x] \approx \phi_d(y) \det(\Sigma)^{-1/2} \text{Vol}(B_d(\sqrt{x})) = \phi_d(y) \sqrt{\det(\Sigma)} \frac{2(\pi x)^{d/2}}{d\Gamma(d/2)}$$

where $B_d(r)$ is the euclidean ball with radius r and $\phi_d(y) = (2\pi)^{-d/2} e^{-\|y\|^2/2}$. Hence, the p th quantile of M is x_p where

$$x_p \approx \frac{1}{\pi} \left(\frac{d\Gamma(d/2)}{2} \frac{(-\log(1 - p)/L) \sqrt{\det(\Sigma)}}{\phi_d(y)} \right)^{2/d}$$

Upper and lower bounds for the approximation are given in the appendix.

Let us now turn to the distribution of V . We have $A \rightarrow \Omega$ in the limit of large Σ . Then,

$$\|Ay + A^{1/2}Z\|_\Sigma^2 \approx \|\Omega y + \Omega^{1/2}Z\|_\Sigma^2 = \|\Omega^{1/2}y + Z\|^2$$

5 Appendix

5.1 Approximation bounds for high-SNR limit

5.1.1 Upper bound

For $x > 0$ we have

$$\Pr[\|y + Z_i\|_\Sigma^2 < x] < K(\Sigma) x^{d/2} \phi_d(\bar{y}_x)$$

where

$$K(\Sigma) = \sqrt{\det(\Sigma)} \frac{2\pi^{d/2}}{d\Gamma(d/2)}$$

and \bar{y}_x is defined as follows.

Consider the optimization problem

$$\text{minimize } \|z - y\|^2 \text{ subject to } \|z\|_\Sigma^2 \leq x$$

We assume ϵ sufficiently small such that the the solution satisfies the hard constraint $\|z\|_\Sigma^2 = \epsilon$. Take the Lagrangian

$$\|z - y\|^2 + \lambda z^T \Sigma z$$

with $\lambda > 0$, and set the derivative equal to zero:

$$0 = 2z - 2y + 2\lambda \Sigma z$$

yielding

$$z = (I + \lambda \Sigma)^{-1} y.$$

Let $\lambda^* > 0$ be the solution to

$$x = y^T (I + \lambda \Sigma)^{-1} \Sigma (I + \lambda \Sigma)^{-1} y$$

and define

$$\bar{y}_x = y - (I + \lambda^* \Sigma)^{-1} y.$$

It follows that defining

$$\underline{x}_p = x \text{ such that } K(\Sigma) \phi_d(\bar{y}_x) = 1 - \sqrt[t]{1 - p},$$

we have

$$\underline{x}_p < x_p.$$

5.1.2 Lower bound

We have the following lower bound:

Lemma. *For any $r \leq \sqrt{\gamma/x}$, where γ is the largest eigenvalue of Σ , we have*

$$\Pr[\|y + Z_i\|_\Sigma^2 < x] < \text{Vol}(B_r) \phi_d(\|y\| + r)$$

where $\phi_d(y) = (2\pi)^{-d/2} \exp(-y^2/2)$.

The lemma follows from the fact that $z \in B_r$ implies $\|z\|_\Sigma^2 < x$ and $\phi_d(y - z) \geq \phi_d(\|y\| + r)$. Let r^* be defined by

$$r^* = \arg\max_r \text{Vol}(B_r) \phi_d(\|y\| + r)$$

The lower bound then comes from choosing $r = \min(r^*, \gamma/x)$.

$$\Pr[\|y + Z_i\|_\Sigma^2 < x] > \text{Vol}(B_r) \phi_d(\|y\| + \min(r^*, \gamma/x))$$