

Better-than-chance classification for signal detection

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Abstract

[TODO]

1 Introduction

A common workflow in genetics or neuroimaging consists of fitting a classifier, and estimating its predictive accuracy using cross validation. Given that the cross validated accuracy is a random quantity, it is then common to test if the cross validated accuracy is significantly better than chance using a permutation test. Examples in the genetics literature include Jiang et al. [2008], Radmacher et al. [2002] [TODO: elaborate]. Example sin the neuroscientific literature include [Golland and Fischl, 2003, Kriegeskorte et al., 2006, Pereira et al., 2009, Varoquaux et al., 2016]. The number of citations¹ of these papers attest to the popularity of the above workflow: 956 for Kriegeskorte et al. [2006], and 274 for Radmacher et al. [2002], as examples.

To fix ideas, we will adhere to a neuroscientific example: In Gilron et al. [2016], the authors seek to detect brain regions which encode differences between vocal and non-vocal stimuli. According to the MVPA analysis workflow, the localization problem is cast as a supervised learning problem: if the type of the stimulus can be predicted from the spatial activation pattern, significantly better than chance, then a region is declared to encode vocal/non-vocal information. We call this an *accuracy test*, a.k.a. *class prediction* in Simon et al. [2003].

This same signal detection task can be also approached as a two-group multivariate test: Inferring that a region encodes vocal/non-vocal information, is essentially inferring that the spatial distribution of brain activations

¹Based on GoogleScholar. Accesses on 26.7.2016.

25 is different given a vocal/non-vocal stimulus. A practitioner may then call
 26 upon a two-group location test such as Hotelling’s T^2 [Fujikoshi et al., 2011].
 27 Alternatively, if the size of the brain region is too large compared to the num-
 28 ber of observations, so that the spatial covariance cannot be fully estimated,
 29 then a high dimensional version of Hotelling’s test can be called upon, such
 30 as in Srivastava [2013] or Schäfer et al. [2005]. In contrast to *accuracy tests*,
 31 we call these *location tests*, a.k.a. *class comparison* in Simon et al. [2003].

32 At this point, it becomes unclear which is the preferred test. The compar-
 33 ison between location and accuracy tests was precisely the topic of Ramdas
 34 et al. [2016], who compared the Hotelling location test to the accuracy of
 35 *Fisher’s linear discriminant analysis* classifier (LDA) [Hastie et al., 2003].
 36 Using an asymptotic analysis, Ramdas et al. [2016] concluded that accuracy
 37 and location tests are equivalent with respect to their order of convergence
 38 to a consistent test, while they may differ in constants. Put differently, the
 39 (asymptotic) relative efficiency of the tests is not trivially 0 nor ∞ .

40 The relative efficiency, governing the power of the tests, may prove crucial
 41 when dealing with the finite sample sizes in neuroscience and genetics, and
 42 thus the focus of this study. We thus seek to study which test is to be
 43 preferred in finite samples? Our conclusion will be quite simple: *location*
 44 *tests almost always have more power than accuracy tests*.

45 The main argument for our statement rests upon the observation that
 46 with typical sample sizes, the accuracy test statistic is highly discrete. Dis-
 47 crete test statistics are known to be conservative [Hemerik and Goeman,
 48 2014], since they cannot exhaust the permissible false positive rate. For accu-
 49 racy tests, the degree of discretization is governed by the number of samples.
 50 In our running neuroscience example [Gilron et al., 2016], the classification
 51 is performed based on 40 trials, so that the test statistic may assume only 40
 52 possible values. This number of examples is not unusual if considering this
 53 is the number of subject in a genetic study, or the number of trial-repeats in
 54 an fMRI brain scan.

55 The discretization effect is aggravated if the test statistic is highly concen-
 56 trated. For an intuition consider the usage of the *train* accuracy test statistic
 57 (i.e., not cross validated). In Section 4 we then address our main question-
 58 which test has more power? Based on the finding that the location test is
 59 typically more powerful, we try to offer an intuition for this phenomenon in
 60 the Discussion section.

61 2 Problem setup

62 Adhering to our neuroscientific example, we now formalize terminology and
63 notation. Let $y \in \mathcal{Y}$ be a class encoding. In our vocal/non-vocal example
64 we have $\mathcal{Y} = \{-1, 1\}$. Let $x \in \mathcal{X}$ be a p dimensional feature vector. In our
65 vocal/non-vocal example p is the number of voxels in a brain region. We
66 thus have $\mathcal{X} = \mathbb{R}^{27}$.

67 Given n pairs of (x_i, y_i) , typically assumed i.i.d., the *testing* approach to
68 localization amounts to testing whether $x|y = 1$ has the the same distribution
69 as $x|y = -1$. I.e., the multivariate voxel activation pattern has the same
70 distribution when given a vocal stimulus, as when given a non-vocal stimulus.
71 The *classification* approach to the localization problem amounts to learning a
72 predictive model $\hat{f}(x)$ from some assumed model class $\hat{f} \in \mathcal{F}$. The prediction
73 accuracy, denoted $T_{\hat{f}}^{acc}$, is defined as the probability of a given classifier \hat{f}
74 of making a correct prediction $T_{\hat{f}}^{acc} := P(\hat{f}(x) = y)$ when given a new,
75 randomly drawn data point, (x, y) .

76 2.1 Candidate Tests

77 The design of a permutation test using the prediction accuracy, requires the
78 following design choices:

79 **What test statistic?**

80 **Cross validated or not?** Is the statistic cross validated or not?

81 **Refolding?** For a K-fold cross validated test statistic: is the data refolded
82 in each permutation?

83 **Permute labels of features?** Should the y be permuted or should the x ?

84 **Balanced folding?** For a K-fold cross validated test statistic: is the data
85 folding balanced? (a.k.a. stratified).

86 **How many folds?** We will now address these questions while bearing in
87 mind that unlike the typical supervised learning setup, we are not in-
88 terested in an unbiased estimate of the prediction error, but rather in
89 the mere detection of a difference between two groups, leading to a
90 better-than-chance accuracy.

What test statistic? Given a predictor \hat{f} , a natural test statistic is some estimate of its accuracy $T_{\hat{f}}^{acc}$. Then again, very low accuracies, even 0, is evidence that the classes are separated, and we only need to invert the predictions. We can thus consider some estimate of $|T_{\hat{f}}^{acc} - 0.5|$ as the test statistic. This, however, implies that if the classes are identical, random guessing has a 0.5 accuracy. This is not true if the classes are not balanced. The chance level in which case is the prevalence of the dominant class, we denote by \hat{p}_{max} . This suggests the following test statistic $|T_{\hat{f}}^{acc} - \hat{p}_{max}|$. Since we will latter be aggregating these statistic over random data foldings, where the dominant class may have varying frequencies, it seems appropriate to standardize the scale of this statistic. We thus also consider a z-scored accuracy: $|T_{\hat{f}}^{acc} - \hat{p}_{max}| / \sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$.

Cross validated or not? Were we interested in an unbiased estimator of the prediction error, there is no question that some validation is in order. Since we are merely interested in detecting a difference between groups, a biased error estimate is not an issue provided that it is consistent over all permutations. The underlying intuition is that if the exact same computation is performed over all permutations, then a permutation test will be “fair”, i.e., will not inflate the false positive rate. We will thus be considering both cross validated accuracies, and train accuracies as our test statistics.

Refolding? The standard practice in neuroimaging is to refold the data after each permutation. This is imperative if permuting labels while aiming at balanced data folds. This is not, however, imperative in general. In this work, we will adhere to the standard practice of refolding the data within each permutation.

Permute labels of features? While seemingly identical, the compounding of permutations with data foldings renders these two approaches distinct. As an example, consider balanced (stratified) K-fold cross validation where the initial data folding is balanced. After a label permutation, the folds will probably not be balanced, and will thus have to be refolded. If the features are permuted, then the labels conserve their original fold assignments, and the data need not be refolded. Since we only report results while refolding the data in each permutation, then the only difference between permuting labels and permuting

127 features seems to be a computational one. We thus adhere to the more
128 common, albeit less efficient practice, of permuting labels.

129 **Balanced folding?** A standard practice when cross validating is to
130 constrain the data folds to be balanced (i.e. stratified). This is well
131 justified when aiming at unbiased accuracy estimation. This also sim-
132 plifies matter when aiming at signal detection, as can be seen from the
133 above discussion of the appropriate test statistic. Then again, it may
134 complicate matters, as can be seen from the above discussion on label
135 versus feature permutation. In general, it is not imperative in gen-
136 eral, and we will indeed be comparing the effect of balanced foldings
137 versus unbalanced. We will thus report results with both balanced and
138 unbalanced data foldings.

139 **How many folds?** Different authors suggest different rules for the
140 number of folds. We will be varying the number of folds, since it will
141 affect the concentration of the estimated accuracy, which will have a
142 crucial effect on the conservativeness of the permutation test. Our intu-
143 ition suggests that since more folds imply a less concentrated estimate,
144 then leave-one-out should be the less conservative, and 2-fold should
145 be the most conservative.

146 By now, the reader will have observed that there are indeed many ways
147 to perform a permutation test using a cross validated statistic. The subset
148 of tests we will be comparing is collected for convenience in Table 1.

149 3 Controlling the False Positive Rate

150 In the first of our battery of simulations we verify that various test statistics
151 and permutation schemes control the type I error. Figure ?? demonstrates
152 that this is indeed the case. All our candidate tests control the type I error,
153 with varying degrees of conservativeness. In particular: (a) if the folds are
154 balanced or not, (b) if the labels are permuted or the features, (c) if the test
155 statistic is varied, (d) if the regularization level of the support vector machine
156 classifier (SVM) is varied, (e) if the number of folds is varied.

Name	Basis	CV	Accuracy	Parameters
Hotelling	Hotelling	–	–	shrink=FALSE
Hotelling.shrink	Hotelling	–	–	shrink=TRUE
lda.CV.1	LDA	TRUE	accuracy	–
lda.CV.2	LDA	TRUE	z-accuracy	–
lda.noCV.1	LDA	FALSE	accuracy	–
lda.noCV.2	LDA	FALSE	z-accuracy	–
sd	SD	–	–	–
svm.CV.1	SVM	TRUE	accuracy	cost=1e1
svm.CV.2	SVM	TRUE	accuracy	cost=1e-1
svm.CV.3	SVM	TRUE	z-accuracy	cost=1e1
svm.CV.4	SVM	TRUE	z-accuracy	cost=1e-1
svm.noCV.1	SVM	FALSE	accuracy	cost=1e1
svm.noCV.2	SVM	FALSE	accuracy	cost=1e-1
svm.noCV.3	SVM	FALSE	z-accuracy	cost=1e1
svm.noCV.4	SVM	FALSE	z-accuracy	cost=1e-1

Table 1: This table enumerates the various test statistics we will be studying. Three are location tests: Hotelling, Hotelling.shrink, and sd. *Hotelling* is the classical two-group T^2 statistic. *Hotelling.shrink* is a high dimensional version with the regularized covariance in Schäfer et al. [2005]. *sd* is another high dimensional version of the T^2 , from Srivastava et al. [2013]. The rest of the tests are variations of the linear SVM, and Fisher’s LDA, with varying accuracy measures, cross validated or not, and varying tuning parameters. For example, *svm.CV.4* is a linear SVM, with *libsvm*’s cost parameter set at 0.1, using the cross validated z-scored accuracy ($|T_{\hat{f}}^{acc} - \hat{p}_{max}|/\sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$, see Section 2.1). Another example is *lda.noCV.1*, which is Fisher’s LDA, returning the train accuracy, without cross validation, and without z-scoring.

157 4 Power

158 Having established that all of the tests in our battery control the false po-
159 sitive rate, it remains to be seen if they have similar power– at least when
160 comparing the power of the various classifiers and multivariate tests. The re-
161 sults of Ramdas et al. [2016] suggest that power should be of the same order.
162 On the other hand, the results of our previous sections suggest that the con-
163 servativeness of some of the considered tests can be considerable, rendering
164 them underpowered.

165 [TODO: discuss power of various tests after finishing simulations]

166 We see by now that the use of accuracy tests for signal detection is un-
167 derpowered compared to location tests. The above simulations can hardly
168 support such a universal statement. We will thus verify on a neuroimaging
169 dataset, and discuss the causes for this phenomenon thus the scope of the

Figure 1: The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. They are assumed to be equal in all the 23 dimensions, and vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square). The various statistics on the y axis. Their details are given in Table 1. Simulation code available at [TODO].



statement.

5 Neuroimaging Example

Figure 2 is an application of our battery of tests to the data of Pernet et al. [2015]. The authors of Pernet et al. [2015] collected fMRI data while subjects were exposed to the sounds of human speech (vocal), and other non-vocal sounds. Each subject was exposed to 20 sounds of each type, totalling in $n = 40$ trials in each scan. The study was rather large and consisted of about 200 subjects. The data was kindly made available by the authors at the OpenfMRI website².

To verify the observation that location tests have more power than accuracy tests, we perform permutation inference using the pipeline of Stelzer et al. [2013], which was also used in Gilron et al. [2016]. For completeness, the pipeline is described in Appendix A. To demonstrate our point, we compare the *sd* location test with the *svm.cv.1* accuracy test (see Table 1 for the definition of these statistics).

²<https://openfmri.org/>

185 In agreement with our simulation results, the location test (*sd*) discovers
186 more brain regions that encode information discriminating between vocal and
187 non-vocal stimuli when compared to an accuracy test (*svm.cv.1*). The former
188 discovers 1,232 regions, while the latter only 441, 399 of which are common
189 to both as reported in Figure 2. We emphasize that both test statistics were
190 compared with the same permutation scheme, and the same error controls,
191 so that any difference in detections is due to their different power.

192 Having established that accuracy tests are underpowered both in simula-
193 tion and in application, we wish to identify the conditions under which this
194 will occur, and discuss implications on the practice of accuracy tests.

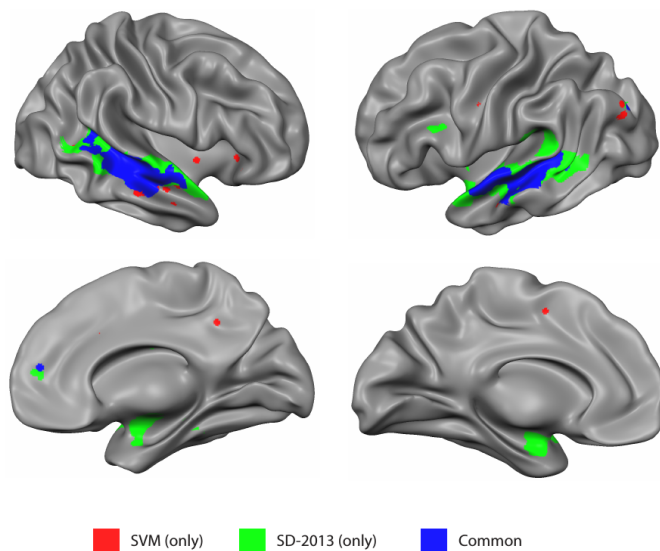


Figure 2: Brain regions encoding information discriminating between vocal and non-vocal stimuli. Map reports the centres of 27-voxel sized spherical regions, as discovered by an accuracy test (*svm.cv.1*), and a location test (*sd*). *svm.cv.1* was computed using 5-fold cross validation, and a cost parameter of 1. Region-wise significance was determined using the permutation scheme of Stelzer et al. [2013], followed by region-wise $FDR \leq 0.05$ control using the Benjamini-Hochberg procedure [Benjamini and Hochberg, 1995]. Number of permutations equals 400. The location test detect 1,232 regions, and the accuracy test 441. The overlap is such that 90% of the accuracy test regions, are also detected by the location test. For the details of the analysis see Appendix A and Gilron et al. [2016].

195 6 Discussion

196 We have set out to understand which of the tests is more powerful: the
197 accuracy test or the location test. Using simulations, we have concluded
198 that the location tests are preferable. We attribute this to the discretization
199 introduced in finite samples by the accuracy test statistic. This also explains
200 why an asymptotic analysis, such as Ramdas et al. [2016], did not find a
201 qualitative difference.

202 At this point some reservations to the generality of our findings are in
203 order. Firstly, not all accuracy tests are concerned with signal detection.
204 Indeed, it is possible that the purpose of the test is not to detect a differ-
205 ence between classes, but to actually test if a particular classifier is better
206 than chance. This would be the case, for instance, with brain-machine inter-
207 faces, where the detection of a signal is not enough [Olivetti et al., 2012]. In
208 such cases, the performance of a particular classifier is the object of study,
209 rendering the accuracy test the appropriate choice.

210 Secondly, there may be cases where the accuracy test does have more
211 power than the location test. Our simulations were unable to point out such
212 a scenario, but the fact that in our neuroimaging example (Section 5) some
213 brain regions were detected with the accuracy test, and not the location test,
214 suggest that the accuracy test does have more power for particular types of
215 signal. [TODO: signal in scale? heavy tails?]

216 A very important point is the ease of implementation. The need for cross
217 validation of the accuracy test greatly increases its computational complexity.
218 Moreover, anyone who has actually implemented tests with discrete statistics,
219 will attest they are considerably harder to implement. This is because their
220 unforgiveness to the type of inequality. Indeed, replacing a weak inequality
221 with a strong inequality may considerably change the results. This is not the
222 case for continuous test statistics.

223 Given all the above, we find the popularity of accuracy tests quite puz-
224 zling. We believe this is due to a reversal of the inference cascade. Re-
225 searchers first fit a classifier, and then ask if the classes are any different.
226 Were they to start by asking if classes are any different, and only then try
227 to classify, then location tests would naturally arise as the preferred method.
228 As put by Ramdas et al. [2016]:

229 The recent popularity of machine learning has resulted in the ex-
230 tensive teaching and use of prediction in theoretical and applied
231 communities and the relative lack of awareness or popularity of
232 the topic of Neyman-Pearson style hypothesis testing in the com-
233 puter science and related “data science” communities.

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298 A Analysis pipeline

299 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in
 300 Gilron et al. [2016]. Denoting by $i = 1, \dots, I$ the subject index, $v = 1, \dots, V$
 301 the voxel index, and $s = 1, \dots, S$ the permutation index. Since regions³ are
 302 centred around a unique voxel, the voxel index v also serves as a unique
 303 region index. Algorithm 1 computes a region-wise test statistic, which is
 304 compared to its permutation null distribution computed by Algorithm 2.

Algorithm 1: Compute a group parametric map.

Data: fMRI scans, and experimental design.

Result: Brain map of group statistics: $\{\bar{T}_v\}_{v=1}^V$

1 **for** $v \in 1, \dots, V$ **do**
 2 **for** $i \in 1, \dots, I$ **do**
 3 $T_{i,v} \leftarrow$ test statistic for subject i in a region centered at v .
 4 $\bar{T}_v \leftarrow \frac{1}{I} \sum_{i=1}^I T_{i,v}$.

Algorithm 2: Compute a permutation p-value map.

Data: fMRI scans of 20 subjects, experimental design.

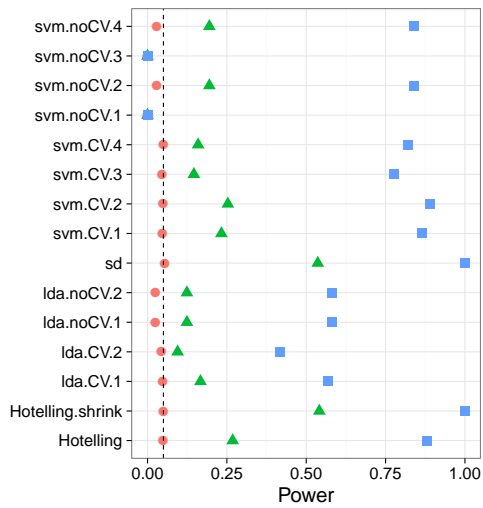
Result: Brain map of permutation p-values: $\{p_v\}_{v=1}^V$

1 **for** $s \in 1, \dots, S$ **do**
 2 permute labels;
 3 $\bar{T}_v^s \leftarrow$ parametric map

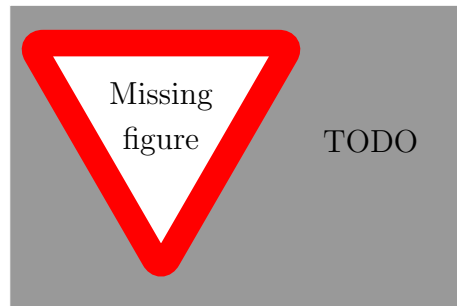
³*searchlight* or *sphere* in the MVPA parlance

B More Simulations

Figure 3: [TODO].



(a) 2 Folds.



(b) 20 Folds.

Figure 4: [TODO].

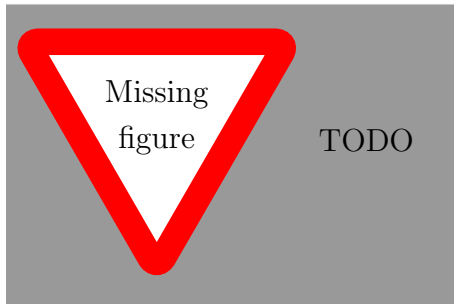


(a) Scale Change.

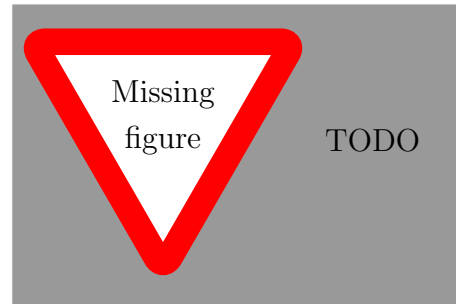


(b) t Null

Figure 5: [TODO].

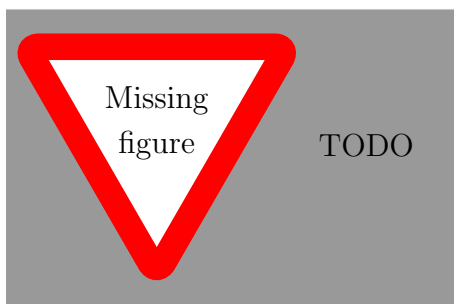


(a) Compound symmetry

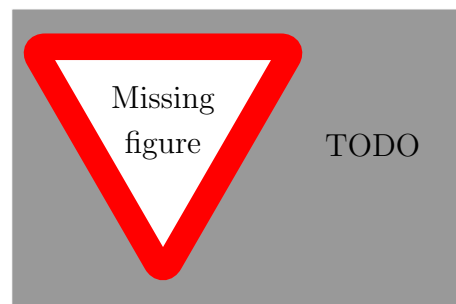


(b) AR(1)

Figure 6: [TODO].



(a) $n=400$



(b) ?