

Better-Than-Chance Classification for Signal Detection

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August 11, 2016

Abstract

[TODO]

1 Introduction

A common workflow in 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 neuroscientific literature include Golland and Fischl [2003], Pereira et al. [2009], Varoquaux et al. [2016], and especially the recently popularized *multivariate pattern analysis* (MVPA) framework of Kriegeskorte et al. [2006]. This practice is also observed in very high profile publications in the genetics literature: Golub et al. [1999], Slonim et al. [2000], Radmacher et al. [2002], Mukherjee et al. [2003], Juan and Iba [2004], Jiang et al. [2008].

To fix ideas, we will adhere to a concrete example. In Gilron et al. [2016], the authors seek to detect brain regions which encode differences between vocal and non-vocal stimuli. Following the MVPA 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*, or *pattern discrimination*.

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 is different given a vocal/non-vocal stimulus. As put in Pereira et al. [2009]:

26 ... the problem of deciding whether the classifier learned to dis-
 27 criminate the classes can be subsumed into the more general ques-
 28 tion as to whether there is evidence that the underlying distribu-
 29 tions of each class are equal or not.

30 A practitioner may then call upon a two-group location test such as Hotelling’s
 31 T^2 [Anderson, 2003]. Alternatively, if the size of a brain region is too large
 32 compared to the number of observations, so that the spatial covariance can-
 33 not be fully estimated, then a high dimensional version of Hotelling’s test can
 34 be called upon, such as in Schäfer and Strimmer [2005] or Srivastava [2013].
 35 For brevity, and in contrast to *accuracy tests*, we will call any two-sample
 36 multivariate tests simply *location tests*, also termed *class comparisons*.

37 At this point, it becomes unclear which is preferable: a location test or an
 38 accuracy test? The former with a heritage dating back to Hotelling [1931],
 39 and the latter being extremely popular, as the 959 citations¹ of Kriegeskorte
 40 et al. [2006] suggest.

41 The comparison between location and accuracy tests was precisely the
 42 goal of Ramdas et al. [2016], who compared the T^2 location test to the accu-
 43 racy of *Fisher’s linear discriminant analysis* classifier (LDA). By comparing
 44 the rates of convergence of the powers to 1, Ramdas et al. [2016] concluded
 45 that accuracy and location tests are rate equivalent.

46 Asymptotic relative efficiency measures (ARE) are typically used by statis-
 47 ticians to compare between test statistics with similar rates [van der Vaart,
 48 1998]. Ramdas et al. [2016] derive the asymptotic power functions of the
 49 two test statistics, which allow to extract the ARE between Hotelling’s T^2
 50 (location) test and Fisher’s LDA (accuracy) test. Using the Theorem 14.7 in
 51 van der Vaart [1998], we deduce that the ARE is lower bounded by $2\pi \approx 6.3$.
 52 This means that Fisher’s LDA requires at least 6.3 more samples to achieve
 53 the same (asymptotic) power than the T^2 test. In this light, the accuracy test
 54 is remarkably inefficient compared to the location test. For comparison, the
 55 t-test is only 1.04 more (asymptotically) efficient than Wilcoxon’s rank-sum
 56 test [Lehmann, 2009], so that an ARE of 2.5 is strong evidence in favor of
 57 the location test.

58 Before discarding accuracy tests as inefficient, we recall that Ramdas
 59 et al. [2016] analyzed a *half-sample* holdout. The authors conjectured that a
 60 leave-one-out approach, which makes more efficient use of the data, may have
 61 better performance. Also, the analysis in Ramdas et al. [2016] is asymptotic.
 62 This eschews the discrete nature of the accuracy statistic, which will be
 63 shown to have crucial impact. Since typical sample sizes in neuroscience are
 64 not large, we seek to study which test is to be preferred in finite samples?

¹GoogleScholar. Accessed on Aug 4, 2016.

65 Our conclusion will be quite simple: *location tests almost always have more*
 66 *power than accuracy tests.*

67 The main argument for our statement rests upon the observation that
 68 with typical sample sizes, the accuracy test statistic is highly discrete. Dis-
 69 crete test statistics are known to be conservative [Hemerik and Goeman,
 70 2014], since they are insensitive to mild perturbations of the data, and they
 71 cannot exhaust the permissible false positive rate. The degree of discretiza-
 72 tion is governed by the number of samples. In our neuroscience example
 73 from Gilron et al. [2016], the classification is performed based on 40 trials,
 74 so that the test statistic may assume only 40 possible values. This number
 75 of examples is not unusual if considering this is the number of subjects, or
 76 the number of trial-repeats in an neuroimaging study.

77 The discretization effect is aggravated if the test statistic is highly concen-
 78 trated. For an intuition consider the usage of a the *resubstitution accuracy*
 79 as a test statistic. This statistic simply means that the accuracy is not cross
 80 validated. If the data is high dimensional, the resubstitution accuracy will be
 81 very high due to over fitting. In a very high dimensional model, the resubsti-
 82 tution accuracy will be 1 for the observed data [McLachlan, 1976, Theorem
 83 1], but also for any permutation. The concentration of resubstitution accu-
 84 racy near 1, and its discreteness, render this test completely useless, with a
 85 power tending to 0 as the dimension of the model grows.

86 To compare the power of accuracy tests and location tests in finite sam-
 87 ples, we perform a simulation study of a battery of test statistics. The main
 88 findings are reported in Sections 4 and 5, and the intuition for our findings
 89 is provided in Section 6, but first, the problem’s setup.

90 2 Problem setup

91 Let $y \in \mathcal{Y}$ be a class encoding. Let $x \in \mathcal{X}$ be a p dimensional feature vector.
 92 In our vocal/non-vocal example we have $\mathcal{Y} = \{-1, 1\}$ and p , the number of
 93 voxels in a brain region so that $\mathcal{X} = \mathbb{R}^{27}$.

94 Given n pairs of (x_i, y_i) , typically assumed i.i.d., a location test amounts
 95 to testing whether $x|y = 1$ has the the same distribution as $x|y = -1$. I.e.,
 96 we test if the multivariate voxel activation pattern has the same distribution
 97 when given a vocal stimulus, as when given a non-vocal stimulus. An accu-
 98 racy test amounts to learning a predictive model $\hat{f}(x)$ from some assumed
 99 model class $\hat{f} \in \mathcal{F}$. The prediction accuracy, denoted $\mathcal{E}_{\hat{f}}$, is defined as the
 100 probability of a given classifier \hat{f} of making a correct prediction. Denoting
 101 by $I(A)$ the indicator function of the event A , we have $\mathcal{E}_{\hat{f}} := \mathbf{E} \left[I(\hat{f}(x) = y) \right]$

when given a randomly drawn data point, (x, y) . A statistically significant “better than chance” estimate of $\mathcal{E}_{\hat{f}}$ is evidence that the classes are distinct.

2.1 Candidate Tests

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

1. How to estimate accuracy?
2. Is the statistic cross validated or not?
3. For a K-fold cross validated test statistic: should the data be refolded in each permutation?
4. Permute labels of features?
5. For a K-fold cross validated test statistic: should the data folding be balanced (a.k.a. stratified)?
6. How many folds?

We will now address these questions while bearing in mind that unlike the typical supervised learning setup, we are not interested in an unbiased estimate of the prediction error, but rather in the mere detection of a difference between two groups.

How to estimate accuracy? Given a predictor \hat{f} , a natural test statistic is some estimate of its accuracy $\mathcal{E}_{\hat{f}}$. Complicating matters: very low accuracies, even 0, is evidence that the classes are separated, and we only need to invert the predictions. We can thus consider $|\mathcal{E}_{\hat{f}} - 0.5|$ as the test statistic. This, however, implies that if the classes are identical, random guessing has 0.5 accuracy. This is not true if the classes are not balanced. For unbalanced data the accuracy chance level is the probability of the majority class, we denote by \hat{p}_{max} [Golland et al., 2005, Sec 4.1]. This suggests the following test statistic $|\mathcal{E}_{\hat{f}} - \hat{p}_{max}|$. Since we will be aggregating these statistics over random data sets where \hat{p}_{max} may vary, it seems appropriate to standardize the scale of this statistic. We thus also consider the z-scored accuracy: $|\mathcal{E}_{\hat{f}} - \hat{p}_{max}| / \sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$.

131 **Cross validate or not?** Were we interested in an unbiased estimator of
132 the prediction error, there is no question that some independent validation
133 is in order. Since we are merely interested in detecting a difference between
134 classes, a biased error estimate is not an issue provided that bias is consistent
135 over all permutations. The underlying intuition is that if the exact same
136 computation is performed over all permutations, then a permutation test
137 will be “fair”, i.e., will not inflate the false positive rate. We will thus be
138 considering both cross validated accuracies, and resubstitution accuracies as
139 our test statistics, a.k.a. *resubstitution classification*.

140 **Refolding?** The standard practice in neuroimaging is to refold the data
141 after each permutation [Pereira et al., 2009]. This is imperative if permuting
142 labels while aiming at balanced data folds. This is not, however, imperative
143 in general. For simplicity, we will adhere to the standard practice of refolding
144 the data within each permutation.

145 **Permute labels of features?** While seemingly identical, the compound-
146 ing of permutations with data foldings renders these two approaches distinct.
147 As an example, consider balanced (stratified) K-fold cross validation where
148 the initial data folding is balanced. After a label permutation, the original
149 folds will probably not be balanced. If the *features* are permuted, then the
150 labels conserve their original fold assignments, and the original folds are bal-
151 anced after each permutation. Since we only report results while refolding
152 the data in each permutation, then the only difference between permuting
153 labels and permuting features seems to be a computational one. We thus
154 adhere to the more common, albeit computationally less efficient practice of
155 permuting labels.

156 **Balanced folding?** As already implied, a standard practice when cross
157 validating is to constrain the data folds to be balanced (i.e. stratified) [e.g.
158 Ojala and Garriga, 2010]. This is well justified when aiming at unbiased accu-
159 racy estimation. This also simplifies matter when aiming at signal detection,
160 as can be seen from the above discussion of the appropriate test statistic. On
161 the other hand, it may complicate matters, as can be seen from the above
162 discussion on label versus feature permutation. We will report results with
163 both balanced and unbalanced data foldings, only to discover, it does not
164 really matter.

165 **How many folds?** Different authors suggest different rules for the num-
166 ber of folds. We will be varying the number of folds. This will affect the

concentration of permutation distribution of the estimated accuracy, which will have a crucial effect on the conservativeness of the accuracy test. Our intuition suggests that since more folds imply a less concentrated estimate, then leave-one-out should be the less conservative, and 2-fold should be the most conservative.

The of tests we will be comparing is collected for convenience in Table 1.

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 and Strimmer [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 ($|\mathcal{E}_{\hat{f}} - \hat{p}_{max}|/\sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$, see Section 2.1). Another example is *lda.noCV.1*, which is Fisher’s LDA, returning the resubstitution accuracy, without cross validation, and without z-scoring.

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3 Controlling the False Positive Rate

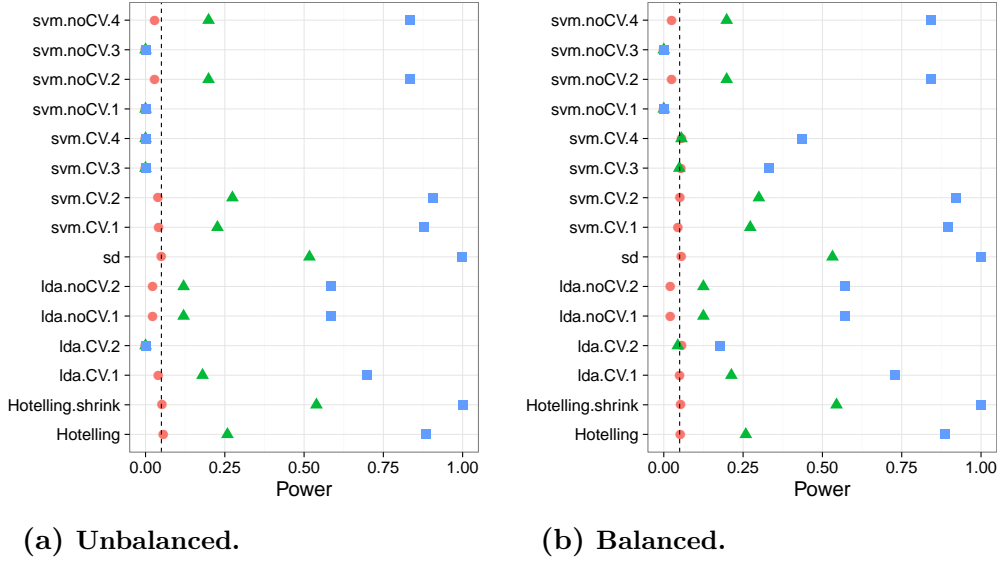
174

Figure 1 demonstrates that all of the tests considered conserve the desired 0.05 false positive rate, up to varying levels of conservatism. This can be seen from the fact that the probability of rejection is no larger than 0.05 in

177

the absence of any effect, encoded by a red circle. This is true, in particular if: (a) the folds are balanced or not, (b) the tuning parameters of some test statistic are varied, (d) the number of folds is varied. We also observe that the most conservative tests are the resubstitution accuracy measures. We return to this matter in the Discussion.

Figure 1: The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. The various statistics on the y axis. Their details are given in Table 1. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square). Simulation details in Appendix B. Cross-validation was performed with balanced (stratified) and unbalanced data folding. See sub-captions.



4 Power

Having established that all of the tests in our battery control the false positive rate, it remains to be seen if they have similar power— especially when comparing the power of location tests to accuracy tests. From the simulation results reported in Appendix C we collect the following insights:

1. Location tests have more power than accuracy tests in all our configurations.

- 190 2. The conservativeness decays as the sample grows (Figures 8a, 8b and
191 9a), suggesting that either concentration or discretization is responsible
192 for power loss.
- 193 3. The power may increase or decrease with the number of folds (Figure 5).
- 194 4. The z-scoring of the accuracies was introduced to deal with unbalanced
195 foldings. If the z-scoring has any effect at all, it merely kills power.
196 There is really no reason to use it.
- 197 5. Both accuracy and location tests are inappropriate for scale alternatives
198 (Figure 7a). This was to be expected and is reported mostly as a sanity
199 check.
- 200 6. The presence of heavy tails (Figure 7b) may reduce power, but does
201 not quantitatively change results.
- 202 7. Balanced folding typically has no effect. It increased power only for
203 the z-scored statistics (Figure 1). This is surprising given they were
204 precisely designed to deal with the presence of imbalance.
- 205 8. Varying the accuracy test's tuning parameter, such as the cost (i.e.
206 margins) has no effect on the power of the test.
- 207 9. Correlation between coordinates, mimicking temporal correlation in
208 fMRI data, has no effect on conclusions, since all test statistics account
209 for this correlation (Figure 9b).

210 The major insight from simulations is that the use of accuracy tests for
211 signal detection is underpowered compared to location tests. We now verify
212 this finding on a neuroimaging dataset.

213 5 Neuroimaging Example

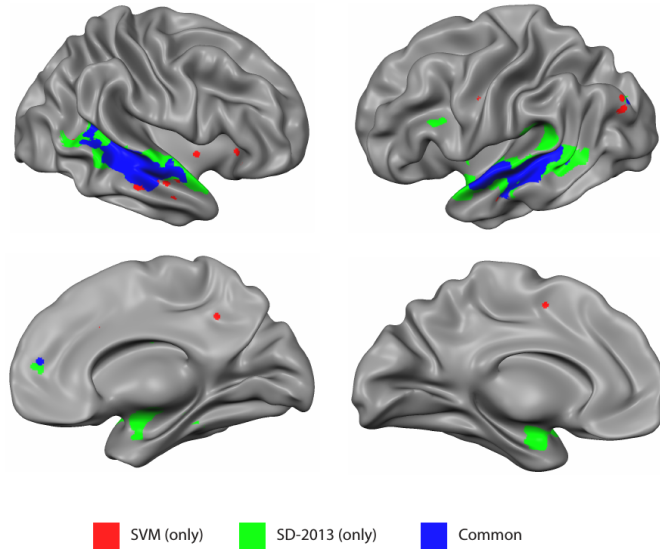
214 Figure 2 is an application of both a location and an accuracy test to the data
215 of Pernet et al. [2015]. The authors of Pernet et al. [2015] collected fMRI
216 data while subjects were exposed to the sounds of human speech (vocal),
217 and other non-vocal sounds. Each subject was exposed to 20 sounds of each
218 type, totaling in $n = 40$ trials in each scan. The study was rather large and
219 consisted of about 200 subjects. The data was kindly made available by the
220 authors at the OpenfMRI website².

²<https://openfmri.org/>

221 We perform group inference using within-subject permutations using the
 222 pipeline of Stelzer et al. [2013], which was also reported in Gilron et al. [2016].
 223 For completeness, the pipeline is described in Appendix A. To demonstrate
 224 our point, we compare the *sd* location test with the *svm.cv.1* accuracy test
 225 (see Table 1 for the definition of these statistics).

226 In agreement with our simulation results, the location test (*sd*) discovers
 227 more brain regions when compared to an accuracy test (*svm.cv.1*). The
 228 former discovers 1,232 regions, while the latter only 441, as depicted in
 229 Figure 2. We emphasize that both test statistics were compared with the
 230 same permutation scheme, and the same error controls, so that any difference
 231 in detections is due to their different power.

232 Having established that accuracy tests are underpowered both in simula-
 233 tion and in application, we wish to identify the conditions under which this
 234 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 centers 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, 399 of which are common to both. For the details of the analysis see Appendix A and Gilron et al. [2016].*

235 6 Discussion

236 We have set out to understand which of the tests is more powerful: the ac-
237 curacy test or the location test. Using simulations, we have concluded that
238 the location tests are preferable. Their high dimensional versions such as
239 Srivastava [2013] and Schäfer and Strimmer [2005] are preferable for typical
240 neuroimaging problems such as MVPA. We attribute this to several phe-
241 nomena: (a) Discretization introduced in finite samples by the accuracy test
242 statistic. (b) Inefficient use of the data for the validation holdout set. In our
243 high dimensional setup, we also confirmed that high-dimensional versions of
244 the T^2 test, such as Srivastava [2013] or Schäfer and Strimmer [2005] are
245 preferable over the original T^2 .

246 The sensitivity of the power to the number of folds suggests that most
247 of the power is lost due to the discretization and not to the holdout. The
248 degree of discretization is governed by the sample size. For this reason, an
249 asymptotic analysis such as Ramdas et al. [2016] may uncover the holdout
250 inefficiency, but will not uncover the discretization effect. The practical ad-
251 vice for the practitioner, is that for the purpose of signal detection, there
252 is typically a multivariate test (be it a location test or other), that is more
253 powerful than an accuracy test. There is also a good chance that it would
254 be easier to implement, since no validation will be involved.

255 6.1 Ease of implementation

256 A very important point is the ease of implementation. The need for cross
257 validation of the accuracy test greatly increases its computational complexity.
258 Moreover, anyone who has actually implemented tests with discrete statistics,
259 will attest they are considerably harder to implement. This is because their
260 unforgiveness to the type of inequality. Indeed, mistakenly replacing a weak
261 inequality with a strong inequality in one's program may considerably change
262 the results. This is not the case for continuous test statistics.

263 6.2 A good accuracy test

264 In Section 6.6 we discuss cases where an accuracy test cannot replace a
265 location test. For such cases we collect some conclusions from our simulations
266 on the best practices for accuracy tests.

- 267 1. The conservativeness due to discretization decreases with sample size.
- 268 2. Cross validating the accuracy statistic increases power in moderate
269 sample sizes. The power loss due to the holdout inefficiency is smaller

- 270 than the power loss due to the concentration of the resubstitution ac-
 271 curacy. For large sample sizes, discretization and concentration have
 272 weaker effects, and the cross validated accuracy may be replaced with
 273 the computationally more efficiency resubstitution accuracy.
- 274 3. Permuting features is easier than permuting labels. It allows to preserve
 275 balanced folds after a permutation without refolding, thus reducing
 276 computational complexity.
 - 277 4. There is no gain in z-scoring the accuracy scores.
 - 278 5. Cross validated accuracy with balanced folds has more power than un-
 279 balanced folds. We currently have no intuition to offer for this phe-
 280 nomenon.
 - 281 6. It is unclear what is the effect of the number of folds. More folds in-
 282 crease power by reducing the number of holdout samples. On the other
 283 hand, it increases the concentration of the accuracy statistic. Com-
 284 pounded with the discreteness of the accuracy statistic, this decreases
 285 power.
 - 286 7. The value of the tuning parameters of a classifier have little to no
 287 effect.

288 6.3 Smoothing accuracy estimates

289 It may be possible to alleviate the effect of discretization by appropriate cross-
 290 validation. The discreteness of the accuracy statistic can be “smoothed” by
 291 allowing the test sample to be drawn with replacement. The *bootstrap* may
 292 seem like a candidate approach, but since the original data always serves as
 293 a test set, the accuracy can still only assume $1/n$ values. This is not the case,
 294 however, for the *leave-one-out bootstrap estimator* (B-LOO) and the *0.632*
 295 *bootstrap estimator* (B-0.632) [Hastie et al., 2003, Sec 7.11], which we define
 296 below for completeness. By the same rational, the degree of conservatism
 297 should decrease with the number of bootstrap samples.

Definition 1 (B-LOO). Denoting by $C^{(i)}$ the index set of bootstrap samples,
 b , where observation i is not in the train set, *leave-one-out bootstrap* estimate
 is defined as:

$$\mathcal{E}_{BLOO} := \frac{1}{n} \sum_{i=1}^n \frac{1}{|C^{(i)}|} \sum_{b \in C^{(i)}} I(\hat{f}^b(x_i) = y_i).$$

Equivalently, denoting by $S^{(b)}$ the indexes of observations, i , that are not in the bootstrap train sample b ,

$$\mathcal{E}_{BLOO} := \frac{1}{B} \sum_{b=1}^B \frac{1}{|S^{(b)}|} \sum_{i \in S^{(b)}} I(\hat{f}^b(x_i) = y_i).$$

Definition 2 (B-0.632). Denoting by \mathcal{E}_{resub} the resubstitution accuracy estimate, the B-0.632 accuracy estimator, $\mathcal{E}_{0.632}$, is defined as

$$\mathcal{E}_{0.632} := 0.368 \mathcal{E}_{resub} + 0.632 \mathcal{E}_{BLOO}.$$

298 The simulation results reported in Figure 3, with naming conventions in
 299 Table 2. It can be seen that selecting test sets with replacement does increase
 300 the power, when compared to V-fold cross validation, but still falls short from
 301 the power of location tests. It can also be seen that power increases with the
 302 number of Bootstrap replications, itself reducing the level of discretization.
 303 The type of Bootstrap, B-LOO versus B-0.632, does not change the power.
 304 Again, consistent with the observation that it is discretization that drives
 305 the power loss.

Name	Basis	Boot Type	B	Accuracy	Parameters
lda.Boot.1	LDA	B-0.632	10	accuracy	—
lda.Boot.2	LDA	B-LOO	10	accuracy	—
svm.Boot.1	SVM	B-0.632	10	accuracy	cost=1e1
svm.Boot.2	SVM	B-LOO	10	accuracy	cost=1e1
svm.Boot.3	SVM	B-0.632	50	accuracy	cost=1e1
svm.Boot.4	SVM	B-LOO	50	accuracy	cost=1e1

Table 2: The same as Table 1 for bootstrapped accuracy estimates. B-LOO and B-0.632 are defined in definitions 1 and 2 respectively. B denotes the number of Bootstrap samples.

307 6.4 High dimensional classifiers

308 It is known that when $p > n$ Hotelling’s T^2 , and Fisher’s LDA are not
 309 computable. In our simulations, in which $p = 23$ and $n = 40$ is “almost”
 310 high dimensional, but still allows to compute both tests. We have simulated
 311 two high dimensional versions of Hotelling’s T^2 : *sd* [Srivastava, 2013] and
 312 *Hotelling.shrink* [Schäfer and Strimmer, 2005]. The former solves the dimen-
 313 sionality problem by assuming independence over coordinates, and the latter

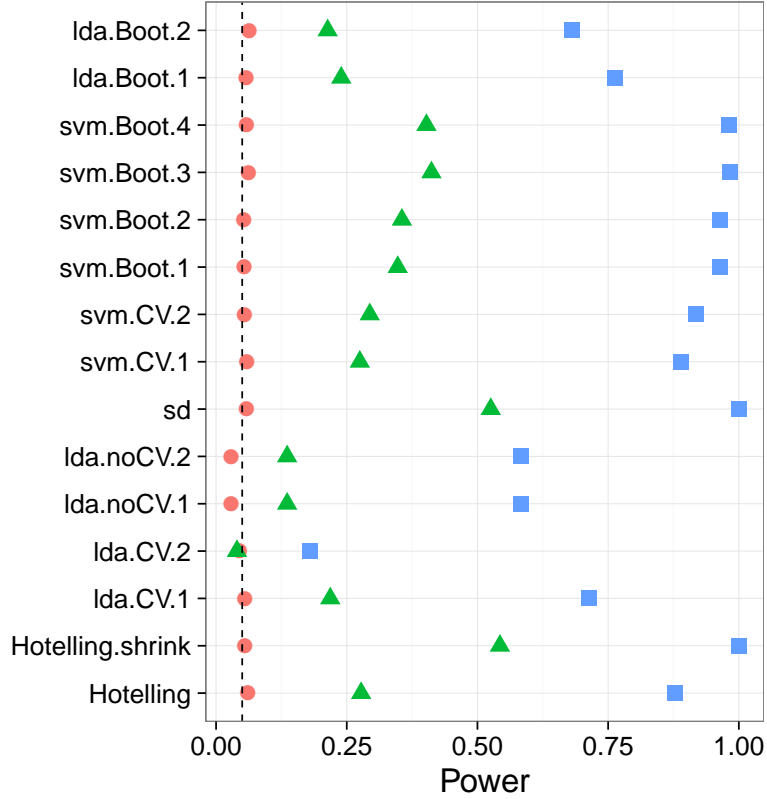


Figure 3: *Bootstrap: The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. The various statistics on the y axis. Their details are given in tables 1 and 2. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square). Simulation details in Appendix B.*

by Tikhonov regularization of the covariance, a-la ridge regression. The corresponding high dimensional accuracy tests would be a *naive Bayes* classifier, and l_2 regularized SVM [Ramdas et al., 2016]. We conjecture that they would not alter our conclusions, since the main force driving the conservatism is discretization, which they do not solve.

6.5 Related Literature

Olivetti et al. [2012] and Olivetti et al. [2014] looked into the problem of choosing a good accuracy test. They propose a new test they call an *independence test*, and demonstrate by simulation that it has more power than

other accuracy tests, and can deal with non-balanced data sets. We did not include this test in the battery we compared, but we note the following: (a) The independence test of Olivetti et al. [2012] relies on a discrete test statistic. This means that in the cases that the accuracy test is called upon for discriminating populations, it will probably be underpowered compared to location tests. (b) In contrast with the underlying motivation of Olivetti et al. [2012]’s independence test, we did not find that balancing the data folds is crucial for an accuracy test.

Golland et al. [2005] study accuracy tests using simulation, neuroimaging data, genetic data, and analytically. Their analytic results formalize our intuition from Section 1 on the effect of concentration of the accuracy statistic: The finite Vapnik–Chervonenkis (VC) dimension requirement [Golland and Fischl, 2003, Sec 4.3] prevents the permutation p-value from (asymptotically) concentrating. They also find that the power decreases with the level of discretization of the statistic. This is seen in their Figure 4, where the size of the test-set, K , governs the discretization. Since they permute features, and not labels, then all their permutation samples are balanced, and there is no issue of refolding.

Golland et al. [2005] simulate the power of an accuracy test using a multivariate Gaussian mixture, with a parameter p governing the separation between classes. Under their model $(x_i|y_i = 1) \sim p\mathcal{N}(\mu_1, I) + (1 - p)\mathcal{N}(\mu_2, I)$ and $(x_i|y_i = -1) \sim (1 - p)\mathcal{N}(\mu_1, I) + p\mathcal{N}(\mu_2, I)$. Varying p interpolates between the null distribution ($p = 0.5$) and a location shift model ($p = 0$). We perform the same simulation as Golland et al. [2005], after reparametrizing p so that $p = 0$ corresponds to the null model, and $p = 23$ to be comparable to our other simulations. We find that in this mixture class of models, like the location class of models, a location test has more power than an accuracy test (Figure 4).

6.6 Reservations

Some reservations to the generality of our findings are in order. Firstly, not all accuracy tests are concerned with signal detection. Consider brain decoding for machine interfaces, and clinical diagnosis, where the presence of a medical condition is predicted from imaging data [e.g. Olivetti et al., 2012, Wager et al., 2013]. In those examples, the purpose of the test is not to detect a difference between classes, but to actually test the performance of a particular classifier. As put by Ojala and Garriga [2010]:

...these tests study whether the classifier is using the described properties and not whether the plain data contain such properties.

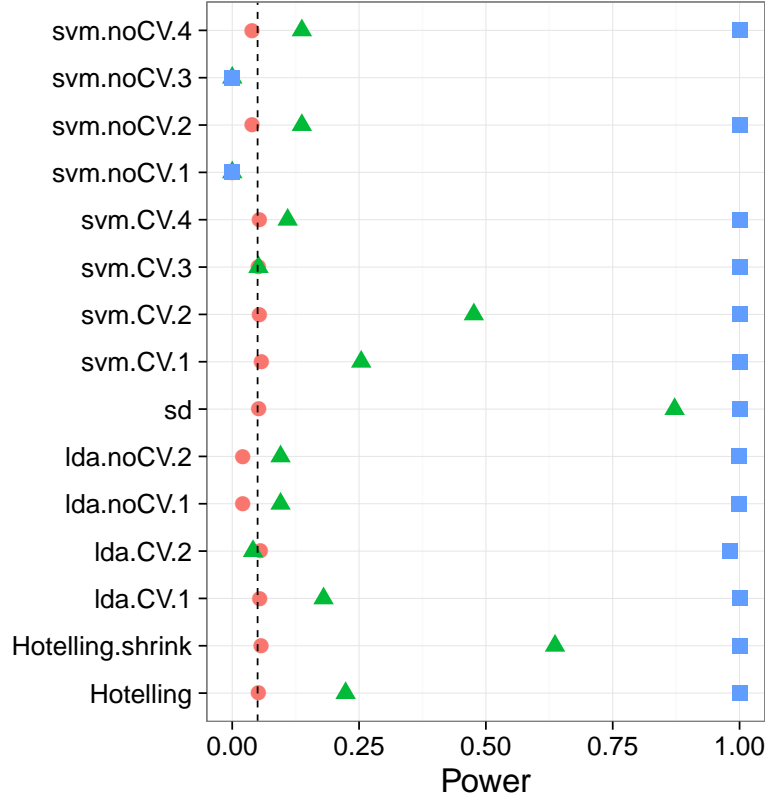


Figure 4: **Mixture:** $\mathbf{x}_i = \chi_i \mu + \eta_i$; $\chi_i = \{-1, 1\}$ and $\text{Prob}(\chi_i = 1) = (1/2 - p)^{y_i^*} (1/2 + p)^{1 - y_i^*}$. μ is a p -vector with $3/\sqrt{p}$ in all coordinates. The effect, p , is color and shape coded and varies over 0 (red circle), $1/4$ (green triangle) and $1/2$ (blue square).

361 For studying the characteristics of a population represented by
 362 the data, standard statistical test could be used.

363 This is because classification is harder than detection. We may be able
 364 to detect a difference between classes, but not be able to classify examples
 365 significantly better than chance.

366 Secondly, it may be argued that accuracy tests permits the separation
 367 between classes in high dimensions, such as in *reproducing kernel Hilbert*
 368 *spaces* (RKHS) by using non-linear predictors. This is a false argument—
 369 accuracy test do not have any more flexibility than location tests. Indeed, it
 370 is possible to test for location in the same dimension the classifier is learned.
 371 Gretton et al. [2012] is an example where the test for location is performed
 372 in the RKHS of the data. It is also possible to test for the equality of two
 373 multivariate distributions without specifying any a-priori alternative [e.g. ?]).

374 On the other hand, based on our reported neuroimaging example, and others,
375 we find that a location test in the original feature space is indeed a simple
376 and powerful approach to signal detection.

377 6.7 Epilogue

378 Given all the above, we find the popularity of accuracy tests quite puzzling.
379 We believe this is due to a reversal of the inference cascade. Researchers
380 first fit a classifier, and then ask if the classes are any different. Were they
381 to start by asking if classes are any different, and only then try to classify,
382 then location tests would naturally arise as the preferred method. As put by
383 Ramdas et al. [2016]:

384 The recent popularity of machine learning has resulted in the ex-
385 tensive teaching and use of prediction in theoretical and applied
386 communities and the relative lack of awareness or popularity of
387 the topic of Neyman-Pearson style hypothesis testing in the com-
388 puter science and related “data science” communities.

389 And more simply by Frank Harrell in the CrossValidated Q&A site³:

390 ... your use of proportion classified correctly as your accuracy
391 score. This is a discontinuous improper scoring rule that can be
392 easily manipulated because it is arbitrary and insensitive.

393 7 Acknowledgments

³[http://stats.stackexchange.com/questions/17408/
how-to-assess-statistical-significance-of-the-accuracy-of-a-classifier](http://stats.stackexchange.com/questions/17408/how-to-assess-statistical-significance-of-the-accuracy-of-a-classifier).

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504 A Analysis pipeline

505 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in
 506 Gilron et al. [2016]. Denoting by $i = 1, \dots, I$ the subject index, $v = 1, \dots, V$
 507 the voxel index, and $s = 1, \dots, S$ the permutation index. Since regions⁴ are
 508 centered around a unique voxel, the voxel index v also serves as a unique
 509 region index. Algorithm 1 computes a region-wise test statistic, which is
 510 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
```

⁴*searchlight* or *sphere* in the MVPA parlance

513 B Simulation Details

514 The following details are common to all the reported simulations, unless stated
515 otherwise in a figure’s caption. The R code for the simulations can be found
516 in [TODO].

517 Each simulation is based on 4,000 replications. In each replication, we
518 generate n i.i.d. samples from a shift model $\mathbf{x}_i = \mu \mathbf{y}_i^* + \eta_i$. Where $y_i^* = \{0, 1\}$
519 is the class of subject i in dummy coding. Recalling that $y_i = \{-1, 1\}$ is the
520 class in effect coding, then clearly $y_i = 2y_i^* - 1$. The noise is distributed as
521 $\eta_i \sim \mathcal{N}_p(0, \Sigma)$. The sample size $n = 40$. The dimension of the data is $p = 23$.
522 The covariance $\Sigma = I$. Effects, i.e. shifts μ , are equal coordinate p -vectors
523 with coordinates that vary over $\mu \in \{0, 1/4, 1/2\}$.

524 Having generated the data, we compute each of the test statistics in Ta-
525 ble 1. For test statistics that require data folding, we used 8 folds. We then
526 compute a permutation p-value by permuting the class labels, and recomput-
527 ing each test statistic. We perform 400 such permutations. We then reject
528 the $\mu_i = 0$ null hypothesis if the permutation p-value is smaller than 0.05.
529 The reported power is the proportion of replication where the permutation
530 p-value falls below 0.05.

C Simulation Results

Figure 5: Simulation details in Appendix B except the changes in the sub-captions.



(a) 2-fold cross validation.
Balanced folding.



(b) 20-fold cross validation.
Balanced folding

Figure 6: *Simulation details in Appendix B except the changes in the sub-captions.*

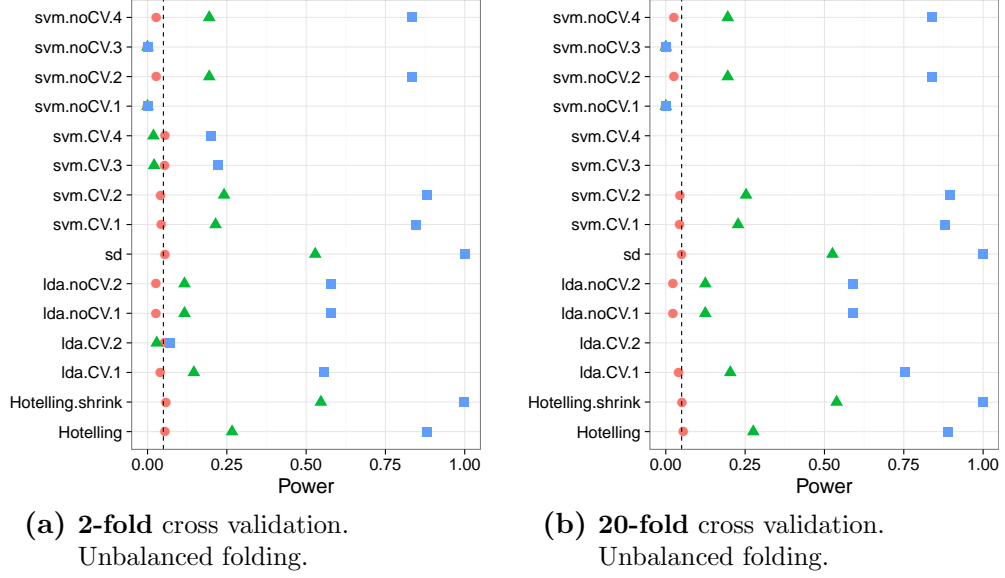
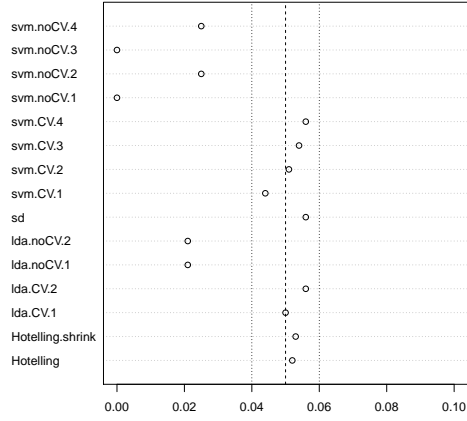


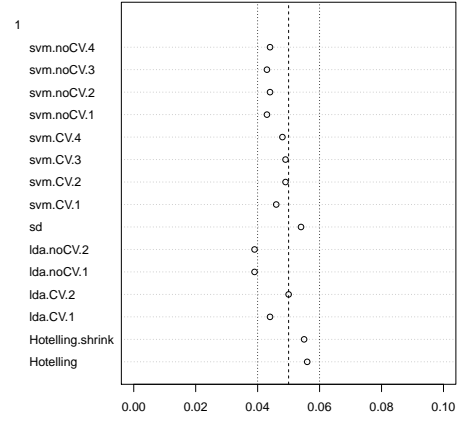
Figure 7: *Simulation details in Appendix B except the changes in the sub-captions.*



Figure 8: *Simulation details in Appendix B except the changes in the sub-captions.*

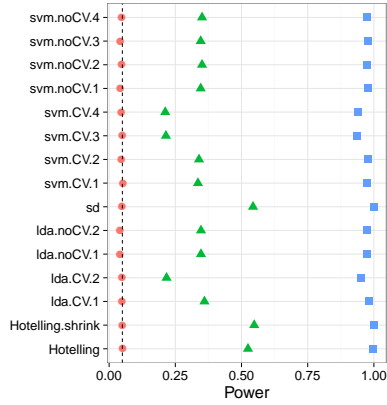


(a) **Low-Dimension:** False positive rates for $n = 40$.

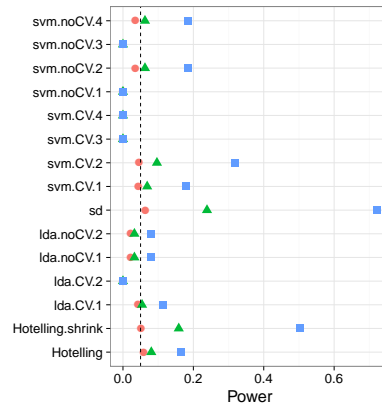


(b) **High-Dimension:** False positive rates for $n = 400$.

Figure 9: *Simulation details in Appendix B except the changes in the sub-captions.*



(a) **High-Dimension, local alternative:**
 $n = 400$,
 $\mu \in \frac{1}{\sqrt{10}} \times \{0, 1/4, 1/2\}$.



(b) **AR(1) dependence:**
 $\Sigma_{k,l} = \rho^{|k-l|}; \rho = 0.8$.