

# Better-Than-Chance Classification for Signal Detection

Jonathan Rosenblatt      Roei Gilron      Roy Mukamel

August 30, 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 some 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 thus approach the signal detection problem with a two-  
 31 group population test such as Hotelling’s  $T^2$  [Anderson, 2003]. Alternatively,  
 32 if the size of brain region of interest is large compared to the number of  
 33 observations, so that the spatial covariance cannot be fully estimated, then  
 34 a high dimensional version of Hotelling’s test can be called upon, such as  
 35 in Schäfer and Strimmer [2005] or Srivastava [2007]. For brevity, and in  
 36 contrast to *accuracy tests*, we will call any two-sample multivariate tests  
 37 simply *population tests*, a.k.a. *class comparisons*. [TODO: rename population  
 38 test to parameter test?]

39 At this point, it becomes unclear which is preferable: a population test or  
 40 an accuracy test? The former with a heritage dating back to Hotelling [1931],  
 41 and the latter being extremely popular, as the 959 citations<sup>1</sup> of Kriegeskorte  
 42 et al. [2006] suggest.

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

48 Asymptotic relative efficiency measures (ARE) are typically used by statis-  
 49 ticians to compare between rate-equivalent test statistics [van der Vaart,  
 50 1998]. Ramdas et al. [2016] derive the asymptotic power functions of the  
 51 two test statistics, which allows to compute the ARE between Hotelling’s  $T^2$   
 52 (population) test and Fisher’s LDA (accuracy) test. Theorem 14.7 of van der  
 53 Vaart [1998] relates asymptotic power functions to ARE. Using this theorem  
 54 and the results of Ramdas et al. [2016] we deduce that the ARE is lower  
 55 bounded by  $2\pi \approx 6.3$ . This means that Fisher’s LDA requires at least 6.3  
 56 more samples to achieve the same (asymptotic) power than the  $T^2$  test. In  
 57 this light, the accuracy test is remarkably inefficient compared to the pop-  
 58 ulation test. For comparison, the t-test is only 1.04 more (asymptotically)  
 59 efficient than Wilcoxon’s rank-sum test [Lehmann, 2009], so that an ARE of  
 60 6.3 is strong evidence in favor of the population test.

61 Before discarding accuracy tests as inefficient, we recall that Ramdas  
 62 et al. [2016] analyzed a *half-sample* holdout. The authors conjectured that a  
 63 leave-one-out approach, which makes more efficient use of the data, may have  
 64 better performance. Also, the analysis in Ramdas et al. [2016] is asymptotic.

---

<sup>1</sup>GoogleScholar. Accessed on Aug 4, 2016.

65 This eschews the discrete nature of the accuracy statistic, which will be  
66 shown to have crucial impact. Since typical sample sizes in neuroscience are  
67 not large, we seek to study which test is to be preferred in finite samples?  
68 Our conclusion will be quite simple: *population tests typically have more*  
69 *power than accuracy tests, and are easier to implement.*

70 Our statement rests upon the observation that with typical sample sizes,  
71 the accuracy test statistic is highly discrete. Permutation testing with dis-  
72 crete test statistics are known to be conservative [Hemerik and Goeman,  
73 2014], since they are insensitive to mild perturbations of the data, and they  
74 cannot exhaust the permissible false positive rate. As simply put by Frank  
75 Harrell in `CrossValidated`<sup>2</sup> post back in 2011:

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

79 The degree of discretization is governed by the number of samples. In our  
80 neuroscience example from Gilron et al. [2016], the classification is performed  
81 based on 40 trials, so that the test statistic may assume only 40 possible  
82 values. This number of examples is not unusual if considering this is the  
83 number of trial-repeats, or the number of subjects, in an neuroimaging study.

84 The discretization effect is aggravated if the test statistic is highly concen-  
85 trated. For an intuition consider the usage of a the *resubstitution accuracy*  
86 as a test statistic. This statistic simply means that the accuracy is not cross  
87 validated, but rather evaluated on the training data. If the data is high  
88 dimensional, the resubstitution accuracy will be very high due to over fit-  
89 ting. In a very high dimensional regime, the resubstitution accuracy will  
90 be 1 for the observed data [McLachlan, 1976, Theorem 1], but also for any  
91 permutation. The concentration of resubstitution accuracy near 1, and its  
92 discreteness, render this test completely useless, with power tending to 0 for  
93 any (fixed) effect size, as the dimension of the model grows.

94 To compare the power of accuracy tests and population tests in finite  
95 samples, we study a battery of test statistics by means of simulation. We start  
96 with formalizing the problem in Section 2. The main findings are reported  
97 in Sections 4, 5 and Appendix C. A discussion follows in Section 6.

---

<sup>2</sup>A Q&A website for statistical questions: <http://stats.stackexchange.com/questions/17408/how-to-assess-statistical-significance-of-the-accuracy-of-a-classifier>

## 98 2 Problem setup

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

102 Given  $n$  pairs of  $(x_i, y_i)$ , typically assumed i.i.d., a population test amounts  
 103 to testing whether  $x|y = 1$  has the the same distribution as  $x|y = -1$ . I.e.,  
 104 we test if the multivariate voxel activation pattern has the same distribution  
 105 when given a vocal stimulus, as when given a non-vocal stimulus.

An accuracy test amounts to learning a predictive model and testing if its  
 predictions  $y|x$  are better than chance. Denoting a dataset by  $\mathcal{S} := (x_i, y_i)_{i=1}^n$ ,  
 the a predictor,  $\mathcal{A}_{\mathcal{S}}(x) : \mathcal{X} \rightarrow \mathcal{Y}$ , is the output of a learning algorithm  $\mathcal{A}$  when  
 applied to the dataset  $\mathcal{S}$ , so that  $\mathcal{A} : \mathcal{S} \rightarrow \mathcal{A}_{\mathcal{S}}(x)$ . The accuracy of predictor,  
 $\mathcal{E}_{\mathcal{A}_{\mathcal{S}}(x)}$ , is defined as the probability of  $\mathcal{A}_{\mathcal{S}}(x)$  making a correct prediction.  
 The accuracy of an algorithm,  $\mathcal{E}_{\mathcal{A}}$ , is defined as the expected accuracy over  
 all possible data sets. Formally– denoting by  $\mathcal{P}$  the probability measure of  
 $(x, y)$ , and by  $\mathcal{P}^n$  the same for the i.i.d sample  $\mathcal{S}$ , then

$$\mathcal{E}_{\mathcal{A}_{\mathcal{S}}(x)} := \int_{(x,y)} \mathcal{I}\{\mathcal{A}_{\mathcal{S}}(x) = y\} d\mathcal{P}(x, y), \quad (1)$$

and

$$\mathcal{E}_{\mathcal{A}} := \int_{\mathcal{S}} \mathcal{E}_{\mathcal{A}_{\mathcal{S}}} d\mathcal{P}^n(\mathcal{S}). \quad (2)$$

106 Denoting an estimate of  $\mathcal{E}_{\mathcal{A}_{\mathcal{S}}(x)}$  by  $\hat{\mathcal{E}}_{\mathcal{A}_{\mathcal{S}}(x)}$ , and  $\mathcal{E}_{\mathcal{A}}$  by  $\hat{\mathcal{E}}_{\mathcal{A}}$ , a statistically sig-  
 107 nificant “better than chance” estimate of either, is evidence that the classes  
 108 are distinct. In a typical application, the predictor is not fixed, so that  $\hat{\mathcal{E}}_{\mathcal{A}}$ ,  
 109 and not  $\hat{\mathcal{E}}_{\mathcal{A}_{\mathcal{S}}(x)}$ , will be used for the testing.

110 Two popular estimates of  $\hat{\mathcal{E}}_{\mathcal{A}}$  are the *resubstitution estimate*, and the  
 111 V-fold cross validation (CV) estimate.

**Definition 1** (Resubstitution estimate). The resubstitution accuracy esti-  
 mator,  $\hat{\mathcal{E}}_{\mathcal{A}}^{Resub}$ , is defined as

$$\hat{\mathcal{E}}_{\mathcal{A}}^{Resub} := \frac{1}{n} \sum_{i=1}^n \mathcal{I}\{\mathcal{A}_{\mathcal{S}}(x_i) = y_i\}, \quad (3)$$

112 where  $\mathcal{I}\{A\}$  is the indicator function of event  $A$ .

**Definition 2** (V-fold CV estimate). Denoting by  $\mathcal{S}^v$  the  $v$ 'th partition, or *fold*, of the dataset, and by  $\mathcal{S}^{(v)}$  its complement, so that  $\mathcal{S}^v \cup \mathcal{S}^{(v)} = \cup_{v=1}^V \mathcal{S}^v = \mathcal{S}$ , the V-fold CV accuracy estimator,  $\hat{\mathcal{E}}_{\mathcal{A}}^{Vfold}$ , is defined as

$$\hat{\mathcal{E}}_{\mathcal{A}}^{Vfold} := \frac{1}{V} \sum_{v=1}^V \frac{1}{|\mathcal{S}^v|} \sum_{i \in \mathcal{S}^v} \mathcal{I}\{\mathcal{A}_{\mathcal{S}^{(v)}}(x_i) = y_i\}, \quad (4)$$

## 113 2.1 Candidate Tests

114 The design of a permutation test using  $\hat{\mathcal{E}}_{\mathcal{A}}$  requires the following design  
115 choices:

- 116 1. Is  $\hat{\mathcal{E}}_{\mathcal{A}}$  cross validated or not?
- 117 2. For a V-fold cross validated test statistic:
  - 118 (a) Should the data be refolded in each permutation?
  - 119 (b) Should the data folding be balanced (a.k.a. stratified)?
  - 120 (c) How many folds?
- 121 3. How to estimate  $\hat{\mathcal{E}}_{\mathcal{A}}$ ?

122 We will now address these questions while bearing in mind that unlike  
123 the typical supervised learning setup, we are not interested in an unbiased  
124 estimate of  $\mathcal{E}_{\mathcal{A}}$ , but rather in the detection of its departure from chance level.

125 **Cross validate or not?** Given our goal, a biased estimate of  $\hat{\mathcal{E}}_{\mathcal{A}}$  is not a  
126 problem provided that bias is consistent over all permutations. The under-  
127 lying intuition is that a permutation test will be unbiased, provided that the  
128 exact same computation is performed over all permutations. We will thus be  
129 considering both cross validated accuracies, and resubstitution accuracies.

130 **Balanced folding?** The standard practice when cross validating is to con-  
131 strain the data folds to be balanced, i.e. stratified [e.g. Ojala and Garriga,  
132 2010]. This means that each fold has the same number of examples from  
133 each class. We will report results with both balanced and unbalanced data  
134 foldings, only to discover, it does not seem to matter.

135 **Refolding?** The standard practice in neuroimaging is to permute labels  
136 and refold the data after each permutation, so that the balance of the classes  
137 in each fold is preserved. We will adhere to this practice due to its popularity,  
138 even though it can be avoided by permuting features instead of labels, as done  
139 by Golland et al. [2005].

140 **How many folds?** Different authors suggest different rules for the number  
 141 of folds. We will look into the effect of the number of folds.

**How to estimate accuracy?** Lower than 0.5 accuracies, known as *anti-learning*, are evidence that signal is present and classes are separated. Given out detection purposes, we should consider the departure from chance level  $|\hat{\mathcal{E}}_{\mathcal{A}} - 0.5|$  as candidate test statistic. For unbalanced classes, chance level is not 0.5, but rather the the probability of the majority class, which we denote by  $\hat{\mathcal{E}}_{Maj}$ . This suggests the following test statistic  $|\hat{\mathcal{E}}_{\mathcal{A}} - \hat{\mathcal{E}}_{Maj}|$ . Since we will be aggregating these statistics over random data sets where  $\hat{\mathcal{E}}_{Maj}$  may vary, it seems appropriate to standardize the scale. We thus study, along with the naive accuracy estimate,  $\hat{\mathcal{E}}_{\mathcal{A}}$ , also the *z-scored accuracy* of algorithm  $\mathcal{A}$ :

$$\hat{\mathcal{Z}}_{\mathcal{A}} := \frac{|\hat{\mathcal{E}}_{\mathcal{A}} - \hat{\mathcal{E}}_{Maj}|}{\sqrt{\hat{\mathcal{E}}_{Maj}(1 - \hat{\mathcal{E}}_{Maj})}}. \quad (5)$$

142 Table 1 collects an initial battery of tests we will be comparing.

Name	Algorithm	Accuracy	Z-scored	Parameters
Hotelling	Hotelling	—	—	—
Hotelling.shrink	Hotelling	—	—	—
sd	Hotelling	—	—	—
lda.CV.1	LDA	V-fold	FALSE	—
lda.CV.2	LDA	V-fold	TRUE	—
lda.noCV.1	LDA	Resubstitution	FALSE	—
lda.noCV.2	LDA	Resubstitution	TRUE	—
svm.CV.1	SVM	V-fold	FALSE	cost=10
svm.CV.2	SVM	V-fold	FALSE	cost=0.1
svm.CV.3	SVM	V-fold	TRUE	cost=10
svm.CV.4	SVM	V-fold	TRUE	cost=0.1
svm.noCV.1	SVM	Resubstitution	FALSE	cost=10
svm.noCV.2	SVM	Resubstitution	FALSE	cost=0.1
svm.noCV.3	SVM	Resubstitution	TRUE	cost=10
svm.noCV.4	SVM	Resubstitution	TRUE	cost=0.1

Table 1: This table collects the various test statistics we will be studying. Three are population 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 from 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 (implemented with the *svm* R function [Meyer et al., 2015]), the cost parameter set at 0.1, and using the cross validated z-scored accuracy in Eq. 5. Another example is *lda.noCV.1*, which is Fisher’s LDA, returning the resubstitution accuracy.

143

### 144 3 Controlling the False Positive Rate

145 Our simulations show that all of the tests considered conserve the desired  
146 0.05 false positive rate, up to varying levels of conservatism. This can be  
147 seen from the fact that the probability of rejection is no larger than 0.05 in  
148 the absence of any effect, encoded by a red circle. This is true, in particular  
149 if:

- 150 (a) The folds are balanced or not (Figures 5,6 and 7).
- 151 (b) The tuning parameters are varied (cost=10 versus cost=0.1).
- 152 (c) The number of folds is varied (Figures 6 and 7).
- 153 (d) The noise is heavytailed (Figure 8b).

- 154 (e) The problem is high or low dimensional (Figure 9.)
- 155 (f) The noise is correlated (Figure 10b).
- 156 We also observe that the most conservative tests are the resubstitution ac-
- 157 curacy statistics. We return to this matter in the Discussion.

## 158 4 Power

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

- 163 1. Population tests have no less— and typically more— power than accuracy  
 164 tests in our simulations.
- 165 2. The conservativeness of accuracy tests decays as the sample grows (Fig-  
 166 ures 9a, 9b and 10a)
- 167 3. For heavy tailed distributions (Figure 8b), the difference in power be-  
 168 tween population tests and accuracy tests vanishes.
- 169 4. Regularization is critical to power as can be seen by comparing *Hotelling*  
 170 to *Hotelling.shrink* and *sd*.
- 171 5. The z-scoring of the accuracies was introduced to deal with unbalanced  
 172 foldings. If the z-scoring has any effect at all, it merely kills power. The  
 173 non-z-scored accuracy tests are unaffected by the balance of the folding.
- 174 6. Both accuracy and population tests are inappropriate for scale alter-  
 175 natives (Figure 8a). This was to be expected and is reported mostly as  
 176 a sanity check (cost=10 vs. cost=0.1 statistics).
- 177 7. Balanced folding only affects the z-scored accuracy, in the opposite  
 178 direction than we anticipated.
- 179 8. Increasing the SVM’s cost parameter, which reduces the number of  
 180 support vectors entering the classifier, reduces power.

181 The major insight from simulations is that the use of accuracy tests for  
 182 signal detection is underpowered compared to population tests. We have not  
 183 established, however, that the dominance of the population tests is not due to  
 184 their regularization. Indeed, the unregularized *Hotelling* test, is only slightly  
 185 superior to the accuracy tests. We return to this matter in Section 6.4, by  
 186 adding some regularized accuracy tests to our battery. We now verify our  
 187 finding on a neuroimaging dataset.



## 188 5 Neuroimaging Example

189 Figure 1 is an application of both a population and an accuracy test to the  
190 data of Pernet et al. [2015]. The authors of Pernet et al. [2015] collected fMRI  
191 data while subjects were exposed to the sounds of human speech (vocal), and  
192 other non-vocal sounds. Each subject was exposed to 20 sounds of each type,  
193 totaling in  $n = 40$  trials. The study was rather large and consisted of about  
194 200 subjects. The data was kindly made available by the authors at the  
195 OpenfMRI website<sup>3</sup>.

196 We perform group inference using within-subject permutations along the  
197 analysis pipeline of Stelzer et al. [2013], which was also reported in Gilron  
198 et al. [2016]. For completeness, the pipeline is described in Appendix A. To  
199 demonstrate our point, we compare the *sd* population test with the *svm.cv.1*  
200 accuracy test.

201 In agreement with our simulation results, the population test (*sd*) dis-  
202 covers more brain regions of interest when compared to an accuracy test  
203 (*svm.cv.1*). The former discovers 1,232 regions, while the latter only 441, as  
204 depicted in Figure 1. We emphasize that both test statistics were compared  
205 with the same permutation scheme, and the same error controls, so that any  
206 difference in detections is due to their different power.

## 207 6 Discussion

208 We have set out to understand which of the tests is more powerful: accu-  
209 racy tests or population tests. No amount of simulations can replace the  
210 insight provided by a closed-form analytic result. The finite sample power  
211 of permutation tests is a formidable mathematical problem, so we currently  
212 content ourselves with simulations. We have concluded that the population  
213 tests are typically preferable. Their high dimensional versions, such as Sri-  
214 vastava [2007] and Schäfer and Strimmer [2005], are particularly well suited  
215 for neuroimaging problems such as MVPA. We attribute this to several ef-  
216 fects:

- 217 (a) The discrete nature of the accuracy test in finite samples.
- 218 (b) Inefficient use of the data when validating with a holdout set.
- 219 (c) The lack of regularization in high SNR regimes (high dimension and/or  
220 strong correlations).

221  
222 The degree of discretization is governed by the sample size. For this  
223 reason, an asymptotic analysis such as Ramdas et al. [2016] may uncover

---

<sup>3</sup><https://openfmri.org/>



*Figure 1:* 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 population 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 population 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].

224 the holdout inefficiency, but will not uncover the discretization effect. An  
 225 asymptotic analysis of a finite complexity model, such as [Golland et al.,  
 226 2005, Sec 4.3], would also fail to reveal the effect of the concentration of the  
 227 resubstitution accuracy near 1. This effect would render the resubstitution  
 228 estimates a legitimate asymptotic test, and a terrible finite sample test.

229 Simulations do show cases where population tests have no advantage over  
 230 accuracy tests. One such scenario is when the noise is heavytailed, as seen  
 231 in Figure 8b. The second scenario will be discussed in Section 6.4.

232 The practical advice for the practitioner, is that for the purpose of signal  
 233 detection, there is typically a population test that is more powerful than an  
 234 accuracy test. The class of population tests we examined, in particular their  
 235 regularized versions, are good performers in a wide range of simulation setups  
 236 and empirically. They are also typically easier to implement, and faster to  
 237 run, since no cross validation will be involved.

## 238 6.1 Ease of implementation

239 A very important consideration is the ease of implementation. The need  
240 for cross validation of the accuracy test greatly increases its computational  
241 complexity. Moreover, programming with discrete statistics is more prone to  
242 errors. This is because their unforgiveness to the type of inequalities used.  
243 Indeed, mistakenly replacing a weak inequality with a strong inequality in  
244 one’s program may considerably change the results. This is not the case for  
245 continuous test statistics.

## 246 6.2 Reservations

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

254 Secondly, it may be argued that accuracy tests permits the separation  
255 between classes in high dimensions, such as in *reproducing kernel Hilbert*  
256 *spaces* (RKHS) by using non-linear predictors while population tests do not.  
257 This is a false argument— accuracy test do not have any more flexibility  
258 that population tests. Indeed, it is possible to test for location in the same  
259 space the classifier is learned. For independence tests in high dimensional  
260 spaces see for example Székely and Rizzo [2009] or Gretton et al. [2012].  
261 On the other hand, based on our experience, and the reported neuroimaging  
262 example, we find that a population test in the original feature space is a  
263 simple and powerful approach to signal detection.

## 264 6.3 Smoothing accuracy estimates

265 It may be possible to alleviate the effect of discretization by via the cross-  
266 validation scheme. The discreteness of the accuracy statistic is governed by  
267 the number of examples in the union of holdout test sets, over all retesting  
268 iterations. For V-fold CV, for instance, the accuracy may assume as many  
269 values as the sample size. This suggests that the accuracy can be “smoothed”  
270 by allowing the test sample to be drawn with replacement. An algorithm that  
271 samples test sets with replacement is the *leave-one-out bootstrap estimator*,  
272 and its derivatives, such as the *0.632 bootstrap*, and *0.632+ bootstrap* [Hastie  
273 et al., 2003, Sec 7.11].

**Definition 3** (bLOO). The *leave-one-out bootstrap* estimate, bLOO, is the average accuracy of the holdout observations, over all bootstrap samples. Denote by  $\mathcal{S}^b$ , a bootstrap sample  $b$  of size  $n$ , sampled with replacement from  $\mathcal{S}$ . Also denote by  $C^{(i)}$  the index set of bootstrap samples,  $b$ , not containing observation  $i$ . The leave-one-out bootstrap estimate,  $\hat{\mathcal{E}}_{\mathcal{A}}^{bLOO}$ , is defined as:

$$\hat{\mathcal{E}}_{\mathcal{A}}^{bLOO} := \frac{1}{n} \sum_{i=1}^n \frac{1}{|C^{(i)}|} \sum_{b \in C^{(i)}} \mathcal{I}\{\mathcal{A}_{\mathcal{S}^b}(x_i) = y_i\}. \quad (6)$$

where  $|A|$  is the cardinality of set  $A$ . Equivalently [TODO: verify], denoting by  $S^{(b)}$  the indexes of observations,  $i$ , that are *not* in the bootstrap sample  $b$  and are not empty,

$$\hat{\mathcal{E}}_{\mathcal{A}}^{bLOO} = \frac{1}{B} \sum_{b=1}^B \frac{1}{|S^{(b)}|} \sum_{i \in S^{(b)}} \mathcal{I}\{\mathcal{A}_{\mathcal{S}^b}(x_i) = y_i\}. \quad (7)$$

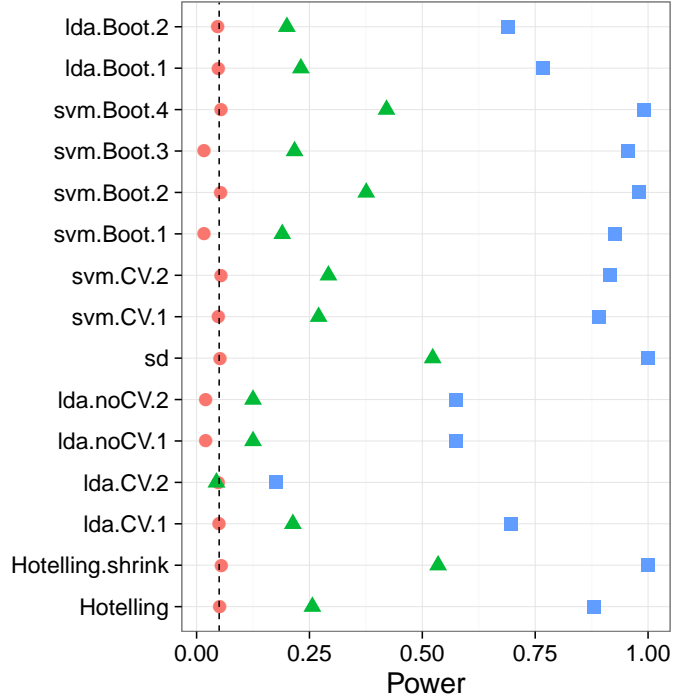
**Definition 4** (b0.632). The *0.632 bootstrap* accuracy estimate, b0.632, is a wighted average of the resubstitution error and the bLOO. Formally:

$$\hat{\mathcal{E}}_{\mathcal{A}}^{0.632} := 0.368 \hat{\mathcal{E}}_{\mathcal{A}}^{Resub} + 0.632 \hat{\mathcal{E}}_{\mathcal{A}}^{bLOO}. \quad (8)$$

Simulation results reported in Figure 2 with naming conventions in Table 2. It can be seen that selecting test sets with replacement does increase the power, when compared to V-fold cross validation, but still falls short from the power of population tests. It can also be seen that power increases with the number of bootstrap replications, as was to be expected, since more replications reduce the level of discretization. The type of bootstrap, bLOO versus b0.632, does not change the power.

Name	Algorithm	Accuracy	B	Z-scored	Parameters
lda.Boot.1	LDA	b0.632	10	FALSE	—
lda.Boot.2	LDA	bLOO	10	FALSE	—
svm.Boot.1	SVM	b0.632	10	FALSE	cost=10
svm.Boot.2	SVM	bLOO	10	FALSE	cost=10
svm.Boot.3	SVM	b0.632	50	FALSE	cost=10
svm.Boot.4	SVM	bLOO	50	FALSE	cost=10

Table 2: The same as Table 1 for bootstrapped accuracy estimates. bLOO and b0.632 are defined in definitions 3 and 4 respectively.  $B$  denotes the number of Bootstrap samples.



*Figure 2: 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.

## 6.4 High dimensional classifiers

Inspecting Figure 5a (for instance), it can be seen that Hotelling’s unregularized  $T^2$  test has similar power as accuracy tests. It should thus be argued that the real advantage of the population tests is due to their adaptation to high dimension by regularization, and not only to discretization. To study this, we call upon several *regularized classifiers*, designed for high dimensional problems. In the spirit of the regularized covariance of *Hotelling.shrink*, we try an  $l_2$  regularized SVM [?], and shrinkage based LDA [Pang et al., 2009, Ramey et al., 2016]. In the spirit of the diagonalized covariance of *sd*, we try a diagonalized LDA [Dudoit et al., 2002], a.k.a. *Gaussian naïve Bayes*.

Simulation results reported in Figure 3 with naming conventions in Table 3. It can be seen that regularizing a classifier in high dimension, just like a parameter test, improves power. It can also be seen that (regularized) parameter tests are still more powerful than (regularized) accuracy tests. This was to be expected, since we already saw in (e.g.) Figure 5a that the unregularized parameter test, *Hotelling*, is slightly more powerful than unregularized

298 accuracy tests such as (e.g.) *svm.CV.1*.

299 We can compound the regularization with the bootstrapping from Sec-  
 300 tion 6.3, to improve finite sample power of the accuracy tests. This is done in  
 301 the *svm.highdim.2* and *lda.highdim.4* tests. The latter being one of the very  
 302 few accuracy tests that achieve the same power as population tests. This is  
 303 exciting news since it shows how to design powerful new high-powered accu-  
 304 racy tests: by sampling test sets with replacement, and by regularizing the  
 305 classifiers.

Name	Algorithm	Accuracy	Z-scored	Parameters
svm.highdim.1	SVM	V-fold	FALSE	cost=10, V=4
svm.highdim.2	SVM	b0.632	FALSE	cost=10, B=50
lda.highdim.1	LDA	V-fold	FALSE	V=4
lda.highdim.2	LDA	V-fold	FALSE	V=4
lda.highdim.3	LDA	V-fold	FALSE	V=4
lda.highdim.4	LDA	b0.632	FALSE	B=50

Table 3: The same as Table 1 for regularized (high dimensional) predic-  
 tors. *svm.highdim.1* is an  $l_2$  regularized SVM [Friedman et al., 2010].  
*svm.highdim.2* is the same with b0.632 instead of V-fold cross valida-  
 tion. *lda.highdim.1* is the Diagonal Linear Discriminant Analysis of  
 Dudoit et al. [2002]. *lda.highdim.2* is the High-Dimensional Regular-  
 ized Discriminant Analysis of Ramey et al. [2016]. *lda.highdim.3* is the  
 Shrinkage-based Diagonal Linear Discriminant Analysis of Pang et al.  
 [2009]. *lda.highdim.4* is the same with b0.632.

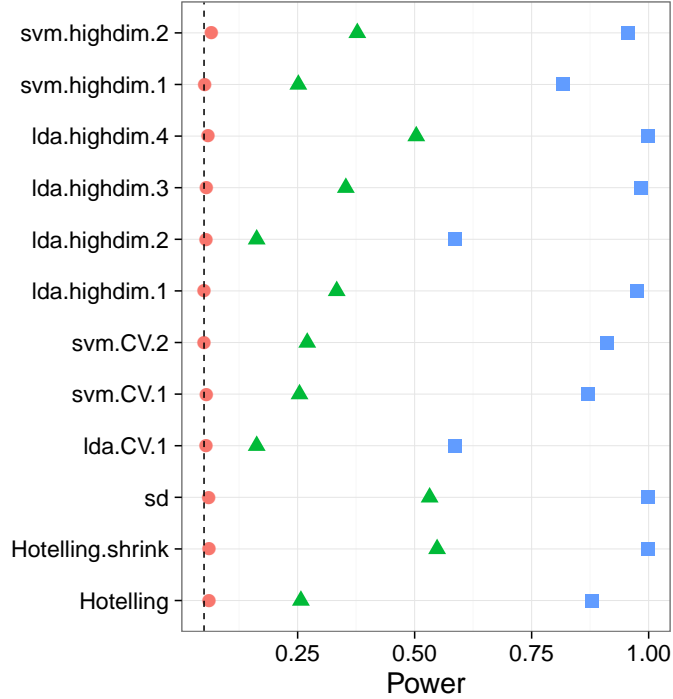
306

## 307 6.5 A good accuracy test

308 For the cases a population test cannot replace an accuracy test, we collect  
 309 some conclusions and best practices.

310 **Sample size.** The conservativeness of accuracy tests decrease with sample  
 311 size.

312 **Regularize.** Regularization proves crucial to detection power in low signal  
 313 to noise regimes: in high dimension and/or in the presence of strong correla-  
 314 tions. We find that the Shrinkage-based Diagonal Linear Discriminant Anal-  
 315 ysis of Pang et al. [2009] is a particularly good performer, but more research



*Figure 3: HighDim Classifier*— 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 3. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square). Simulation details in Appendix B.

316 is required on this matter. We also conjecture that the power-maximizing  
317 regularization is larger than the error-minimizing regularization.

318 **Smooth accuracy.** Smooth accuracy estimate by cross validating with  
319 replacement. The bLOO estimator, in particular, is preferable over V-fold.

320 **Permute features.** Permuting features, such as in Golland et al. [2005], is  
321 easier than permuting labels. It allows to preserve the balance of folds after  
322 a permutation, without refolding.

323 **Resubstitution accuracy in low dimension.** Resubstitution accuracy  
324 is useful in low SNR regimes, such as low dimensional problems, because it  
325 avoids cross validation without compromising power. In high dimension, the  
326 power loss is considerable compared to a cross validated approach. We at-  
327 tribute this to the compounding of discretization and concentration effects:  
328 the difference between the sampling distribution of the resubstitution accu-

329 racy is simply indistinguishable under the null and under the alternative.  
 330 In low dimensional problems, the discretization is less impactful, and the  
 331 computational burden of cross validation can be avoided by using the resub-  
 332 stitution accuracy. There is a fundamental difference between V-folding and  
 333 resubstitution. The latter should not be thought of as the limit of the former.

334 **Don’t z-score.** There is no gain in z-scoring the accuracy scores. Our  
 335 motivating rational was clearly flawed. [TODO: why?]

## 336 6.6 Related Literature

337 Ojala and Garriga [2010] study the power of two accuracy tests differing in  
 338 the permutation scheme: One testing the “no signal” null hypothesis, and  
 339 the other testing the “independent features” null hypothesis. They perform  
 340 an asymptotic analysis, and a simulation study. They also apply various  
 341 classifiers to various data sets. Their emphasis is the effect of the underlying  
 342 classifier on the power, and the potential of the “independent features” test  
 343 for feature selection. This is a very different emphasis from our own.

344 Olivetti et al. [2012] and Olivetti et al. [2014] looked into the problem  
 345 of choosing a good accuracy test. They propose a new test they call an  
 346 *independence test*, and demonstrate by simulation that it has more power  
 347 than other accuracy tests, and can deal with non-balanced data sets. We did  
 348 not include this test in the battery we compared, but we note the following:  
 349 (a) The independence test of Olivetti et al. [2012] relies on a discrete test  
 350 statistic. It may probably be improved with the methods discussed in this  
 351 section, before the application of Olivetti et al. [2012]’s independence test.  
 352 (b) In contrast with the underlying motivation of Olivetti et al. [2012]’s  
 353 independence test, we did not find that balancing the data folds affects the  
 354 power of the test.

355 Golland and Fischl [2003] and Golland et al. [2005] study accuracy tests  
 356 using simulation, neuroimaging data, genetic data, and analytically. Their  
 357 analytic results formalize our intuition from Section 1 on the effect of concen-  
 358 tration of the accuracy statistic: The finite Vapnik–Chervonenkis dimension  
 359 requirement [Golland et al., 2005, Sec 4.3] prevents the permutation p-value  
 360 from (asymptotically) concentrating near 1. Like ourselves, they also find  
 361 that the power increases with the size of the test set. This is seen in Fig.4 of  
 362 Golland et al. [2005], where the size of the test-set,  $K$ , governs the discretiza-  
 363 tion. Since they permute features, not labels, then all their permutation  
 364 samples are balanced, and there is no issue of refolding.

Golland et al. [2005] simulate the power of accuracy tests by sampling  
 from a Gaussian mixture family of models, and not from a location family



as our own simulations. Under their model

$$(x_i|y_i = 1) \sim p\mathcal{N}(\mu_1, I) + (1 - p)\mathcal{N}(\mu_2, I)$$

and

$$(x_i|y_i = -1) \sim (1 - p)\mathcal{N}(\mu_1, I) + p\mathcal{N}(\mu_2, I).$$

365 Varying  $p$  interpolates between the null distribution ( $p = 0.5$ ) and a location  
 366 shift model ( $p = 0$ ). We now perform the same simulation as Golland et al.  
 367 [2005], after parameterizing  $p$  so that  $p = 0$  corresponds to the null model,  
 368 and in the same dimensionality as our previous simulations We find that also  
 369 in this mixture class of models a population test has more power than an  
 370 accuracy test (Figure 4).

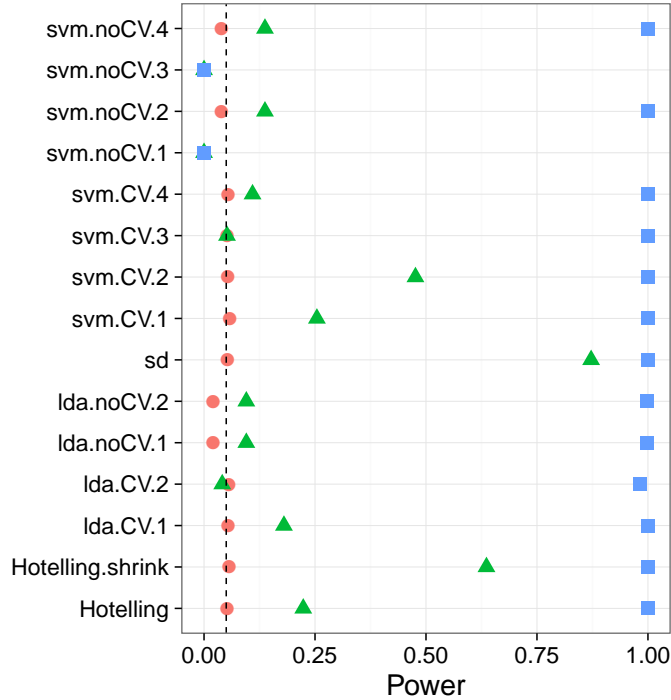


Figure 4: **Mixture**—  $\mathbf{x}_i = \chi_i \mu + \eta_i$ ;  $\chi_i = \{-1, 1\}$  and  $\text{Prob}(\chi_i = 1) = (1/2 - p)^{\mathbf{y}_i^*} (1/2 + p)^{1 - \mathbf{y}_i^*}$ .  $\mu$  is a  $p$ -vector with  $3/\sqrt{p}$  in all coordinates. The effect,  $p$ , is color and shape coded and varies over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

## 371 6.7 Epilogue

372 Given all the above, we find the popularity of accuracy tests for signal de-  
 373 tection quite puzzling. We believe this is due to a reversal of the inference

374 cascade. Researchers first fit a classifier, and then ask if the classes are  
375 any different. Were they to start by asking if classes are any different, and  
376 only then try to classify, then population tests would naturally arise as the  
377 preferred method. As put by Ramdas et al. [2016]:

378       The recent popularity of machine learning has resulted in the ex-  
379       tensive teaching and use of prediction in theoretical and applied  
380       communities and the relative lack of awareness or popularity of  
381       the topic of Neyman-Pearson style hypothesis testing in the com-  
382       puter science and related “data science” communities.

## 383   **7 Acknowledgments**

## References

- T. W. Anderson. *An Introduction to Multivariate Statistical Analysis*. Wiley-Interscience, Hoboken, NJ, 3 edition edition, July 2003. ISBN 978-0-471-36091-9.
- Y. Benjamini and Y. Hochberg. Controlling the false discovery rate: a practical and powerful approach to multiple testing. *JOURNAL-ROYAL STATISTICAL SOCIETY SERIES B*, 57:289–289, 1995.
- S. Dudoit, J. Fridlyand, and T. P. Speed. Comparison of Discrimination Methods for the Classification of Tumors Using Gene Expression Data. *Journal of the American Statistical Association*, 97(457):77–87, Mar. 2002. ISSN 0162-1459. doi: 10.1198/016214502753479248.
- J. Friedman, T. Hastie, and R. Tibshirani. Regularization Paths for Generalized Linear Models via Coordinate Descent. *Journal of Statistical Software*, 33(1):1–22, 2010.
- R. Gilron, J. Rosenblatt, O. Koyejo, R. A. Poldrack, and R. Mukamel. Quantifying spatial pattern similarity in multivariate analysis using functional anisotropy. *arXiv:1605.03482 [q-bio]*, May 2016.
- P. Golland and B. Fischl. Permutation tests for classification: towards statistical significance in image-based studies. In *IPMI*, volume 3, pages 330–341. Springer, 2003.
- P. Golland, F. Liang, S. Mukherjee, and D. Panchenko. Permutation Tests for Classification. In P. Auer and R. Meir, editors, *Learning Theory*, number 3559 in Lecture Notes in Computer Science, pages 501–515. Springer Berlin Heidelberg, June 2005. ISBN 978-3-540-26556-6 978-3-540-31892-7. doi: 10.1007/11503415\_34.
- T. R. Golub, D. K. Slonim, P. Tamayo, C. Huard, M. Gaasenbeek, J. P. Mesirov, H. Coller, M. L. Loh, J. R. Downing, M. A. Caligiuri, C. D. Bloomfield, and E. S. Lander. Molecular Classification of Cancer: Class Discovery and Class Prediction by Gene Expression Monitoring. *Science*, 286(5439):531–537, Oct. 1999. ISSN 0036-8075, 1095-9203. doi: 10.1126/science.286.5439.531.
- A. Gretton, K. M. Borgwardt, M. J. Rasch, B. Schölkopf, and A. Smola. A Kernel Two-sample Test. *J. Mach. Learn. Res.*, 13:723–773, Mar. 2012. ISSN 1532-4435.

- 418 T. Hastie, R. Tibshirani, and J. Friedman. *The Elements of Statistical Learn-*  
419 *ing*. Springer, July 2003. ISBN 0-387-95284-5.
- 420 J. Hemerik and J. Goeman. Exact testing with random permutations.  
421 *arXiv:1411.7565 [math, stat]*, Nov. 2014.
- 422 H. Hotelling. The Generalization of Student’s Ratio. *The Annals of Math-*  
423 *ematical Statistics*, 2(3):360–378, Aug. 1931. ISSN 0003-4851, 2168-8990.  
424 doi: 10.1214/aoms/1177732979.
- 425 W. Jiang, S. Varma, and R. Simon. Calculating confidence intervals for  
426 prediction error in microarray classification using resampling. *Statistical*  
427 *Applications in Genetics and Molecular Biology*, 7(1), 2008.
- 428 L. Juan and H. Iba. Prediction of tumor outcome based on gene expression  
429 data. *Wuhan University Journal of Natural Sciences*, 9(2):177–182, Mar.  
430 2004. ISSN 1007-1202, 1993-4998. doi: 10.1007/BF02830598.
- 431 N. Kriegeskorte, R. Goebel, and P. Bandettini. Information-based functional  
432 brain mapping. *Proceedings of the National Academy of Sciences of the*  
433 *United States of America*, 103(10):3863–3868, July 2006. ISSN 0027-8424,  
434 1091-6490. doi: 10.1073/pnas.0600244103.
- 435 E. L. Lehmann. Parametric versus nonparametrics: two alternative method-  
436 ologies. *Journal of Nonparametric Statistics*, 21(4):397–405, 2009. ISSN  
437 1048-5252. doi: 10.1080/10485250902842727.
- 438 G. J. McLachlan. The bias of the apparent error rate in discriminant analysis.  
439 *Biometrika*, 63(2):239–244, Jan. 1976. ISSN 0006-3444, 1464-3510. doi:  
440 10.1093/biomet/63.2.239.
- 441 D. Meyer, E. Dimitriadou, K. Hornik, A. Weingessel, and F. Leisch. *e1071:*  
442 *Misc Functions of the Department of Statistics, Probability Theory Group*  
443 *(Formerly: E1071), TU Wien*. 2015. R package version 1.6-7.
- 444 S. Mukherjee, P. Tamayo, S. Rogers, R. Rifkin, A. Engle, C. Campbell,  
445 T. R. Golub, and J. P. Mesirov. Estimating dataset size requirements  
446 for classifying DNA microarray data. *Journal of Computational Biology:*  
447 *A Journal of Computational Molecular Cell Biology*, 10(2):119–142, 2003.  
448 ISSN 1066-5277. doi: 10.1089/106652703321825928.
- 449 M. Ojala and G. C. Garriga. Permutation Tests for Studying Classifier Perfor-  
450 mance. *Journal of Machine Learning Research*, 11(Jun):1833–1863, 2010.  
451 ISSN 1533-7928.

- 452 E. Olivetti, S. Greiner, and P. Avesani. Induction in Neuroscience with  
 453 Classification: Issues and Solutions. In G. Langs, I. Rish, M. Grosse-  
 454 Wentrup, and B. Murphy, editors, *Machine Learning and Interpretation*  
 455 *in Neuroimaging*, number 7263 in Lecture Notes in Computer Science,  
 456 pages 42–50. Springer Berlin Heidelberg, 2012. ISBN 978-3-642-34712-2  
 457 978-3-642-34713-9. doi: 10.1007/978-3-642-34713-9\_6.
- 458 E. Olivetti, S. Greiner, and P. Avesani. Statistical independence for the  
 459 evaluation of classifier-based diagnosis. *Brain Informatics*, 2(1):13–19, Dec.  
 460 2014. ISSN 2198-4018, 2198-4026. doi: 10.1007/s40708-014-0007-6.
- 461 H. Pang, T. Tong, and H. Zhao. Shrinkage-based Diagonal Discriminant  
 462 Analysis and Its Applications in High-Dimensional Data. *Biometrics*, 65  
 463 (4):1021–1029, Dec. 2009. ISSN 1541-0420. doi: 10.1111/j.1541-0420.2009.  
 464 01200.x.
- 465 F. Pereira, T. Mitchell, and M. Botvinick. Machine learning classifiers and  
 466 fMRI: A tutorial overview. *NeuroImage*, 45(1, Supplement 1):S199–S209,  
 467 Mar. 2009. ISSN 1053-8119. doi: 10.1016/j.neuroimage.2008.11.007.
- 468 C. R. Pernet, P. McAleer, M. Latinus, K. J. Gorgolewski, I. Charest, P. E. G.  
 469 Bestelmeyer, R. H. Watson, D. Fleming, F. Crabbe, M. Valdes-Sosa, and  
 470 P. Belin. The human voice areas: Spatial organization and inter-individual  
 471 variability in temporal and extra-temporal cortices. *NeuroImage*, 119:164–  
 472 174, Oct. 2015. ISSN 1053-8119. doi: 10.1016/j.neuroimage.2015.06.050.
- 473 M. D. Radmacher, L. M. McShane, and R. Simon. A Paradigm for  
 474 Class Prediction Using Gene Expression Profiles. *Journal of Computa-*  
 475 *tional Biology*, 9(3):505–511, June 2002. ISSN 1066-5277. doi: 10.1089/  
 476 106652702760138592.
- 477 A. Ramdas, A. Singh, and L. Wasserman. Classification Accuracy as a Proxy  
 478 for Two Sample Testing. *arXiv:1602.02210 [cs, math, stat]*, Feb. 2016.
- 479 J. A. Ramey, C. K. Stein, P. D. Young, and D. M. Young. High-Dimensional  
 480 Regularized Discriminant Analysis. *arXiv preprint arXiv:1602.01182*,  
 481 2016.
- 482 J. Schäfer and K. Strimmer. A Shrinkage Approach to Large-Scale Covariance  
 483 Matrix Estimation and Implications for Functional Genomics. *Statistical*  
 484 *Applications in Genetics and Molecular Biology*, 4(1), Jan. 2005. ISSN  
 485 1544-6115. doi: 10.2202/1544-6115.1175.

- 486 D. K. Slonim, P. Tamayo, J. P. Mesirov, T. R. Golub, and E. S. Lander. Class  
487 Prediction and Discovery Using Gene Expression Data. In *Proceedings of*  
488 *the Fourth Annual International Conference on Computational Molecular*  
489 *Biology*, RECOMB '00, pages 263–272, New York, NY, USA, 2000. ACM.  
490 ISBN 978-1-58113-186-4. doi: 10.1145/332306.332564.
- 491 M. S. Srivastava. Multivariate Theory for Analyzing High Dimensional Data.  
492 *Journal of the Japan Statistical Society*, 37(1):53–86, 2007. doi: 10.14490/  
493 jjss.37.53.
- 494 M. S. Srivastava, S. Katayama, and Y. Kano. A two sample test in high  
495 dimensional data. *Journal of Multivariate Analysis*, 114:349–358, Feb.  
496 2013. ISSN 0047-259X. doi: 10.1016/j.jmva.2012.08.014.
- 497 J. Stelzer, Y. Chen, and R. Turner. Statistical inference and multiple test-  
498 ing correction in classification-based multi-voxel pattern analysis (MVPA):  
499 Random permutations and cluster size control. *NeuroImage*, 65:69–82, Jan.  
500 2013. ISSN 1053-8119. doi: 10.1016/j.neuroimage.2012.09.063.
- 501 G. J. Székely and M. L. Rizzo. Brownian distance covariance. *The Annals of*  
502 *Applied Statistics*, 3(4):1236–1265, Dec. 2009. ISSN 1932-6157, 1941-7330.  
503 doi: 10.1214/09-AOAS312.
- 504 A. W. van der Vaart. *Asymptotic Statistics*. Cambridge University Press,  
505 Cambridge, UK ; New York, NY, USA, Oct. 1998. ISBN 978-0-521-49603-  
506 2.
- 507 G. Varoquaux, P. R. Raamana, D. Engemann, A. Hoyos-Idrobo, Y. Schwartz,  
508 and B. Thirion. Assessing and tuning brain decoders: cross-validation,  
509 caveats, and guidelines. working paper or preprint, June 2016.
- 510 T. D. Wager, L. Y. Atlas, M. A. Lindquist, M. Roy, C.-W. Woo, and E. Kross.  
511 An fMRI-Based Neurologic Signature of Physical Pain. *New England Jour-*  
512 *nal of Medicine*, 368(15):1388–1397, Apr. 2013. ISSN 0028-4793. doi:  
513 10.1056/NEJMoa1204471.

## 514 A Analysis pipeline

515 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in  
 516 Gilron et al. [2016]. Denoting by  $i = 1, \dots, I$  the subject index,  $v = 1, \dots, V$   
 517 the voxel index, and  $s = 1, \dots, S$  the permutation index. Since regions<sup>4</sup> are  
 518 centered around a unique voxel, the voxel index  $v$  also serves as a unique  
 519 region index. Algorithm 1 computes a region-wise test statistic, which is  
 520 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
```

---

<sup>4</sup>*searchlight* or *sphere* in the MVPA parlance

## 523 B Simulation Details

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

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

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



## C Simulation Results

*Figure 5:* 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 and unbalanced data folding. See sub-captions.

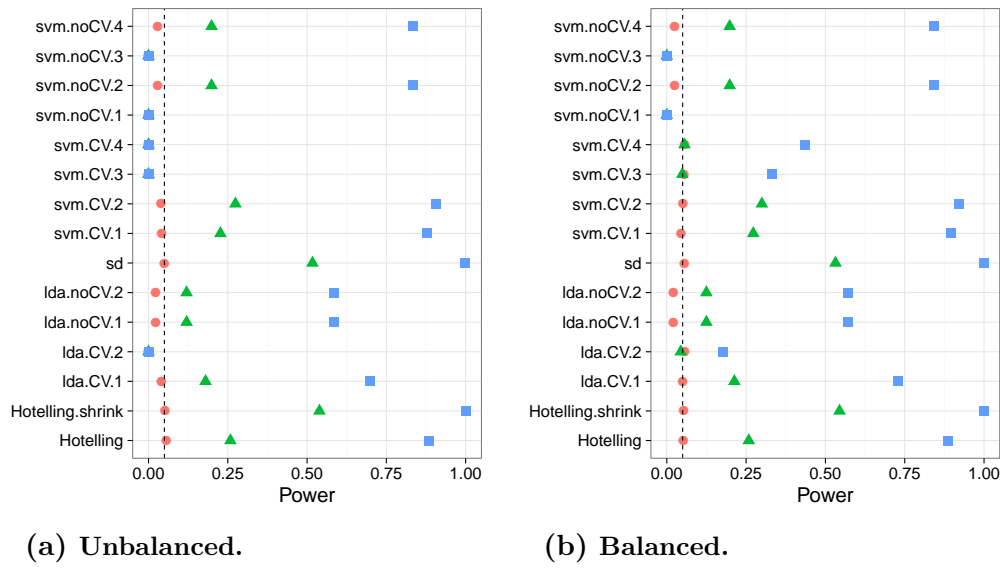


Figure 6: Simulation details in Appendix B except the changes in the sub-captions.

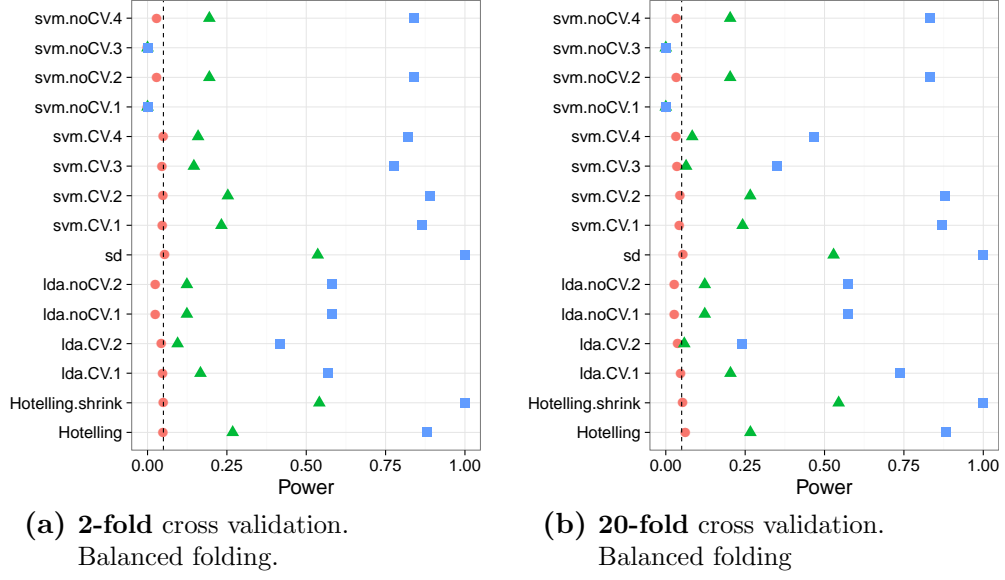


Figure 7: Simulation details in Appendix B except the changes in the sub-captions.

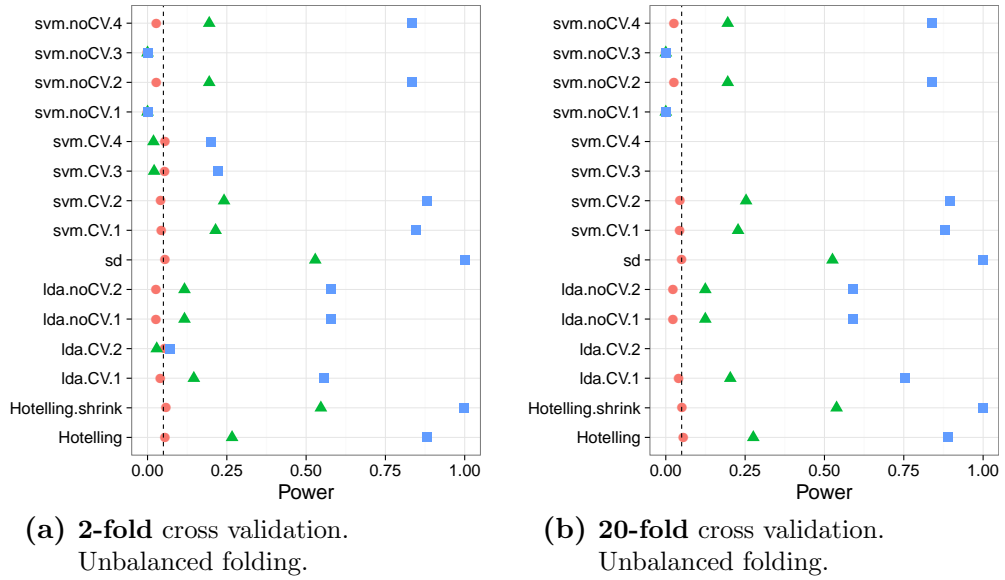


Figure 8: Simulation details in Appendix B except the changes in the sub-captions.

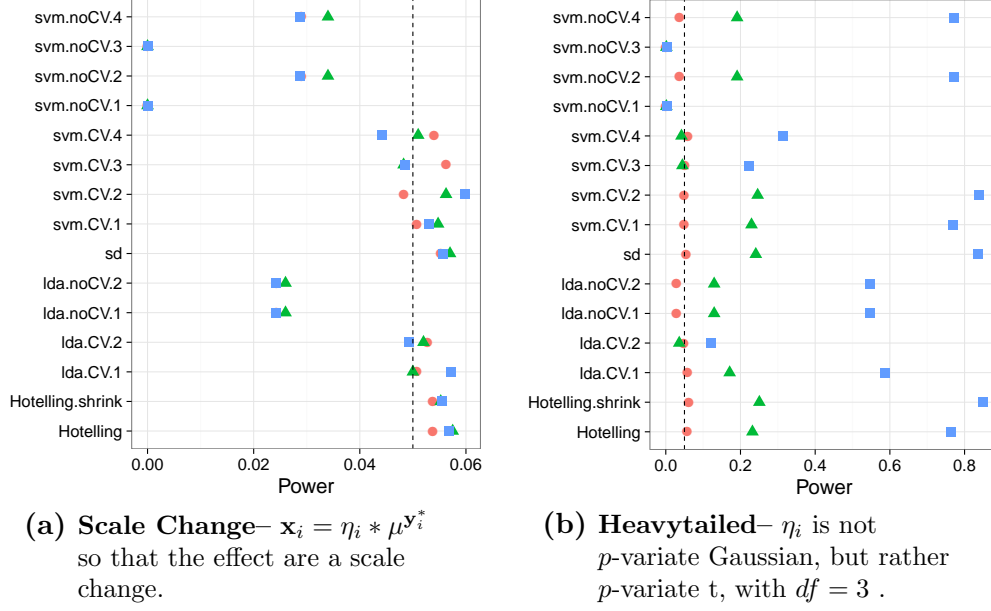


Figure 9: Simulation details in Appendix B except the changes in the sub-captions.

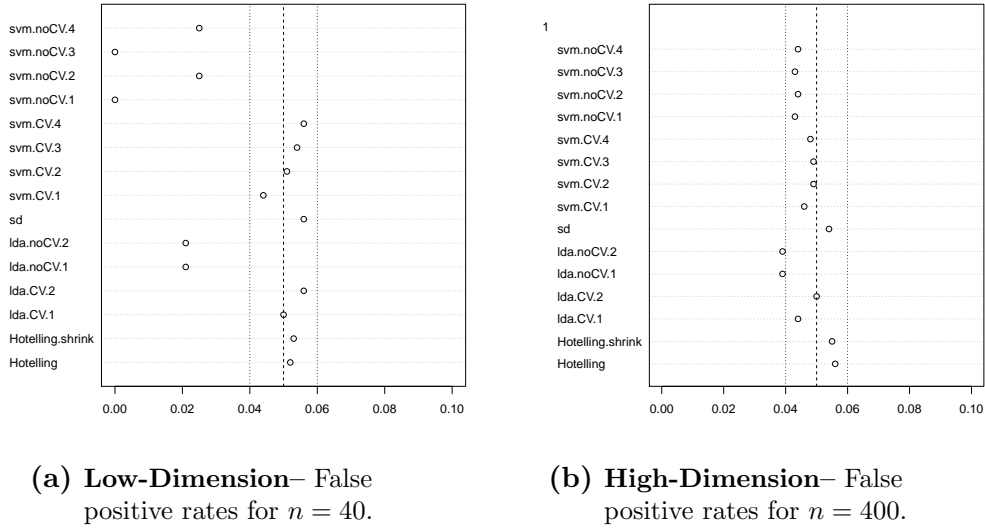
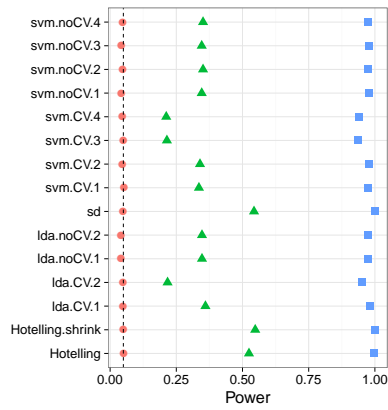
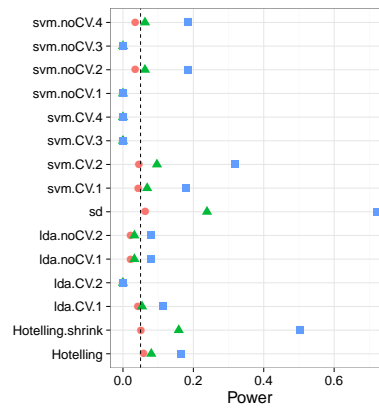


Figure 10: Simulation details in Appendix B except the changes in the sub-captions.



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



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