

Better-Than-Chance Classification for Signal Detection

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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]:

... the problem of deciding whether the classifier learned to discriminate the classes can be subsumed into the more general question as to whether there is evidence that the underlying distributions of each class are equal or not.

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

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

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

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

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

¹GoogleScholar. 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`² 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.

²A 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 more power than accuracy tests in all our con-
 164 figurations.
- 165 2. The conservativeness decays as the sample grows (Figures 9a, 9b and
 166 10a)
- 167 3. For heavy tailed distributions (Figure 8b), the extra power of the pop-
 168 ulation test vanishes.
- 169 4. Regularization is most beneficial to power in low signal to noise (SNR)
 170 regimes. Low SNR may be the result of a high-dimensional problem,
 171 or due to correlations. Indeed, the presence of positive correlations
 172 amplifies the contribution of regularization to power ((Figure 10b)).
- 173 5. The z-scoring of the accuracies was introduced to deal with unbalanced
 174 foldings. If the z-scoring has any effect at all, it merely kills power.
- 175 6. Both accuracy and population tests are inappropriate for scale alter-
 176 natives (Figure 8a). This was to be expected and is reported mostly as
 177 a sanity check.
- 178 7. Balanced folding only affects the z-scored accuracy, in the opposite
 179 direction than we anticipated.
- 180 8. Increasing the SVM’s cost parameter, which reduces the number of
 181 support vectors entering the classifier, reduces power.

182 The major insight from simulations is that the use of accuracy tests for
 183 signal detection is underpowered compared to population tests. We have not
 184 established, however, that the dominance of the population tests is not due to
 185 their regularization. Indeed, the unregularized *Hotelling* test, is only slightly
 186 superior to the accuracy tests. We return to this matter in Section 6.5. We
 187 now verify our 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 website³.

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: the ac-
209 curacy test or the population test. 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 or cor-
220 relations).

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

³<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 would also fail to reveal the
 226 effect of the concentration of the resubstitution accuracy near 1. This effect
 227 would render the resubstitution estimates a legitimate asymptotic test, and
 228 a terrible finite sample test.

229 The presence of heavy tails shrinks the power advantage of the population
 230 tests over accuracy tests. Our empirical example suggests that even if the
 231 population test does not necessarily dominate the accuracy test in power,
 232 empirically, it does have an advantage.

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

239 6.1 Ease of implementation

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

247 6.2 Reservations

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

255 Secondly, it may be argued that accuracy tests permits the separation
256 between classes in high dimensions, such as in *reproducing kernel Hilbert*
257 *spaces* (RKHS) by using non-linear predictors while population tests do not.
258 This is a false argument— accuracy test do not have any more flexibility
259 that population tests. Indeed, it is possible to test for location in the same
260 space the classifier is learned. Gretton et al. [2012] is an example where
261 the test for location is performed in RKHS. It is also possible to test for
262 the equality of two multivariate distributions on an arbitrary, unspecified
263 manifold [e.g. Heller et al., 2013][TODO: verify]. On the other hand, based
264 on our experience, and the reported neuroimaging example, we find that a
265 population test in the original feature space is a simple and powerful approach
266 to signal detection.

267 6.3 A good accuracy test

268 For the cases a population test cannot replace an accuracy test, we collect
269 some conclusions and best practices from our simulations. We give particular
270 emphasis in this section to V-fold cross validation due to its popularity, but
271 note that sampling the test set with replacement is actually preferable, as
272 we discuss in Section 6.4.

273 **Sample size.** The conservativeness of accuracy tests decrease with sample
274 size.

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

278 **Resubstitution accuracy in low dimension.** Resubstitution accuracy
279 is useful in low SNR regimes, such as low dimensional problems, because it
280 avoids cross validation without compromising power. In high dimension, the
281 power loss is considerable compared to a cross validated approach. We at-
282 tribute this to the compounding of discretization and concentration effects:
283 the difference between the sampling distribution of the resubstitution accu-
284 racy is simply indistinguishable under the null and under the alternative.
285 In low dimensional problems, the discretization is less impactful, and the
286 computational burden of cross validation can be avoided by using the resub-
287 stitution accuracy. There is a fundamental difference between V-folding and
288 resubstitution. The latter should not be thought of as the limit of the former.

289 **Regularize** Regularizing a classifier proves crucial to detection power in
290 low SNR regimes; in high dimension in particular. We also conjecture that
291 the power-maximizing regularization is larger than the error-minimizing reg-
292 ularization.

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

295 6.4 Smoothing accuracy estimates

296 It may be possible to alleviate the effect of discretization by appropriate
297 cross-validation. The discreteness of the accuracy statistic is governed by the
298 number of examples in the union of test sets, over all validation iterations.
299 For V-fold CV, for instance, the accuracy may assume as many values as the
300 sample size. This suggests that the accuracy can be “smoothed” by allowing
301 the test sample to be drawn with replacement. An algorithm that samples
302 test sets with replacement is the *leave-one-out bootstrap estimator*, and its
303 derivatives, such as the *0.632 bootstrap*, and *0.632+ bootstrap* [Hastie et al.,
304 2003, Sec 7.11].

Definition 3 (bLOO). The *leave-one-out bootstrap* estimate is the average
accuracy of the holdout observations, over all bootstrap samples. Denoting

by \mathcal{S}^b , a bootstrap sample b , 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* estimator, $\hat{\mathcal{E}}_{\mathcal{A}}^{0.632}$, is defined as

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

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=1e1
svm.Boot.2	SVM	bLOO	10	FALSE	cost=1e1
svm.Boot.3	SVM	b0.632	50	FALSE	cost=1e1
svm.Boot.4	SVM	bLOO	50	FALSE	cost=1e1

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.

313 6.5 High dimensional classifiers

314 Inspecting Figure 5a (for instance), it can be seen that Hotelling’s T^2 test
 315 has similar power as accuracy tests. It should thus be argued that the real
 316 advantage of the population tests is due to their adaptation to high dimension
 317 by regularization, and not only to discretization. To study this, we call
 318 upon several *regularized classifiers*, designed for high dimensional problems.
 319 In the spirit of the regularized covariance of *Hotelling.shrink*, we try an l_2
 320 regularized SVM Friedman et al. [2010], and shrinkage based LDA [Pang
 321 et al., 2009, Ramey et al., 2016]. In the spirit of the diagonalized covariance
 322 of *sd*, we try a diagonalized LDA [Dudoit et al., 2002], a.k.a. *Gaussian naive*
 323 *Bayes*.

324 Simulation results reported in Figure 3 with naming conventions in Ta-
 325 ble 3. It can be seen that regularizing a classifier in high dimension, just like
 326 a parameter test, improves power. It can also be seen that (regularized) pa-
 327 rameter tests are still more powerful than (regularized) accuracy tests. This
 328 was to be expected, since we already saw in (e.g. Figure 5a) that the unregu-

larized parameter test, *Hotelling*, is slightly more powerful than unregularized accuracy tests— *svm.CV.1* for instance.

We can compound the regularization with the bootstrapping from Section 6.4, to improve finite sample power of the accuracy tests. This is done in the *svm.highdim.2* and *lda.highdim.4* tests. The latter being the first accuracy test that achieves the same power as the best of population tests. This is exciting news for the cases a population test cannot replace an accuracy test. The implication for practitioners is that powerful accuracy tests can be constructed by sampling test sets with replacement, and regularizing the classifier.

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

Table 3: The same as Table 1 for regularized (high dimensional) predictors. *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 validation. *lda.highdim.1* is the Diagonal Linear Discriminant Analysis of Dudoit et al. [2002]. *lda.highdim.2* is the High-Dimensional Regularized 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.

6.6 Related Literature

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

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

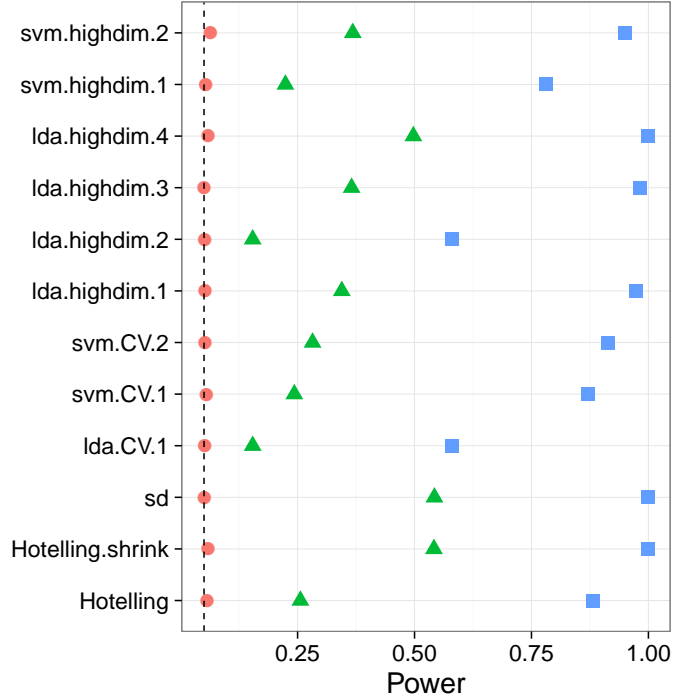


Figure 3: HighDim Classifier— The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. The various statistics on the y axis. Their details are given in tables 1 and 3. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue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

350 *independence test*, and demonstrate by simulation that it has more power
351 than other accuracy tests, and can deal with non-balanced data sets. We did
352 not include this test in the battery we compared, but we note the following:
353 (a) The independence test of Olivetti et al. [2012] relies on a discrete test
354 statistic. It may probably be improved with the methods discussed in this
355 section, before the application of Olivetti et al. [2012]’s independence test.
356 (b) In contrast with the underlying motivation of Olivetti et al. [2012]’s
357 independence test, we did not find that balancing the data folds affects the
358 power of the test.

359 Golland and Fischl [2003] and Golland et al. [2005] study accuracy tests
360 using simulation, neuroimaging data, genetic data, and analytically. Their
361 analytic results formalize our intuition from Section 1 on the effect of concen-
362 tration of the accuracy statistic: The finite Vapnik–Chervonenkis dimension
363 requirement [Golland et al., 2005, Sec 4.3] prevents the permutation p-value
364 from (asymptotically) concentrating near 1. Like ourselves, they also find
365 that the power increases with the size of the test set. This is seen in Fig.4 of

366 Golland et al. [2005], where the size of the test-set, K , governs the discretiza-
 367 tion. Since they permute features, not labels, then all their permutation
 368 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

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

369 Varying p interpolates between the null distribution ($p = 0.5$) and a location
 370 shift model ($p = 0$). We now perform the same simulation as Golland et al.
 371 [2005], after parameterizing p so that $p = 0$ corresponds to the null model,
 372 and in the same dimensionality as our previous simulations We find that also
 373 in this mixture class of models a population test has more power than an
 374 accuracy test (Figure 4).

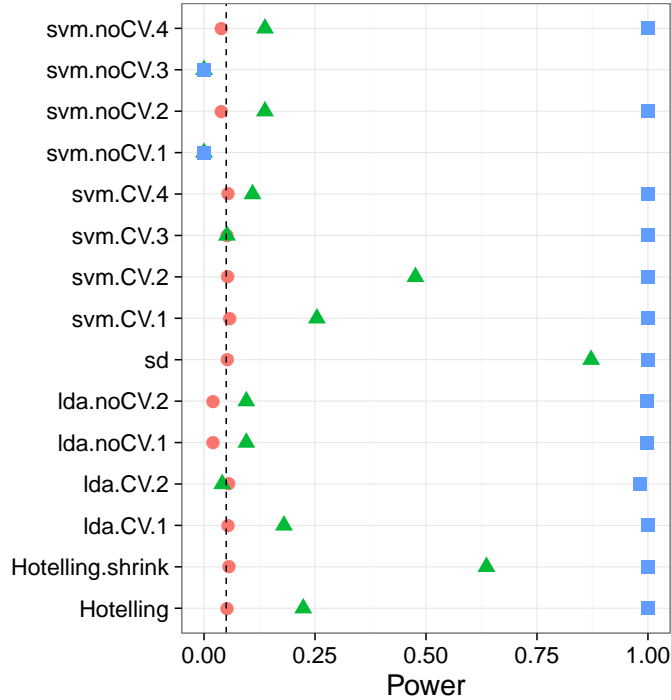


Figure 4: **Mixture**— $\mathbf{x}_i = \chi_i \mu + \eta_i$; $\chi_i = \{-1, 1\}$ and $Prob(\chi_i = 1) = (1/2 - p)^{\mathbf{y}_i^*} (1/2 + p)^{1 - \mathbf{y}_i^*}$. μ is a p -vector with $3/\sqrt{p}$ in all coordinates. The effect, p , is color and shape coded and varies over 0 (red circle), 1/4 (green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

375 6.7 Epilogue

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

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

387 7 Acknowledgments

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518 A Analysis pipeline

519 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in
 520 Gilron et al. [2016]. Denoting by $i = 1, \dots, I$ the subject index, $v = 1, \dots, V$
 521 the voxel index, and $s = 1, \dots, S$ the permutation index. Since regions⁴ are
 522 centered around a unique voxel, the voxel index v also serves as a unique
 523 region index. Algorithm 1 computes a region-wise test statistic, which is
 524 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

527 B Simulation Details

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

531 Each simulation is based on 4,000 replications. In each replication, we
532 generate n i.i.d. samples from a shift model $\mathbf{x}_i = \mu \mathbf{y}_i^* + \eta_i$. Where $y_i^* = \{0, 1\}$
533 is the class of subject i in dummy coding. Recalling that $y_i = \{-1, 1\}$ is the
534 class in effect coding, then clearly $y_i = 2y_i^* - 1$. The noise is distributed as
535 $\eta_i \sim \mathcal{N}_p(0, \Sigma)$. The sample size $n = 40$. The dimension of the data is $p = 23$.
536 The covariance $\Sigma = I$. Effects, i.e. shifts μ , are equal coordinate p -vectors
537 with coordinates that vary over $\mu \in \{0, 1/4, 1/2\}$.

538 Having generated the data, we compute each of the test statistics in Ta-
539 ble 1. For test statistics that require data folding, we used 8 folds. We then
540 compute a permutation p-value by permuting the class labels, and recomput-
541 ing each test statistic. We perform 400 such permutations. We then reject
542 the $\mu_i = 0$ null hypothesis if the permutation p-value is smaller than 0.05.
543 The reported power is the proportion of replication where the permutation
544 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.

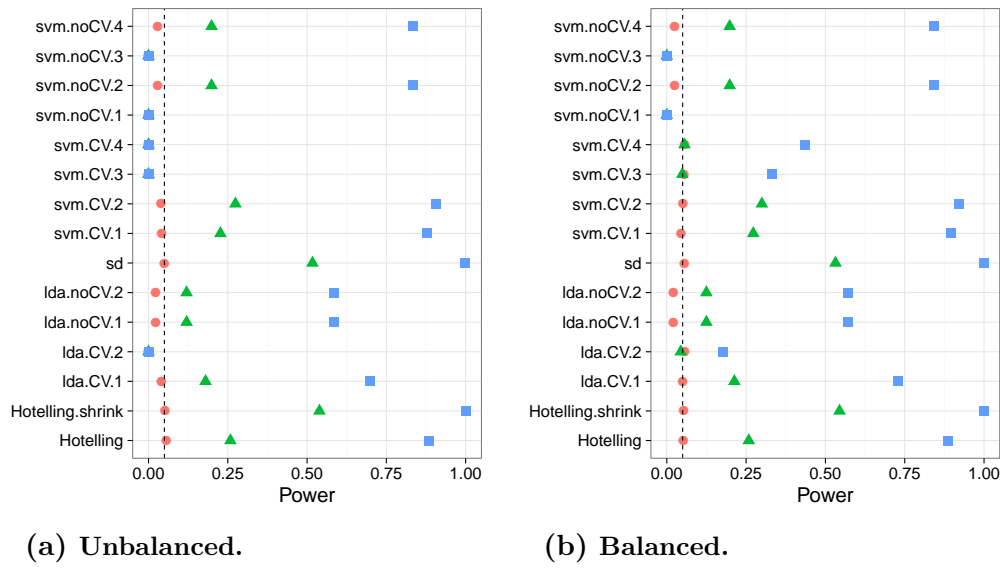


Figure 6: Simulation details in Appendix B except the changes in the sub-captions.

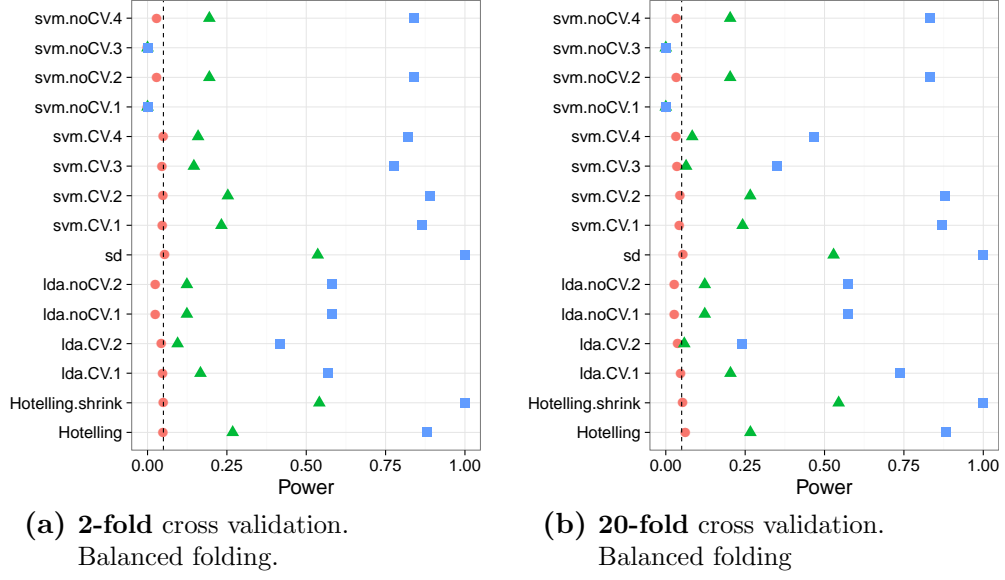


Figure 7: Simulation details in Appendix B except the changes in the sub-captions.

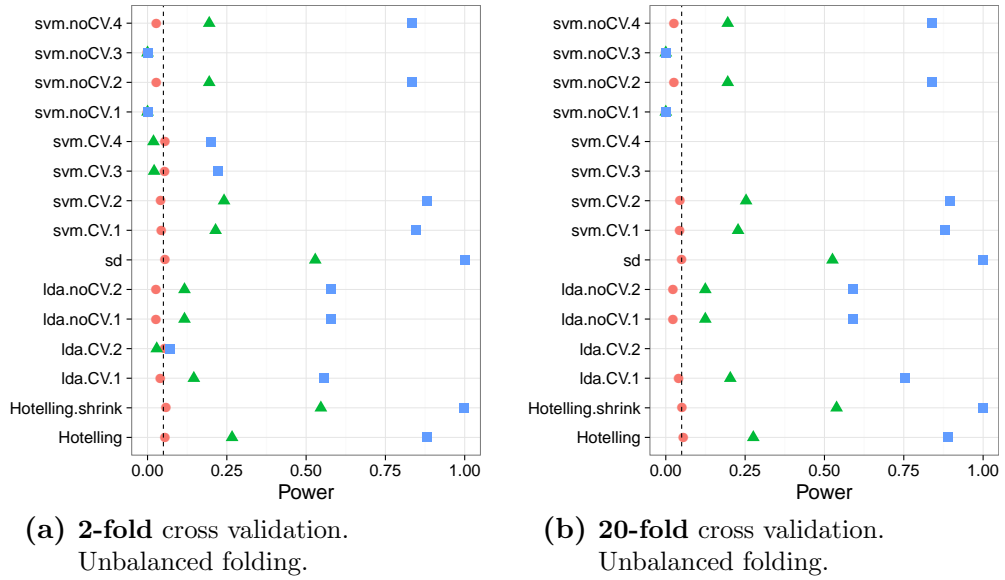


Figure 8: Simulation details in Appendix B except the changes in the sub-captions.

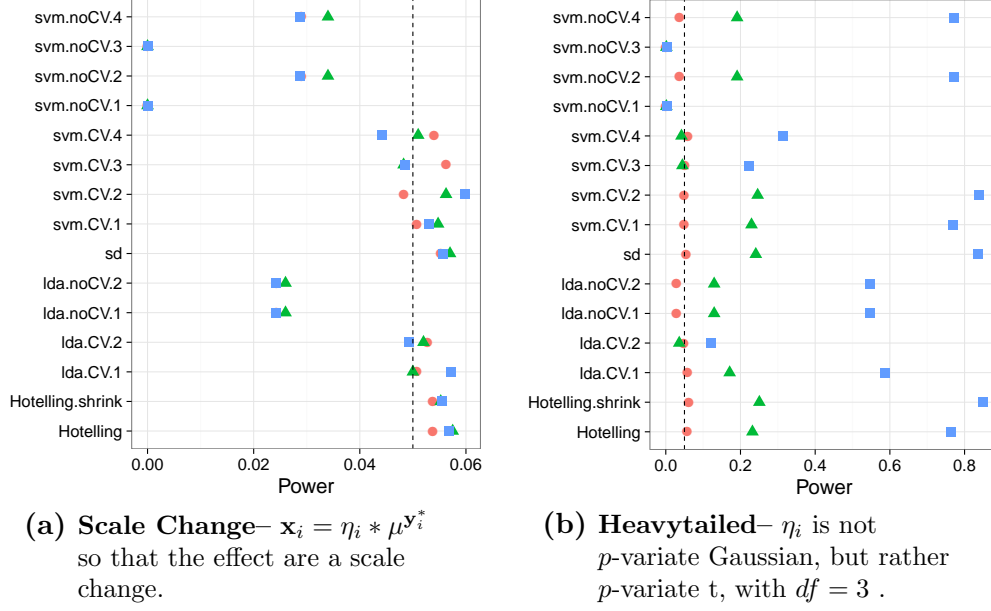


Figure 9: Simulation details in Appendix B except the changes in the sub-captions.

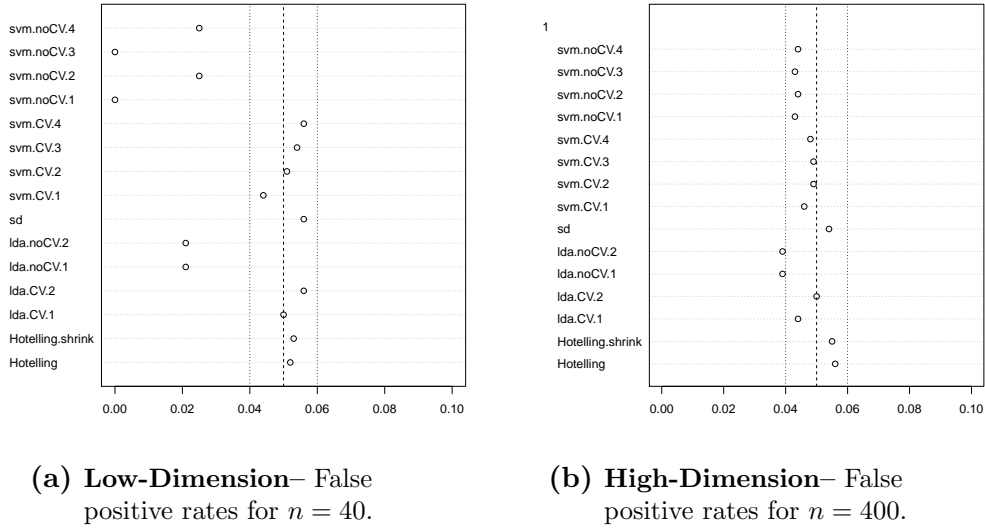


Figure 10: Simulation details in Appendix B except the changes in the sub-captions.

