

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 very high profile publications in the genetics literature: Golub et al. [1999], Slonim et al. [2000], Radmacher et al. [2002], Mukherjee et al. [2003], Juan and Iba [2004], Jiang et al. [2008].

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

This same signal detection task can be also approached as a two-group multivariate test. Inferring that a region encodes vocal/non-vocal information, is essentially inferring that the spatial distribution of brain activations is different given a vocal/non-vocal stimulus. As put in Pereira et al. [2009]:

... 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 then call upon a two-group population test such as Hotelling’s T^2 [Anderson, 2003]. Alternatively, if the size of a brain region 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*, also termed *class comparisons*. [TODO: rename 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 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. This eschews the discrete nature of the accuracy statistic, which will be

¹GoogleScholar. Accessed on Aug 4, 2016.

65 shown to have crucial impact. Since typical sample sizes in neuroscience are
 66 not large, we seek to study which test is to be preferred in finite samples?
 67 Our conclusion will be quite simple: *population tests almost always have more*
 68 *power than accuracy tests.*

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

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

89 To compare the power of accuracy tests and population tests in finite sam-
 90 ples, we perform a simulation study of a battery of test statistics. We start
 91 with formalizing the problem in Section 2. The main findings are reported
 92 in Sections 4 and 5. A discussion follows in Section 6.

93 2 Problem setup

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

97 Given n pairs of (x_i, y_i) , typically assumed i.i.d., a population test amounts
 98 to testing whether $x|y = 1$ has the the same distribution as $x|y = -1$. I.e.,
 99 we test if the multivariate voxel activation pattern has the same distribution
 100 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, $\mathcal{A} : \mathcal{S} \rightarrow \mathcal{A}_{\mathcal{S}}(x)$. The accuracy of predictor $\mathcal{A}_{\mathcal{S}}(x)$ is defined as the probability of $\mathcal{A}_{\mathcal{S}}(x)$ making a correct prediction. 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

$$\mathcal{E}_{\mathcal{A}_{\mathcal{S}}(x)} := \mathcal{P}(\mathcal{A}_{\mathcal{S}}(x) = y). \quad (1)$$

The accuracy of an algorithm \mathcal{A} is defined as the average accuracy, over all possible data sets

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

101 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-
 102 nificant “better than chance” estimate of either, is evidence that the classes
 103 are distinct. In a typical application, the predictor is not fixed, so that $\hat{\mathcal{E}}_{\mathcal{A}}$,
 104 and not $\hat{\mathcal{E}}_{\mathcal{A}_{\mathcal{S}}(x)}$, will be used for the testing.

105 Two popular estimates of $\hat{\mathcal{E}}_{\mathcal{A}}$ are the *resubstitution estimate*, and the
 106 V-fold cross validation (CV) estimate [Hastie et al., 2003].

Definition 1 (Resubstitution accuracy). The resubstitution accuracy estimator, $\hat{\mathcal{E}}_{\mathcal{A}}^{resub}$, is defined as

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

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

Definition 2 (V-fold CV). Denoting by \mathcal{S}^v the v 'th partition 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

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

108 2.1 Candidate Tests

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

- 111 1. Is $\hat{\mathcal{E}}_{\mathcal{A}}$ cross validated or not?

112 2. For a V-fold cross validated test statistic:

113 (a) Should the data be refolded in each permutation?

114 (b) Should the data folding be balanced (a.k.a. stratified)?

115 (c) How many folds?

116 3. How to estimate $\hat{\mathcal{E}}_{\mathcal{A}}$?

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

120 **Cross validate or not?** Given our goal, a biased estimate of $\hat{\mathcal{E}}_{\mathcal{A}}$ is not a
121 problem provided that bias is consistent over all permutations. The under-
122 lying intuition is that a permutation test will be unbiased, provided that the
123 exact same computation is performed over all permutations. We will thus
124 be considering both cross validated accuracies, and *resubstitution accuracies*,
125 where the accuracy is evaluated on the training set and not on a holdout.

126 **Balanced folding?** The standard practice when cross validating is to con-
127 strain the data folds to be balanced, i.e. stratified [e.g. Ojala and Garriga,
128 2010]. This means that each fold has the same number of examples from
129 each class. We will report results with both balanced and unbalanced data
130 foldings, only to discover, it does not really matter.

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

136 **How many folds?** Different authors suggest different rules for the number
137 of folds. We will be varying the number of folds, and ultimately discover that
138 the power *decreases with the number of folds*.

How to estimate accuracy? Low accuracies, even 0, are evidence that
the classes are separated so that for our purposes, we should consider the
departure from chance level $|\hat{\mathcal{E}}_{\mathcal{A}} - 0.5|$ as candidate test statistic. For un-
balanced classes, chance level is not 0.5, but rather the probability of
the majority class, we denote by $\hat{\pi}$. This suggests the following test statistic

$|\hat{\mathcal{E}}_{\mathcal{A}} - \hat{\pi}|$. Since we will be aggregating these statistics over random data sets where $\hat{\pi}$ 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} :

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

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

Name	Algorithm	Accuracy	Z-scored	Parameters
Hotelling	Hotelling	—	—	—
Hotelling.shrink	Hotelling	—	—	—
sd	SD	—	—	—
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.

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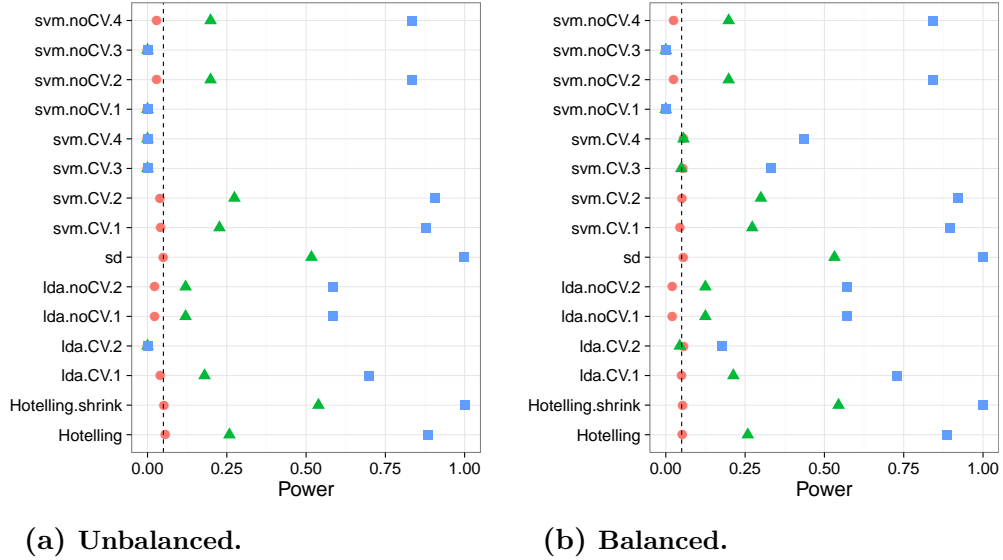
3 Controlling the False Positive Rate

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

- (a) The folds are balanced or not (Figures 1,6 and 7)
- (b) The tuning parameters are varied (cost=10 versus cost=0.1).
- (c) The number of folds is varied (Figures 6 and 7).
- (d) The noise is heavytailed (Figure 8b).
- (e) The problem is high or low dimensional (Figure 9.)
- (f) The noise is correlated (Figure 10b).

We also observe that the most conservative tests are the resubstitution accuracy statistics. We return to this matter in the Discussion.

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



155 4 Power

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

- 160 1. Population tests have more power than accuracy tests in all our con-
161 figurations.
- 162 2. The conservativeness decays as the sample grows (Figures 9a, 9b and
163 10a)
- 164 3. For heavy tailed distributions (Figure 8b), the extra power of the pop-
165 ulation test vanishes.
- 166 4. Regularization is most beneficial to power in low signal to noise (SNR)
167 regimes. Low SNR may be the result of a high-dimensional problem,
168 or due to correlations. Indeed, the presence of positive correlations
169 amplifies the contribution of regularization to power ((Figure 10b)).
- 170 5. The z-scoring of the accuracies was introduced to deal with unbalanced
171 foldings. If the z-scoring has any effect at all, it merely kills power.
- 172 6. Both accuracy and population tests are inappropriate for scale alter-
173 natives (Figure 8a). This was to be expected and is reported mostly as
174 a sanity check.
- 175 7. Balanced folding only affects the z-scored accuracy, in the opposite
176 direction than we anticipated.
- 177 8. Increasing the SVM’s cost parameter, which reduces the number of
178 support vectors entering the classifier, reduces power.

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

185 5 Neuroimaging Example

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

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

198 In agreement with our simulation results, the population test (*sd*) dis-
199 covers more brain regions of interest when compared to an accuracy test
200 (*svm.cv.1*). The former discovers 1,232 regions, while the latter only 441, as
201 depicted in Figure 2. We emphasize that both test statistics were compared
202 with the same permutation scheme, and the same error controls, so that any
203 difference in detections is due to their different power.

204 Having established that accuracy tests are typically underpowered for sig-
205 nal detection compared to population tests, we wish to identify the conditions
206 under which this will occur, and discuss practical implications.

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
210 the insight provided by a good closed-form analytic result. The finite sam-
211 ple power of permutation tests is a formidable mathematical problem, so
212 we currently content ourselves with simulations. We have concluded that the
213 population tests are typically preferable. Their high dimensional versions,
214 such as Srivastava [2007] and Schäfer and Strimmer [2005], are particularly
215 well suited for neuroimaging problems such as MVPA. We attribute this to
216 several phenomena:

- 217 (a) Discretization introduced in finite samples by the accuracy test statistic.
- 218 (b) Inefficient use of the data for the validation holdout set.
- 219 (c) Regularization crucial in high dimensional problems.

220

²<https://openfmri.org/>



Figure 2: Brain regions encoding information discriminating between vocal and non-vocal stimuli. Map reports the centers of 27-voxel sized spherical regions, as discovered by an accuracy test (*svm.cv.1*), and a 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].

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

225 The degree of discretization is governed by the sample size. For this
 226 reason, an asymptotic analysis such as Ramdas et al. [2016] may uncover
 227 the holdout inefficiency, but will not uncover the discretization effect. An
 228 asymptotic analysis of a finite complexity model would also fail to reveal the
 229 effect of the concentration of the resubstitution accuracy near 1. This effect
 230 would render the resubstitution estimates a legitimate asymptotic test, and
 231 a terrible finite sample test.

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
 234 an accuracy test. There is also a good chance that it would be easier to
 235 implement, and faster to run, since no cross validation will be involved.

236 6.1 Ease of implementation

237 A very important consideration is the ease of implementation. The need for
238 cross validation of the accuracy test greatly increases its computational com-
239 plexity. Moreover, anyone who has actually implemented tests with discrete
240 statistics, will attest they are more prone to programming errors. This is
241 because their unforgiveness to the type of inequalities used. Indeed, mistak-
242 enly replacing a weak inequality with a strong inequality in one’s program
243 may considerably change the results. This is not the case for continuous test
244 statistics.

245 6.2 Reservations

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

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

264 6.3 A good accuracy test

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

270 **Sample size.** The conservativeness of accuracy tests decrease with sample
271 size.

272 **Permute features.** Permuting features is easier than permuting labels.
273 It allows to preserve balanced folds after a permutation without refolding.
274 Although we not we did not find a power difference between balanced and
275 unbalanced foldings.

276 **Use less folds.** For V-fold CV, power decreases as the number of folds
277 increases. This is quite interesting since two phenomena compete as the
278 number of folds increase: (a) the train set is larger so that better accuracies
279 are achievable. (b) The test set is smaller so that the accuracy estimate is
280 more variable. The decrease in power with increase fold number suggests
281 that the latter dominates the former. Put differently: it is easier to detect a
282 small stable departure from chance level, than a large but unstable one.

283 **Resubstitution accuracy in low dimension.** Resubstitution accuracy
284 useful in low dimension. In high dimension, the power loss is considerable
285 compared to a cross validated approach. We attribute this to the compound-
286 ing of discretization and concentration effects: the difference between the
287 sampling distribution of the resubstitution accuracy is simply indistinguish-
288 able under the null and under the alternative. In low dimensional problems,
289 the discretization is less impactful, and the computational burden of cross
290 validation can be avoided by using the resubstitution accuracy. There is
291 a fundamental difference between V-folding and resubstitution. The latter
292 should not be thought of as the limit of the former.

293 **Regularize** Regularizing the accuracy test proves very useful in high di-
294 mensional problems. Put differently: reducing variance by adding some bias
295 is very useful to detect better-than-chance classification.

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

298 6.4 Smoothing accuracy estimates

299 It may be possible to alleviate the effect of discretization by appropriate
300 cross-validation. The discreteness of the accuracy statistic is governed by
301 the number of examples in the union (over all validation iterations) of test
302 sets. For V-fold CV, for instance, this number is simply the sample size. This

303 suggests that the accuracy can be “smoothed” by allowing the test sample to
 304 be drawn with replacement. The *bootstrap* may seem like a good candidate
 305 approach since it samples examples with replacement. It does so, however,
 306 for the train set, and not the test set. An algorithm that samples test sets
 307 with replacement is the *leave-one-out bootstrap estimator* (bLOO) and its
 308 derivation– the *0.632 bootstrap estimator* (b0.632) [Hastie et al., 2003, Sec
 309 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 b0.632 accuracy estimator, $\hat{\mathcal{E}}_{\mathcal{A}}^{0.632}$, is defined as

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

310 Simulation results reported in Figure 3 with naming conventions in Ta-
 311 ble 2. It can be seen that selecting test sets with replacement does increase
 312 the power, when compared to V-fold cross validation, but still falls short
 313 from the power of population tests. It can also be seen that power increases
 314 with the number of bootstrap replications, itself reducing the level of dis-
 315 cretization. The type of bootstrap, bLOO versus b0.632, does not change
 316 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.

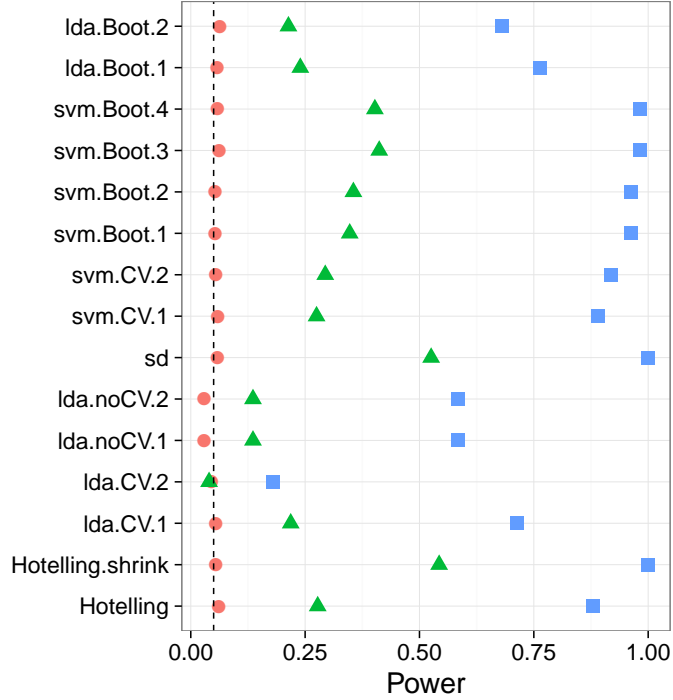


Figure 3: **Bootstrap**— The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. The various statistics on the y axis. Their details are given in tables 1 and 2. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square).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

318 6.5 High dimensional classifiers

319 Inspecting Figure 1a (for instance), it can be seen that Hotelling’s T^2 test
320 has similar power to accuracy tests. It should thus be argued that the real
321 advantage of the population tests is due to their adaptation to high dimen-
322 sion by regularization (*sd* and *Hotelling.shrink*), and not only to discretiza-
323 tion. To study this, we call upon several regularized classifiers, designed
324 for high dimensional problems. In the spirit of the regularized covariance of
325 *Hotelling.shrink*, we try an l_2 regularized svm Friedman et al. [2010], and
326 shrinkage based LDA [Pang et al., 2009, Ramey et al., 2016]. In the spirit of
327 the diagonalized covariance of *sd*, we try a diagonalized LDA [Dudoit et al.,
328 2002], which can be thought of a method intersecting Fisher’s LDA and Naive
329 Bayes.

330 Simulation results reported in Figure 4 with naming conventions in Ta-
331 ble 3. It can be seen that regularizing a classifier in high dimension, just
332 like a parameter test, improves power. It can also be seen that (regularized)
333 parameter tests are still more powerful than (regularized) accuracy tests.
334 This was to be expected, since we already saw in (e.g. Figure 1a) that the
335 unregularized parameter test, *Hotelling*, is slightly more powerful than the
336 regularized accuracy test, *svm.CV.1* for instance.

337 We can compound regularization in this section with the bootstrapping
338 from Section 6.4, to improve finite sample power of the accuracy tests. This
339 is done in the *svm.highdim.2* test, which still falls short from the power of
340 the population tests, but is a much more powerful accuracy test than the
341 original non-regularized, V-fold validated, version of *svm.CV.1*.

Name	Algorithm	Accuracy	Z-scored	Parameters
svm.highdim.1	SVM	V-fold	FALSE	cost=1e-1, V=4
svm.highdim.2	SVM	b0.632	FALSE	cost=1e-1, 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

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].

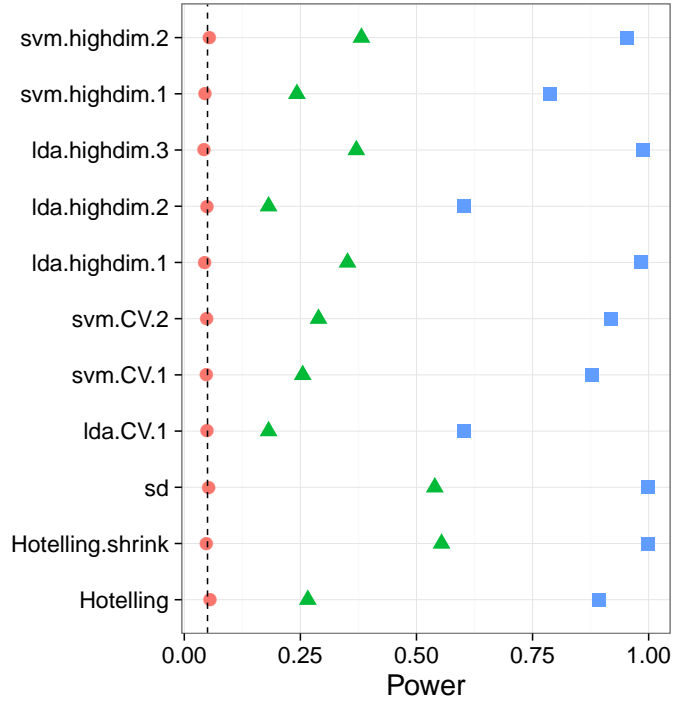


Figure 4: **HighDim Classifier**— The power of a permutation test with various test statistics. The power on the x axis. Effect are color and shape coded. The various statistics on the y axis. Their details are given in tables 1 and 3. Effects vary over 0 (red circle), 0.25 (green triangle), and 0.5 (blue square). Simulation details in Appendix B.

343 6.6 Related Literature

344 Ojala and Garriga [2010] study the power of two accuracy tests: one test-
345 ing the “no signal” null hypothesis, and the other testing the “independent
346 features” null hypothesis. They perform an asymptotic analysis, and a sim-
347 ulation study. They also apply various classifiers to various data sets. Their
348 emphasis is the effect of the underlying classifier on the power, and the po-
349 tential of the “independent features” test for feature selection. This is a very
350 different emphasis from our own.

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

361 Golland et al. [2005] study accuracy tests using simulation, neuroimaging
362 data, genetic data, and analytically. Their analytic results formalize our in-
363 tuition from Section 1 on the effect of concentration of the accuracy statistic:
364 The finite Vapnik–Chervonenkis (VC) dimension requirement [Golland and
365 Fischl, 2003, Sec 4.3] prevents the permutation p-value from (asymptotically)
366 concentrating near 1. Like ourselves, they also find that the power increases
367 with the size of the test set (Figure 4, middle). This is seen in their Figure 4,
368 where the size of the test-set, K , governs the discretization. Since they per-
369 mutate features, not labels, then all their permutation samples are balanced,
370 and there is no issue of refolding.

371 Golland et al. [2005] simulate the power of accuracy tests by sampling
372 from a Gaussian mixture family of models, and not from a location family
373 as our own simulations. Under their model $(x_i|y_i = 1) \sim p\mathcal{N}(\mu_1, I) +$
374 $(1 - p)\mathcal{N}(\mu_2, I)$ and $(x_i|y_i = -1) \sim (1 - p)\mathcal{N}(\mu_1, I) + p\mathcal{N}(\mu_2, I)$. Varying p
375 interpolates between the null distribution ($p = 0.5$) and a location shift model
376 ($p = 0$). We now perform the same simulation as Golland et al. [2005], after
377 parameterizing p so that $p = 0$ corresponds to the null model, and in the
378 same dimensionality as our previous simulations We find that also in this
379 mixture class of models a population test has more power than an accuracy
380 test (Figure 5).

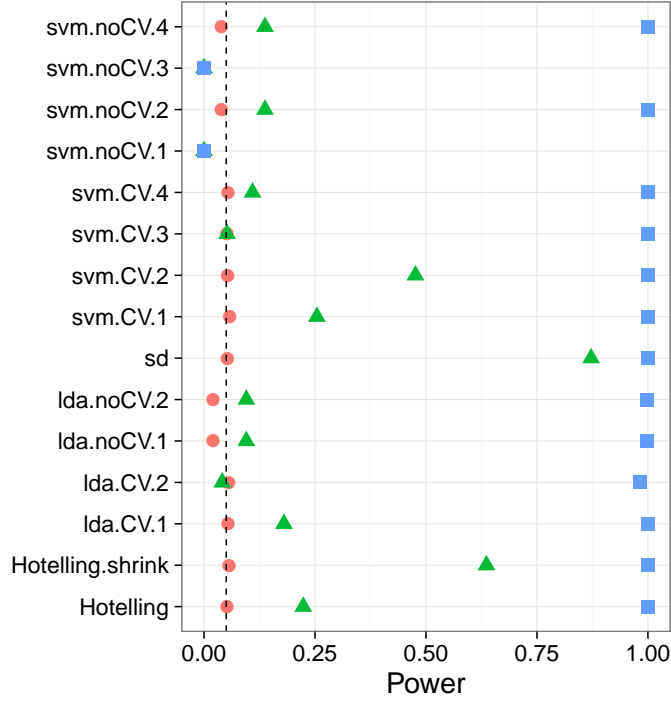


Figure 5: **Mixture**— $\mathbf{x}_i = \chi_i \mu + \eta_i$; $\chi_i = \{-1, 1\}$ and $\text{Prob}(\chi_i = 1) = (1/2 - p)^{y_i^*} (1/2 + p)^{1-y_i^*}$. μ is a p -vector with $3/\sqrt{p}$ in all coordinates. The effect, p , is color and shape coded and varies over 0 (red circle), $1/4$ (green triangle) and $1/2$ (blue square).

6.7 Epilogue

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

The recent popularity of machine learning has resulted in the extensive teaching and use of prediction in theoretical and applied communities and the relative lack of awareness or popularity of the topic of Neyman-Pearson style hypothesis testing in the computer science and related “data science” communities.

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

³<http://stats.stackexchange.com/questions/17408/how-to-assess-statistical-significance-of-the-accuracy-of-a-classifier>.

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

397 **7 Acknowledgments**

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525 A Analysis pipeline

526 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in
 527 Gilron et al. [2016]. Denoting by $i = 1, \dots, I$ the subject index, $v = 1, \dots, V$
 528 the voxel index, and $s = 1, \dots, S$ the permutation index. Since regions⁴ are
 529 centered around a unique voxel, the voxel index v also serves as a unique
 530 region index. Algorithm 1 computes a region-wise test statistic, which is
 531 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
532 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: $\{p_v\}_{v=1}^V$

```

533 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

534 B Simulation Details

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

538 Each simulation is based on 4,000 replications. In each replication, we
539 generate n i.i.d. samples from a shift model $\mathbf{x}_i = \mu \mathbf{y}_i^* + \eta_i$. Where $y_i^* = \{0, 1\}$
540 is the class of subject i in dummy coding. Recalling that $y_i = \{-1, 1\}$ is the
541 class in effect coding, then clearly $y_i = 2y_i^* - 1$. The noise is distributed as
542 $\eta_i \sim \mathcal{N}_p(0, \Sigma)$. The sample size $n = 40$. The dimension of the data is $p = 23$.
543 The covariance $\Sigma = I$. Effects, i.e. shifts μ , are equal coordinate p -vectors
544 with coordinates that vary over $\mu \in \{0, 1/4, 1/2\}$.

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

C Simulation Results

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

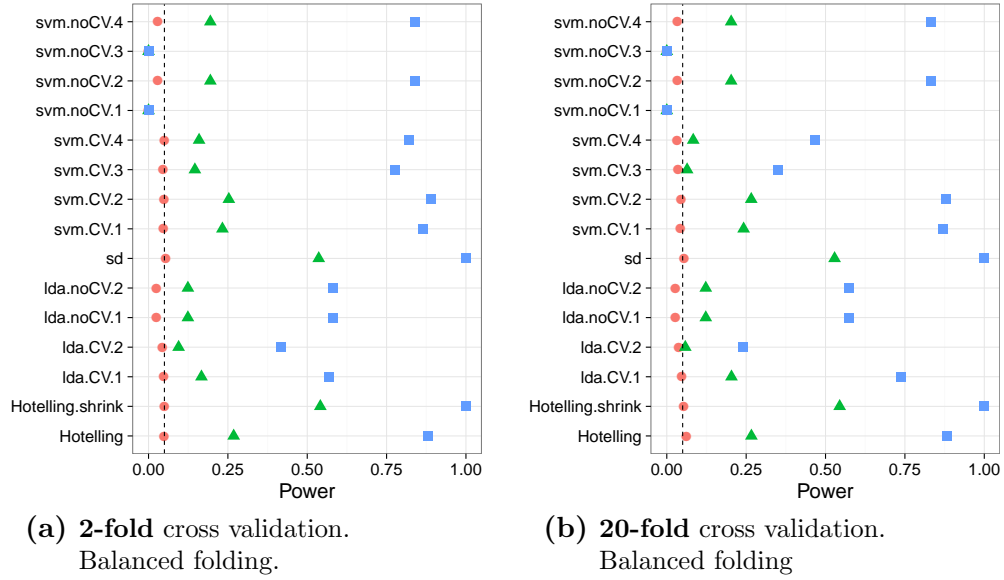


Figure 7: Simulation details in Appendix B except the changes in the sub-captions.

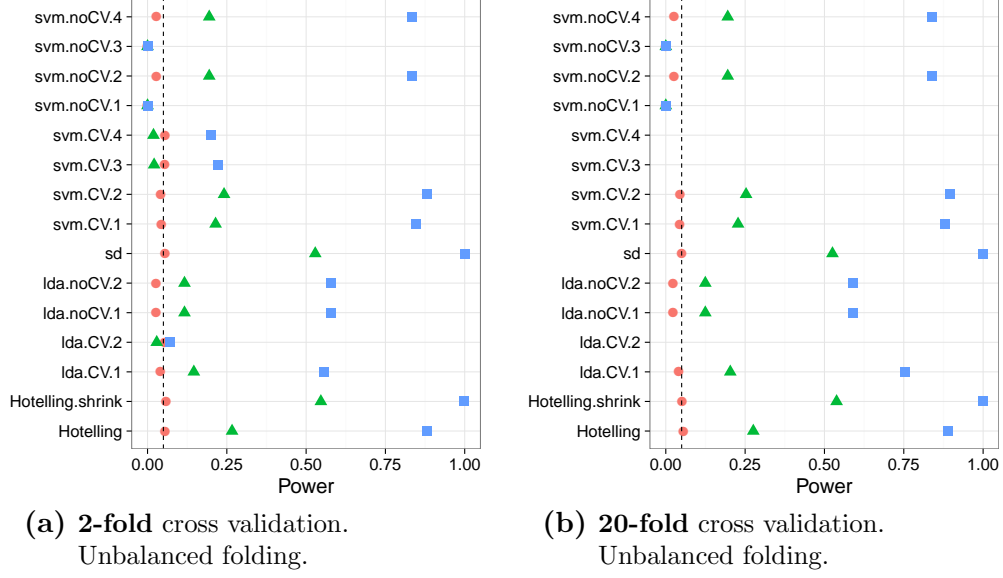


Figure 8: Simulation details in Appendix B except the changes in the sub-captions.

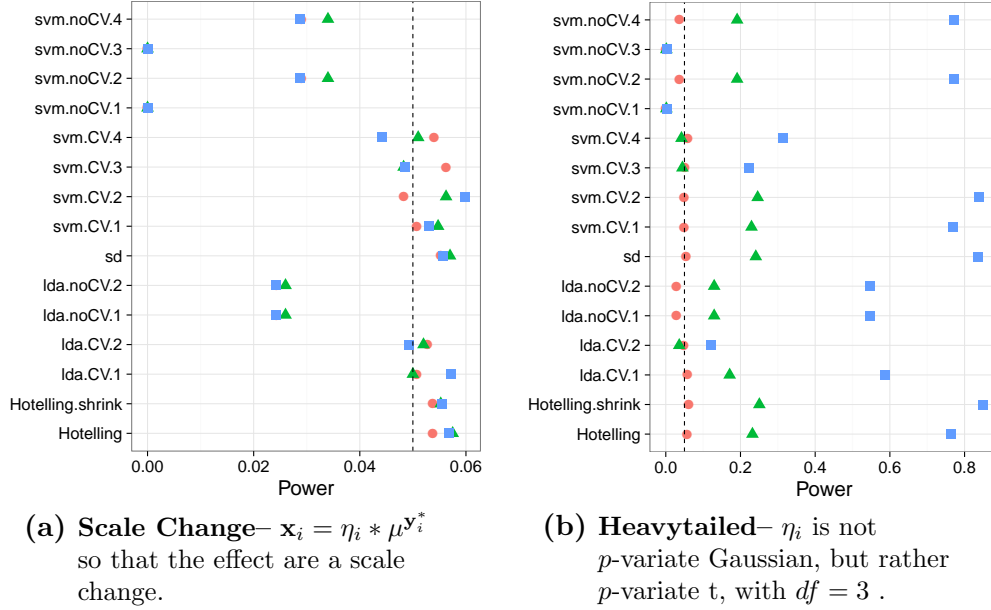
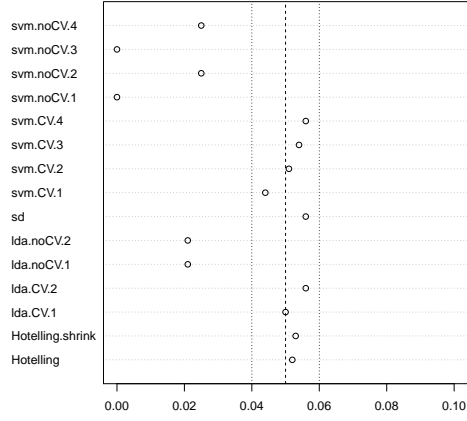
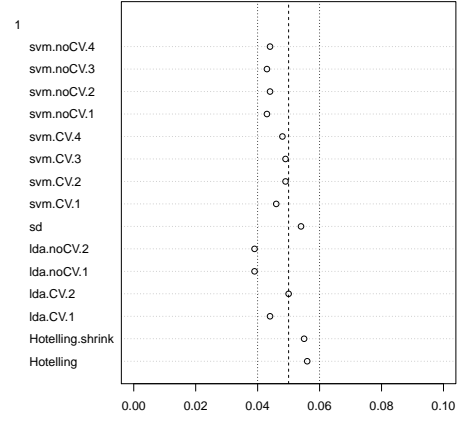


Figure 9: Simulation details in Appendix B except the changes in the sub-captions.

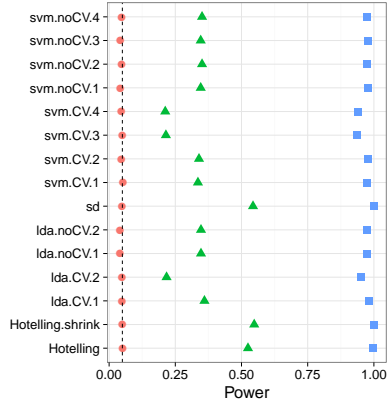


(a) Low-Dimension— False positive rates for $n = 40$.

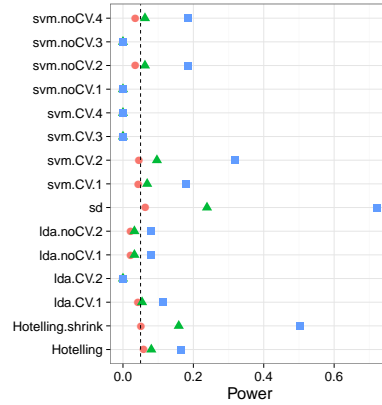


(b) High-Dimension— False positive rates for $n = 400$.

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—
 $\Sigma_{k,l} = \rho^{|k-l|}; \rho = 0.8$.