

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 the genetics literature, but to a lesser extent [Radmacher et al., 2002, 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* in Simon et al. [2003], or *pattern discrimination* in Pereira et al. [2009].

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 location test such as Hotelling’s T^2 [Anderson, 2003]. Alternatively, if the size of a brain region is too 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 [2013]. For brevity, and in contrast to *accuracy tests*, we will call these two-sample multivariate tests simply *location tests*, also termed *class comparisons* in Simon et al. [2003].

At this point, it becomes unclear which is preferable: a location 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 location and accuracy tests was precisely the goal of Ramdas et al. [2016], who compared the T^2 location 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 location tests are rate equivalent. Judging by convergence rates alone, not much is (asymptotically) lost by using an accuracy test. Asymptotic relative efficiency measures (ARE) are typically used by statisticians to compare between test statistics with similar rates [van der Vaart, 1998].

The ARE between Hotelling’s T^2 (location) test and Fisher’s LDA (accuracy) test in Ramdas et al. [2016] is lower bounded by $\sqrt{2\pi} \approx 2.5$. This means that Fisher’s LDA requires at least 2.5 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 location 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 2.5 is strong evidence in favour of the location test.

Before discarding accuracy tests, we recall that Ramdas et al. [2016] analyzed a half-sample holdout. The authors thus conjecture that a leave-one-out approach, which makes more efficient use of the data, may have better performance. On the other hand, the analysis in Ramdas et al. [2016] is asymptotic. This eschews the discrete nature of the accuracy statistic, which will shown to have a crucial impact. Since typical sample sizes in neuroscience

¹GoogleScholar. Accessed on Aug 4, 2016.

are not large, we seek to study which test is to be preferred in finite samples? Our conclusion will be quite simple: *location tests almost always have more power than accuracy tests.*

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

The discretization effect is aggravated if the test statistic is highly concentrated. For an intuition consider the usage of a the *training* accuracy as a test statistic. This is the *resubstitution accuracy* in Ramdas et al. [2016], and simply means that the accuracy is not cross validated. If the data is high dimensional, the train accuracy will be very high due to over fitting. In an extreme case, the train accuracy will be 1 for the observed data, but also for any permutaiton. The concentration of the train accuracy near 1, and its discreteness, render this test completely useless, with a power of 0.

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

2 Problem setup

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

Given n pairs of (x_i, y_i) , typically assumed i.i.d., a location test amounts to testing whether $x|y = 1$ has the the same distribution as $x|y = -1$. I.e., we test if the multivariate voxel activation pattern has the same distribution when given a vocal stimulus, as when given a non-vocal stimulus. An accuracy test amounts to learning a predictive model $\hat{f}(x)$ from some assumed model class $\hat{f} \in \mathcal{F}$. The prediction accuracy, denoted $T_{\hat{f}}^{acc}$, is defined as the probability of a given classifier \hat{f} of making a correct prediction $T_{\hat{f}}^{acc} := Prob(\hat{f}(x) = y)$ when given a randomly drawn data point, (x, y) .

101 A statistically significant “better than chance” estimate of $T_{\hat{f}}^{acc}$ is evidence
 102 that the classes are distinct.

103 2.1 Candidate Tests

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

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

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

118 **How to estimate accuracy?** Given a predictor \hat{f} , a natural test statis-
 119 tic is some estimate of its accuracy $T_{\hat{f}}^{acc}$. Complicating matters: very low
 120 accuracies, even 0, is evidence that the classes are separated, and we only
 121 need to invert the predictions. We can thus consider $|T_{\hat{f}}^{acc} - 0.5|$ as the test
 122 statistic. This, however, implies that if the classes are identical, random
 123 guessing has a 0.5 accuracy. This is not true if the classes are not balanced.
 124 The chance level in which case is the prevalence of the dominant class, we
 125 denote by \hat{p}_{max} . This suggests the following test statistic $|T_{\hat{f}}^{acc} - \hat{p}_{max}|$. Since
 126 we will be aggregating these statistic over random data sets where the dom-
 127 inant class may have varying frequencies, it seems appropriate to standard-
 128 ize the scale of this statistic. We thus also consider the z-scored accuracy:
 129 $|T_{\hat{f}}^{acc} - \hat{p}_{max}| / \sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$.

130 **Cross validate or not?** Were we interested in an unbiased estimator of
131 the prediction error, there is no question that some independent validation
132 is in order. Since we are merely interested in detecting a difference between
133 classes, a biased error estimate is not an issue provided that bias is consistent
134 over all permutations. The underlying intuition is that if the exact same
135 computation is performed over all permutations, then a permutation test
136 will be “fair”, i.e., will not inflate the false positive rate. We will thus be
137 considering both cross validated accuracies, and *train* accuracies as our test
138 statistics, a.k.a. *resubstitution classification* in Ramdas et al. [2016].

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

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

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

162 **How many folds?** Different authors suggest different rules for the num-
163 ber of folds. We will be varying the number of folds. This will affect the
164 concentration of permutation distribution of the estimated accuracy, which
165 will have a crucial effect on the conservativeness of the accuracy test. Our

intuition suggests that since more folds imply a less concentrated estimate, then leave-one-out should be the less conservative, and 2-fold should be the most conservative.

There are indeed many design choices when performing a permutation test using a cross validated statistic. The subset of tests we will be comparing is collected for convenience in Table 1.

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

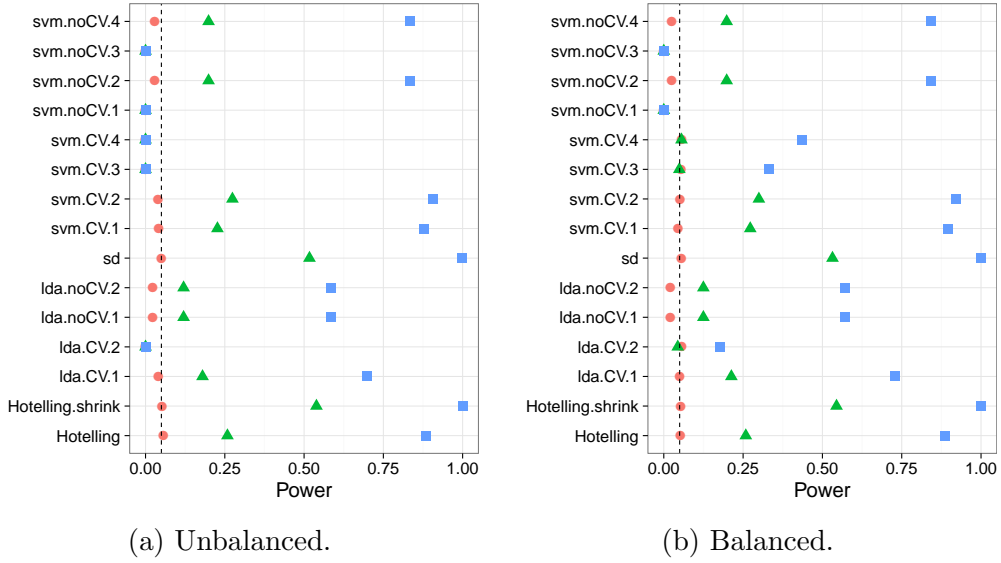
Table 1: This table enumerates the various test statistics we will be studying. Three are location tests: Hotelling, Hotelling.shrink, and sd. *Hotelling* is the classical two-group T^2 statistic. *Hotelling.shrink* is a high dimensional version with the regularized covariance in Schäfer and Strimmer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

3 Controlling the False Positive Rate

We start by verifying that the battery of tests in Table 1 control the false positive rate at the desired 0.05 level, with varying conservativeness levels. Figure 1 demonstrates that this is indeed the case. All our candidate tests

control the type I error, with varying degrees of conservativeness. In particular: (a) if the folds are balanced or not, (b) if the tuning parameters of some test statistic are varied, (d) if the number of folds is varied.

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



4 Power

Having established that all of the tests in our battery control the false positive rate, it remains to be seen if they have similar power; Especially when comparing the power of location tests to accuracy tests. On the other hand, the results of our previous sections suggest that the conservativeness of some of the considered tests can be considerable, rendering them underpowered.

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

We see by now that the use of accuracy tests for signal detection is underpowered compared to location tests. Simulations alone cannot, however, support such a universal statement. We will thus verify on a neuroimaging dataset, and discuss the causes for this phenomenon with implications on the scope of our statement.

191 5 Neuroimaging Example

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

199 We perform permutation inference using the pipeline of Stelzer et al.
200 [2013], which was also used in Gilron et al. [2016]. For completeness, the
201 pipeline is described in Appendix A. To demonstrate our point, we compare
202 the *sd* location test with the *svm.cv.1* accuracy test (see Table 1 for the
203 definition of these statistics).

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

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

213 6 Discussion

214 We have set out to understand which of the tests is more powerful: the
215 accuracy test or the location test. Using simulations, we have concluded
216 that the location tests are preferable. We attribute this to the discretization
217 introduced in finite samples by the accuracy test statistic. This also explains
218 why an asymptotic analysis, such as Ramdas et al. [2016], did not find a rate
219 difference. Their results however are limited in that: (a) they are asymptotic,
220 thus eschew the discretization effect. (b) They assume a half-sample holdout,
221 so that half of the data is available for estimation. (c) They assume a linear
222 classifier.

223 The linear classifier assumption, (c), is immaterial since for every non-
224 linear classifier, one may design a non-linear location test. See ? for an
225 example of a location test in RKHS space. [TODO: relate to large sample

²<https://openfmri.org/>



Figure 2: Brain regions encoding information discriminating between vocal and non-vocal stimuli. Map reports the centres of 27-voxel sized spherical regions, as discovered by an accuracy test (*svm.cv.1*), and a location test (*sd*). *svm.cv.1* was computed using 5-fold cross validation, and a cost parameter of 1. Region-wise significance was determined using the permutation scheme of Stelzer et al. [2013], followed by region-wise $FDR \leq 0.05$ control using the Benjamini-Hochberg procedure [Benjamini and Hochberg, 1995]. Number of permutations equals 400. The location test detect 1,232 regions, and the accuracy test 441, 399 of which are common to both. For the details of the analysis see Appendix A and Gilron et al. [2016].

simulation] [TODO: discuss ARE, and holdout versus leave one out effect].
[TODO: non-linear classification and testing].

Olivetti et al. [2012] and Olivetti et al. [2014] also looked into a similar problem as we do, namely, what is the preferred accuracy test? They propose a new test they call an *independence test*, and demonstrate by simulation that it has more power than other accuracy tests, and can deal with non-balanced data sets. We did not include this test in the battery we compared, but we note the following: (a) The independence test of Olivetti et al. [2012] relies on a discrete test statistic. This means that in the cases that the accuracy test is called upon for discriminating populations, it will probably be under-powered compared to location tests. (b) The problem of the accuracy test with unbalanced data-sets, which motivates Olivetti et al. [2012]’s independence test, can also be remedied by replacing the accuracy statistic with its z-score, as suggested in Section 2.1.

At this point some reservations to the generality of our findings are in

241 order. Firstly, not all accuracy tests are concerned with signal detection.
242 Indeed, it is possible that the purpose of the test is not to detect a difference
243 between classes, but to actually test if a particular classifier is better than
244 chance. This would be the case in decoding applications, like brain-machine
245 interfaces, where the localization of a signal is not enough. Clinical diagnosis is
246 another application, where the presence of a medical condition is “predicted”
247 from imaging data. [e.g. Olivetti et al., 2012, Wager et al., 2013]

248 Secondly, not all signals are manifested in a shift of the null distribution.
249 Put differently, the preferred alternative to an accuracy test is not always a
250 location test. Indeed, one may consider signal, i.e. effects, as a change in
251 scale, such as the *spiked covariance* model. In this case, other-than-Hotelling
252 type tests are appropriate [TODO: cite change in covariance alternative].
253 Tests have been proposed even when the nature of the difference between
254 populations is left unspecified [e.g. ?]. The fact that in our neuroimaging
255 example (Section 5) some brain regions were detected with the accuracy test,
256 and not the location test, is consistent with this observation. On the other
257 hand, the far greater power of the location test, certainly in our example,
258 does serve as empirical evidence that changes in location are a prevalent
259 phenomenon. [TODO: signal in scale? heavy tails?]

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

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

273 The recent popularity of machine learning has resulted in the ex-
274 tensive teaching and use of prediction in theoretical and applied
275 communities and the relative lack of awareness or popularity of
276 the topic of Neyman-Pearson style hypothesis testing in the com-
277 puter science and related “data science” communities.

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357 A Analysis pipeline

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

Algorithm 1: Compute a group parametric map.

Data: fMRI scans, and experimental design.
Result: Brain map of group statistics: $\{\bar{T}_v\}_{v=1}^V$

```

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

Algorithm 2: Compute a permutation p-value map.

Data: fMRI scans of 20 subjects, experimental design.
Result: Brain map of permutation p-values: $\{p_v\}_{v=1}^V$

```

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

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

B More Simulations

Figure 3: [TODO].

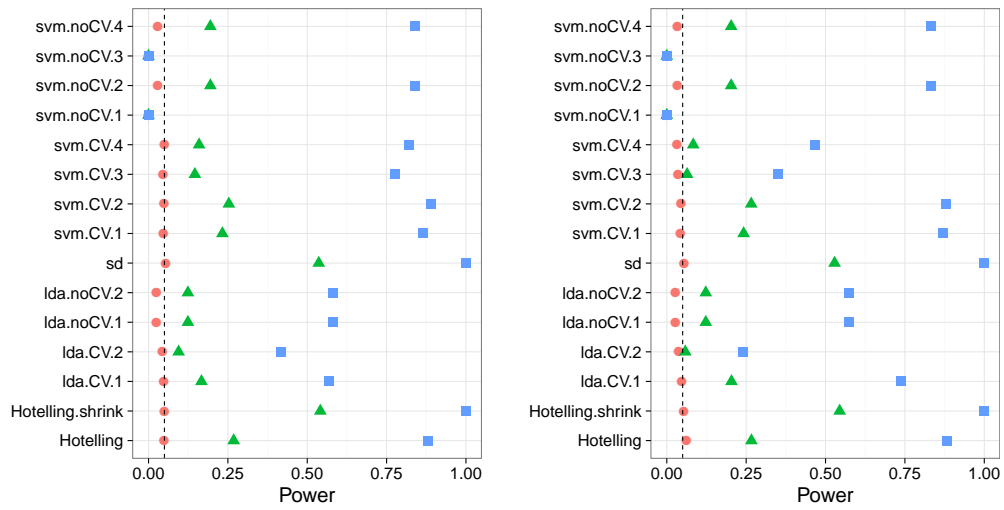


Figure 4: [TODO].

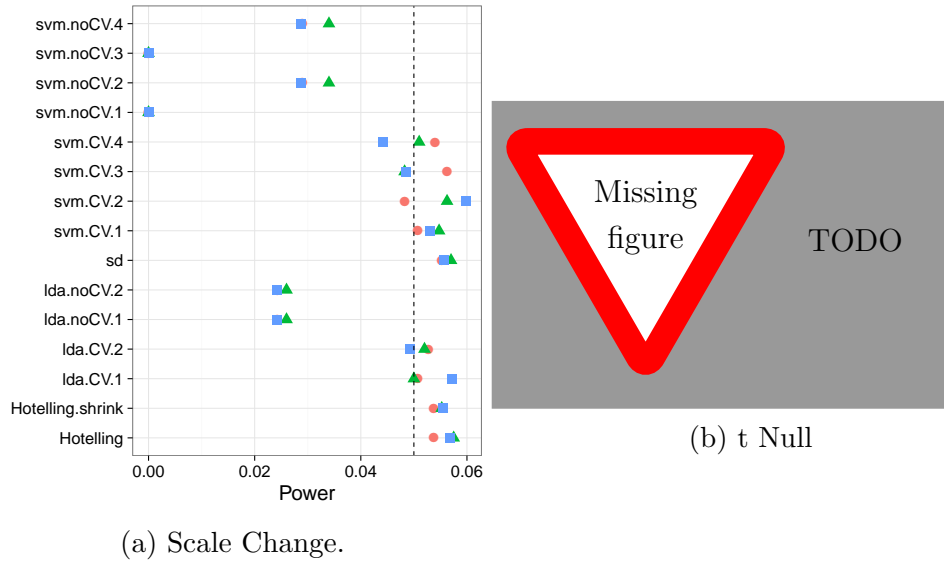


Figure 5: [TODO].

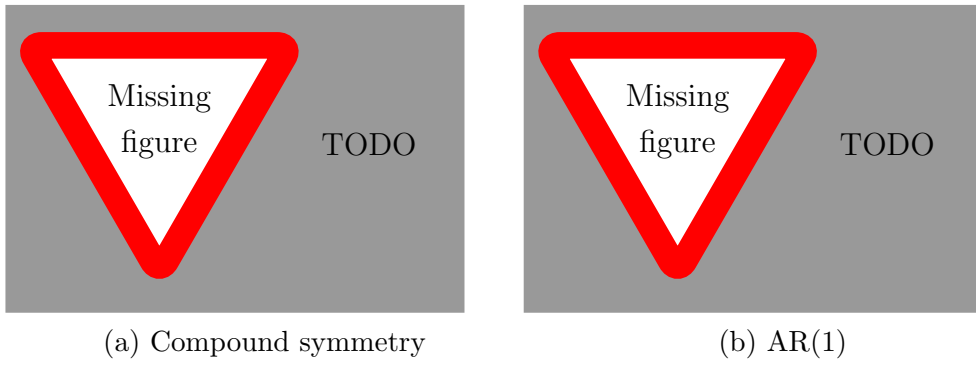


Figure 6: [TODO].

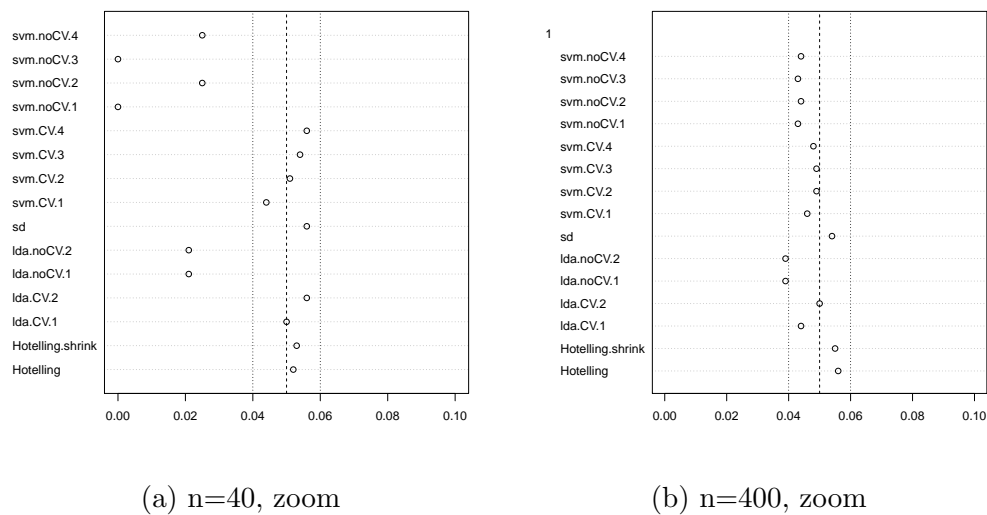


Figure 7: [TODO].

