

Better-than-chance classification for signal detection

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Abstract

[TODO]

1 Introduction

A common workflow in genetics or 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 genetics literature include Jiang et al. [2008], Radmacher et al. [2002] [TODO: elaborate]. Example sin the neuroscientific literature include [Golland and Fischl, 2003, Kriegeskorte et al., 2006, Pereira et al., 2009, Varoquaux et al., 2016]. The number of citations¹ of these papers attest to the popularity of the above workflow: 956 for Kriegeskorte et al. [2006], and 274 for Radmacher et al. [2002], as examples.

To fix ideas, we will adhere to a neuroscientific example: In Gilron et al. [2016], the authors seek to detect brain regions which encode differences between vocal and non-vocal stimuli. According to the MVPA analysis 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].

¹Based on GoogleScholar. Accesses on 26.7.2016.

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

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

31 A practitioner may then call upon a two-group location test such as Hotelling’s
 32 T^2 [Fujikoshi et al., 2011]. Alternatively, if the size of the brain region is too
 33 large compared to the number of observations, so that the spatial covariance
 34 cannot be fully estimated, then a high dimensional version of Hotelling’s test
 35 can be called upon, such as in Srivastava [2013] or Schäfer et al. [2005]. In
 36 contrast to *accuracy tests*, we call these *location tests*, a.k.a. *class comparison*
 37 in Simon et al. [2003].

38 At this point, it becomes unclear which is the preferred test. The compar-
 39 ison between location and accuracy tests was precisely the topic of Ramdas
 40 et al. [2016], who compared the Hotelling location test to the accuracy of
 41 *Fisher’s linear discriminant analysis* classifier (LDA) [Hastie et al., 2003].
 42 Using an asymptotic analysis, Ramdas et al. [2016] concluded that accuracy
 43 and location tests are equivalent with respect to their order of convergence
 44 to a consistent test, while they may differ in constants. Put differently, the
 45 (asymptotic) relative efficiency of the tests is not trivially 0 nor ∞ .

46 The relative efficiency, governing the power of the tests, may prove crucial
 47 when dealing with the finite sample sizes in neuroscience and genetics, and
 48 thus the focus of this study. We thus seek to study which test is to be
 49 preferred in finite samples? Our conclusion will be quite simple: *location*
 50 *tests almost always have more power than accuracy tests*.

51 The main argument for our statement rests upon the observation that
 52 with typical sample sizes, the accuracy test statistic is highly discrete. Dis-
 53 crete test statistics are known to be conservative [Hemerik and Goeman,
 54 2014], since they cannot exhaust the permissible false positive rate. For accu-
 55 racy tests, the degree of discretization is governed by the number of samples.
 56 In our running neuroscience example [Gilron et al., 2016], the classification
 57 is performed based on 40 trials, so that the test statistic may assume only 40
 58 possible values. This number of examples is not unusual if considering this
 59 is the number of subject in a genetic study, or the number of trial-repeats in
 60 an fMRI brain scan.

61 The discretization effect is aggravated if the test statistic is highly concen-
 62 trated. For an intuition consider the usage of the *train* accuracy test statistic

63 (i.e., not cross validated). In Section 4 we then address our main question-
 64 which test has more power? Based on the finding that the location test is
 65 typically more powerful, we try to offer an intuition for this phenomenon in
 66 the Discussion section.

67 2 Problem setup

68 Adhering to our neuroscientific example, we now formalize terminology and
 69 notation. Let $y \in \mathcal{Y}$ be a class encoding. In our vocal/non-vocal example
 70 we have $\mathcal{Y} = \{-1, 1\}$. Let $x \in \mathcal{X}$ be a p dimensional feature vector. In our
 71 vocal/non-vocal example p is the number of voxels in a brain region. We
 72 thus have $\mathcal{X} = \mathbb{R}^{27}$.

73 Given n pairs of (x_i, y_i) , typically assumed i.i.d., a location test amounts
 74 to testing whether $x|y = 1$ has the the same distribution as $x|y = -1$ (or
 75 at least the same location). I.e., the multivariate voxel activation pattern
 76 has the same distribution when given a vocal stimulus, as when given a non-
 77 vocal stimulus. An accuracy test amounts to learning a predictive model $\hat{f}(x)$
 78 from some assumed model class $\hat{f} \in \mathcal{F}$. The prediction accuracy, denoted
 79 $T_{\hat{f}}^{acc}$, is defined as the probability of a given classifier \hat{f} of making a correct
 80 prediction $T_{\hat{f}}^{acc} := Prob(\hat{f}(x) = y)$ when given a new, randomly drawn data
 81 point, (x, y) . A statistically significant “better than chance” estimate of $T_{\hat{f}}^{acc}$
 82 is evidence that the classes are distinct.

83 2.1 Candidate Tests

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

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

94 We will now address these questions while bearing in mind that unlike the
 95 typical supervised learning setup, we are not interested in an unbiased esti-
 96 mate of the prediction error, but rather in the mere detection of a difference
 97 between two groups, leading to a better-than-chance accuracy.

98 **How to estimate accuracy?** Given a predictor \hat{f} , a natural test statis-
 99 tic is some estimate of its accuracy $T_{\hat{f}}^{acc}$. Complicating matters: very low
 100 accuracies, even 0, is evidence that the classes are separated, and we only
 101 need to invert the predictions. We can thus consider $|T_{\hat{f}}^{acc} - 0.5|$ as the test
 102 statistic. This, however, implies that if the classes are identical, random
 103 guessing has a 0.5 accuracy. This is not true if the classes are not balanced.
 104 The chance level in which case is the prevalence of the dominant class, we
 105 denote by \hat{p}_{max} . This suggests the following test statistic $|T_{\hat{f}}^{acc} - \hat{p}_{max}|$. Since
 106 we will be aggregating these statistic over random data sets where the dom-
 107 inant class may have varying frequencies, it seems appropriate to standard-
 108 ize the scale of this statistic. We thus also consider the z-scored accuracy:
 109 $|T_{\hat{f}}^{acc} - \hat{p}_{max}| / \sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$.

110 **Cross validate or not?** Were we interested in an unbiased estimator of
 111 the prediction error, there is no question that some independent validation
 112 is in order. Since we are merely interested in detecting a difference between
 113 classes, a biased error estimate is not an issue provided that bias is consistent
 114 over all permutations. The underlying intuition is that if the exact same
 115 computation is performed over all permutations, then a permutation test
 116 will be “fair”, i.e., will not inflate the false positive rate. We will thus be
 117 considering both cross validated accuracies, and *train* accuracies as our test
 118 statistics.

119 **Refolding?** The standard practice in neuroimaging is to refold the data
 120 after each permutation. This is imperative if permuting labels while aiming
 121 at balanced data folds. This is not, however, imperative in general. For
 122 simplicity, we will adhere to the standard practice of refolding the data within
 123 each permutation.

124 **Permute labels of features?** While seemingly identical, the compound-
 125 ing of permutations with data foldings renders these two approaches distinct.
 126 As an example, consider balanced (stratified) K-fold cross validation where
 127 the initial data folding is balanced. After a label permutation, the original
 128 folds will probably not be balanced. If the *features* are permuted, then the

129 labels conserve their original fold assignments, and the original folds are bal-
 130 anced after each permutation. Since we only report results while refolding the
 131 data in each permutation, then the only difference between permuting labels
 132 and permuting features seems to be a computational one. We thus adhere
 133 to the more common, albeit less efficient practice, of permuting labels.

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

142 **How many folds?** Different authors suggest different rules for the num-
 143 ber of folds. We will be varying the number of folds. This will affect the
 144 concentration of permutation distribution of the estimated accuracy, which
 145 will have a crucial effect on the conservativeness of the accuracy test. Our
 146 intuition suggests that since more folds imply a less concentrated estimate,
 147 then leave-one-out should be the less conservative, and 2-fold should be the
 148 most conservative.

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

152 3 Controlling the False Positive Rate

153 We start by verifying that the battery of tests in Table 1 control the false
 154 positive rate at the desired 0.05 level, with varying conservativeness levels.
 155 Figure 1 demonstrates that this is indeed the case. All our candidate tests
 156 control the type I error, with varying degrees of conservativeness. In particu-
 157 lar: (a) if the folds are balanced or not, (b) if the tuning parameters of some
 158 test statistic are varied, (d) if the number of folds is varied.

159 4 Power

160 Having established that all of the tests in our battery control the false pos-
 161 itive rate, it remains to be seen if they have similar power; Especially, when

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 et al. [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 ($|T_{\hat{f}}^{acc} - \hat{p}_{max}| / \sqrt{\hat{p}_{max}(1 - \hat{p}_{max})}$, 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.

162 comparing the power of the location tests to the accuracy tests. The theo-
163 retical results of Ramdas et al. [2016] suggest that power should be of the
164 same order. On the other hand, the results of our previous sections suggest
165 that the conservativeness of some of the considered tests can be considerable,
166 rendering them underpowered.

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

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

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].



5 Neuroimaging Example

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

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

In agreement with our simulation results, the location test (*sd*) discovers more brain regions when compared to an accuracy test (*svm.cv.1*). The former discovers 1,232 regions, while the latter only 441, as reported in Figure 2. We emphasize that both test statistics were compared with the

²<https://openfmri.org/>

190 same permutation scheme, and the same error controls, so that any difference
 191 in detections is due to their different power.

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

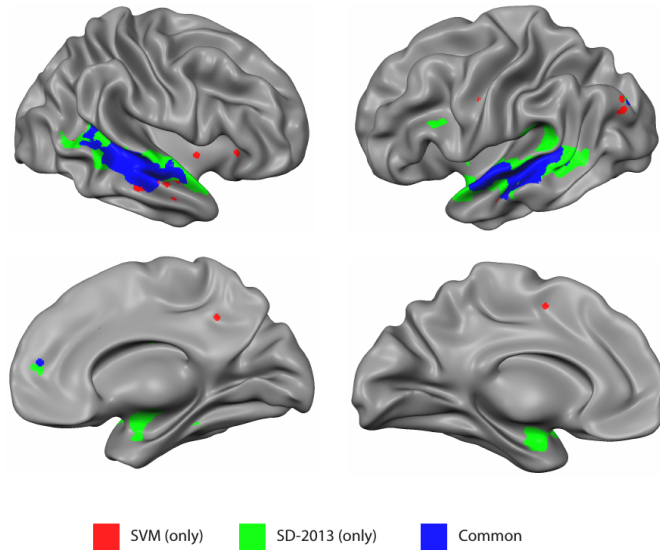


Figure 2: Brain regions encoding information discriminating between vocal and non-vocal stimuli. Map reports the centres of 27-voxel sized spherical regions, as discovered by an accuracy test (*svm.cv.1*), and a location test (*sd*). *svm.cv.1* was computed using 5-fold cross validation, and a cost parameter 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].

195 6 Discussion

196 We have set out to understand which of the tests is more powerful: the
 197 accuracy test or the location test. Using simulations, we have concluded
 198 that the location tests are preferable. We attribute this to the discretization
 199 introduced in finite samples by the accuracy test statistic. This also explains
 200 why an asymptotic analysis, such as Ramdas et al. [2016], did not find a
 201 qualitative difference. [TODO: relate to large sample simulation].

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

213 At this point some reservations to the generality of our findings are in
 214 order. Firstly, not all accuracy tests are concerned with signal detection.
 215 Indeed, it is possible that the purpose of the test is not to detect a difference
 216 between classes, but to actually test if a particular classifier is better than
 217 chance. This would be the case in decoding applications, like brain-machine
 218 interfaces, where the localization of a signal is not enough. Clinical diagnosis is
 219 another application, where the presence of a medical condition is “predicted”
 220 from imaging data. [e.g. Olivetti et al., 2012, Wager et al., 2013]

221 Secondly, there may be cases where the accuracy test does have more
 222 power than the location test. Our simulations were unable to point out such
 223 a scenario, but the fact that in our neuroimaging example (Section 5) some
 224 brain regions were detected with the accuracy test, and not the location test,
 225 suggest that the accuracy test does have more power for particular types of
 226 signal. [TODO: signal in scale? heavy tails?]

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

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

240 The recent popularity of machine learning has resulted in the ex-
 241 tensive 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 com-
puter science and related “data science” communities.

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316 A Analysis pipeline

317 Here is the analysis pipeline of Stelzer et al. [2013] we for the auditory data in
 318 Gilron et al. [2016]. Denoting by $i = 1, \dots, I$ the subject index, $v = 1, \dots, V$
 319 the voxel index, and $s = 1, \dots, S$ the permutation index. Since regions³ are
 320 centred around a unique voxel, the voxel index v also serves as a unique
 321 region index. Algorithm 1 computes a region-wise test statistic, which is
 322 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].

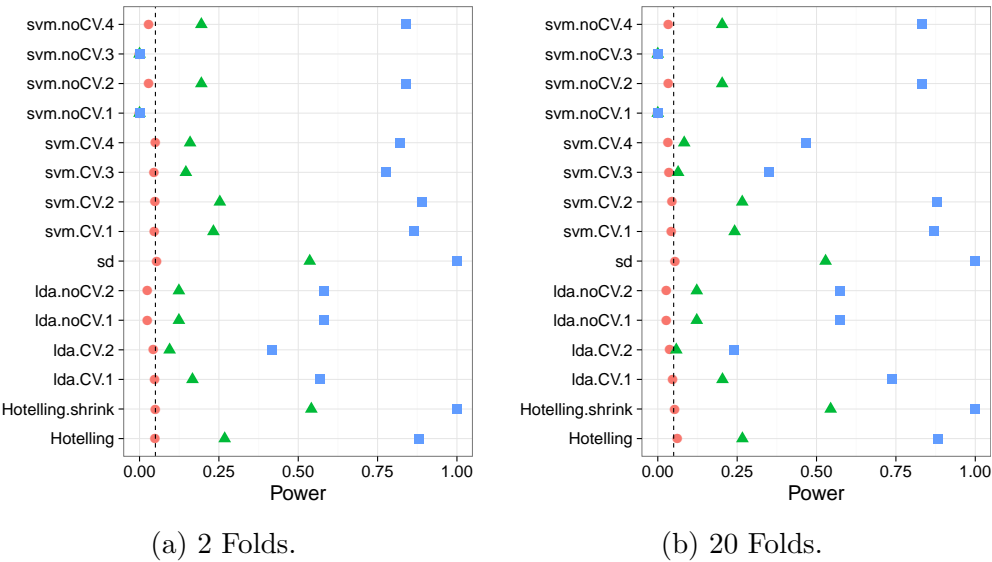


Figure 4: [TODO].

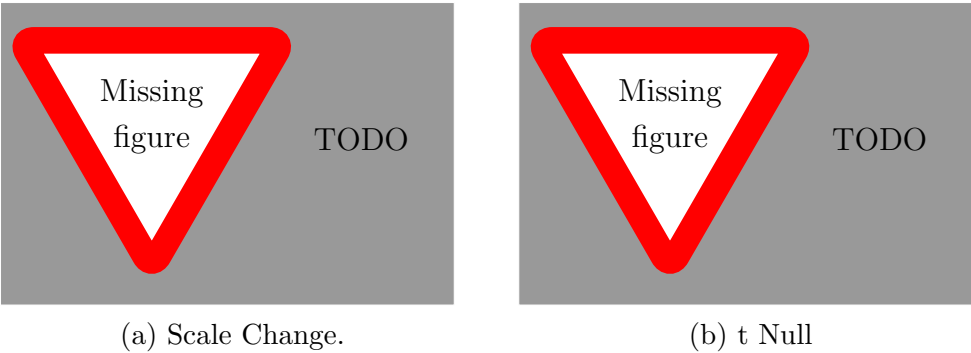
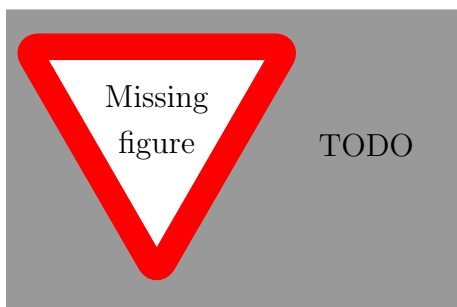
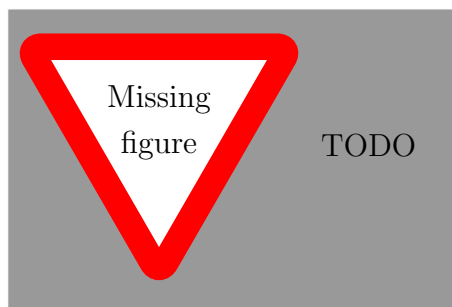


Figure 5: [TODO].



(a) Compound symmetry

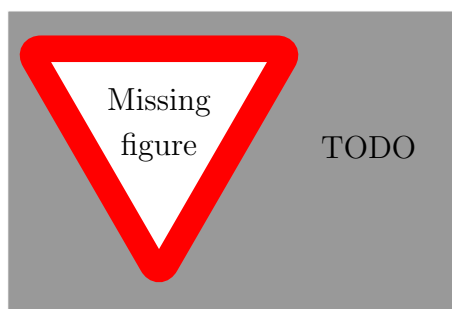


(b) AR(1)

Figure 6: [TODO].



(a) $n=400$



(b) ?