

1 Draft Version for internal usage:  
2 How to evaluate an agent's behaviour to  
3 infrequent events? – Reliable performance  
4 estimation insensitive to class distribution

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7 **Abstract**

8 In everyday life, humans and animals often have to base decisions on in-  
9 frequent relevant stimuli with respect to frequent irrelevant ones. When  
10 research in neuroscience mimics this situation, the effect of this imbalance  
11 in stimulus classes on performance evaluation has to be considered. This  
12 is most obvious for the often used overall accuracy, because the proportion  
13 of correct responses is governed by the more frequent class. This imbal-  
14 ance problem has been widely debated across disciplines and out of the  
15 discussed treatments this review focusses on performance estimation. For  
16 this, a more universal view is taken: an agent performing a classification  
17 task. Commonly used performance measures are characterized when used  
18 with imbalanced classes. Metrics like Accuracy, F-Measure, Matthews  
19 Correlation Coefficient, and Mutual Information are affected by imbal-  
20 ance, while other metrics do not have this drawback, like AUC, d-prime,  
21 Balanced Accuracy, Weighted Accuracy and G-Mean. It is pointed out  
22 that one is not restricted to this group of metrics, but the sensitivity to  
23 the class ratio has to be kept in mind for a proper choice. Selecting an  
24 appropriate metric is critical to avoid drawing misled conclusions.  
25

26 **Keywords:**

27 metrics, decision making, confusion matrix, oddball, imbalance, perfor-  
28 mance evaluation, classification

29 **1 Imbalance Is Common**

30 In their book on signal detection theory, Macmillan and Creelman debate that  
31 comparison is the basic psychophysical process and that all judgements are of  
32 one stimulus relative to another [Macmillan and Creelman, 2004]. Accordingly,

33 many behavioural experimental paradigms are based on comparisons (mostly of  
34 two stimulus classes), like the yes-no, same-different, forced-choice, matching-  
35 to-sample, go/no-go or the rating paradigm. When the correctness of such tasks  
36 is of interest, the overall proportion of correct responses over the two classes,  
37 i.e., the Accuracy (ACC) is the most straightforward measure. It can be easily  
38 computed and gives an intuitive measure of the performance as long as the two  
39 stimulus classes occur with equal probability. However, compared to the con-  
40 trolled situation in a lab where often judgements have to be made on balanced  
41 stimulus classes, natural environments provide generally different and more un-  
42 certain situations: the brain has to select the relevant stimuli irrespective of  
43 the frequency of their occurrence. Humans and animals are experts for this  
44 situation due to selection mechanisms that have been extensively investigated,  
45 e.g., in the visual [Treue, 2003] and the auditory [McDermott, 2009] domain.  
46 The behavioural relevance in a natural environment is not necessarily a matter  
47 of balance: if one is looking for an animal in the woods, the brain would have  
48 to reject many more of the irrelevant stimuli (wood) to successfully detect the  
49 relevant stimulus (animal). If the correctness of behaviour concerning the two  
50 classes is estimated for such an imbalanced case, a measure like the ACC is mis-  
51 leading, because it is biased towards the more frequent class [Kubat et al., 1998,  
52 for discussion]: missing an animal after correctly identifying many trees will not  
53 be revealed using the ACC. This is not only relevant under natural situations,  
54 but also for classical experimental paradigms, e.g., in oddball conditions which  
55 are essentially based on the fact that one class is more frequent than the other.  
56 In addition, such problems get even worse when one compares two situations  
57 with different class ratios or for dynamic situations where ratios may change  
58 over time, such as, e.g., in visual screening tasks [Wolfe et al., 2005].

59 To summarize, the question is how to estimate performance appropriately for  
60 imbalanced stimulus classes, i.e., which metric to use. Approaches to deal with  
61 imbalanced classes have been suggested in a number of disciplines taking differ-  
62 ent perspectives (outlined in Section 2). In this broader context, a more general  
63 view of a human, animal or an artificial system will be taken in the following:  
64 an agent that discriminates incoming (stimulus) classes. Given the high num-  
65 ber of performance measures suggested in the literature of various disciplines,  
66 the choice of an appropriate metric (or a combination) is not straightforward  
67 and often depends on more than one constraint. These constraints have to be  
68 considered carefully to avoid drawing false conclusions from the obtained metric  
69 value.

## 70 2 Existing Approaches To Deal With Imbalance

71 Existing approaches addressing the imbalance problem can be divided into three  
72 types: modification of the underlying data, manipulation of the way the data is  
73 classified, or application of a metric that should not be affected by imbalanced  
74 classes. When the data are modified, the single instances are resampled to a  
75 balanced situation before classification or evaluation [Japkowicz, 2000, Japkow-

76 icz and Stephen, 2002, Guo et al., 2008, Sun et al., 2009, Khoshgoftaar et al.,  
77 2010]. The approaches here use either oversampling of the infrequent class or  
78 undersampling of the frequent class, or a combination of both. On the classi-  
79 fier level, imbalance can be treated by introducing certain biases towards the  
80 infrequent class using internal modifications or by introducing cost matrices for  
81 different misclassification types. This approach is often used for artificial agents  
82 where the classification algorithm can be influenced in an explicit and formal  
83 way, e.g., by using cost-sensitive boosting [Sun et al., 2007]. These two types of  
84 approaches represent the most common in the fields of machine learning, where  
85 one has full access to the training data, the test data and the classification  
86 algorithm.

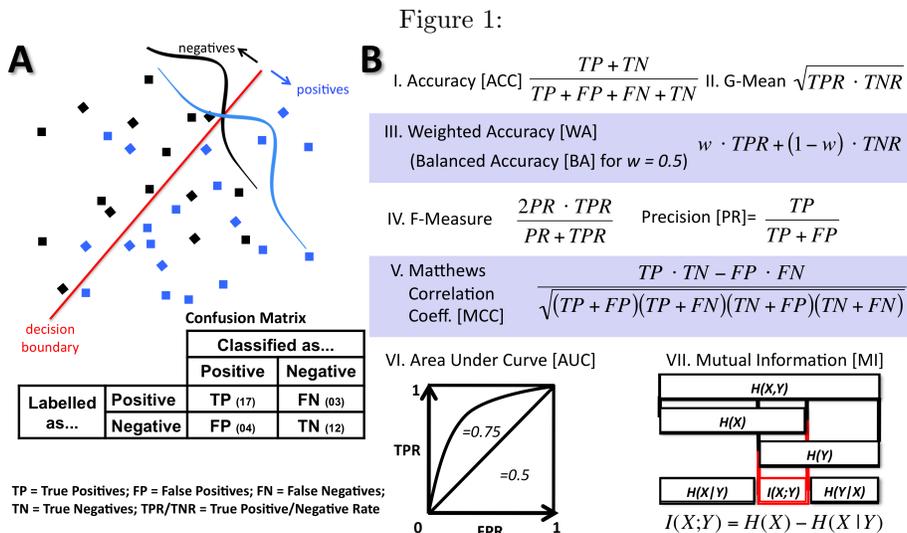
87 However, when one does not want to re-balance the data after the exper-  
88 iment, the third type of approach is the most favourable for investigating the  
89 behaviour of humans, animals or artificial systems. This is the typical situation  
90 in neuroscience where the behaviour is investigated *as is* (within the specific  
91 scope of the experiment). Across research areas different treatments have been  
92 proposed for evaluating imbalanced classes such as genetics [Velez et al., 2007,  
93 Garcia-Pedrajas et al., 2012], bioinformatics [Levner et al., 2006, Rogers and  
94 Ben-Hur, 2009], medical data sets [Cohen et al., 2003, 2004, Li et al., 2010],  
95 data mining, and machine learning [Fawcett and Provost, 1997, Bradley, 1997,  
96 Kubat et al., 1998, Gu et al., 2008, Powers, 2011]. In neuroscience, recent ap-  
97 proaches evaluating the performance of brain-computer interfaces are trying to  
98 find a more direct and intuitive measure of performance in imbalanced cases  
99 [Zhang et al., 2007, Salvaris et al., 2012, Hohne and Tangermann, 2012, Feess  
100 et al., 2013]. However, the decision for a single metric is often avoided by keep-  
101 ing the numbers for the two classes separated [Bollon et al., 2009, Kimura et al.,  
102 2010, e.g.].

103 Still there is no unified concept of how to deal with this problem and which  
104 metric to choose, although this would be highly beneficial: a performance mea-  
105 sure insensitive to imbalance enables straightforward comparisons between sub-  
106 jects or experiments, since individual differences in class ratio have no effect.  
107 While it is also feasible to avoid the imbalance problem by evaluating one class  
108 and ignoring the other, it bears the risk that performance qualities might be  
109 misjudged, as illustrated in Section 4. An agent might yield a high performance  
110 concerning one class, but might completely fail on the other. However, in real  
111 world situations, it is equally important that the agent *accepts* the relevant sig-  
112 nals and *rejects* the irrelevant ones. In most cases, the metric applied should  
113 directly reflect this overall behaviour.

### 114 3 Properties Of Existing Metrics

115 To perform the task, the agent has some learned decision boundary to separate  
116 the two classes as is formalised in Fig. 1A. Due to noise the agent labels instances  
117 to the wrong class, so that overlapping distributions with false positive (FP)  
118 and false negative (FN) decisions are obtained besides the correct ones (TP and

Figure 1 about here



119 TN). The confusion matrix comprises these four values and is the basis for most  
 120 performance metrics (compare Fig. 1A). Since the comparison of two matrices  
 121 is difficult without a way of combining its elements, a metric is often used to  
 122 compress the confusion matrix into a single number.

123 The choice of the metric itself heavily depends on the question addressed.  
 124 Yet, this choice can be justified by certain criteria serving as guidelines: the  
 125 metric should (i) evaluate the results of the agent and not the properties of  
 126 the data, i.e., it should judge true performance improvements or deteriorations  
 127 of the agent, (ii) be as intuitive to interpret as possible, and (iii) be applied  
 128 such that comparisons with the existing literature remain possible. After this  
 129 choice has been made, the results essentially depend on the metric properties.  
 130 In extreme cases, if it has been a bad choice, another metric might lead to  
 131 opposite conclusions.

132 Metrics that compress the confusion matrix into a single number are defined  
 133 in Fig. 1B. The ACC reflects the percentage of the overall correct responses and  
 134 does not distinguish between the two classes. For separate handling of the two  
 135 classes and thus a better approach to cope with imbalanced classes, the follow-  
 136 ing two metrics have been suggested which compute the mean of the TPR and  
 137 TNR. The Balanced Accuracy (BA), on the one hand, uses the arithmetic mean  
 138 [Levner et al., 2006, Velez et al., 2007, Rogers and Ben-Hur, 2009, Brodersen  
 139 et al., 2010, Feess et al., 2013]. The G-Mean [Kubat and Matwin, 1997, Kubat  
 140 et al., 1998], on the other hand, computes the geometric mean. The character-  
 141 istics of the two measures differ slightly: while the BA is still very intuitive to  
 142 interpret since ACC and BA are equal for balanced class ratios, the G-Mean is

143 additionally sensitive to the difference between TPR and TNR. It has also been  
144 suggested to use different weights for TPR and TNR, so that the BA becomes  
145 a special case of the Weighted Accuracy (WA) [Fawcett and Provost, 1997, Co-  
146 hen et al., 2003, 2004]. The additional parameter of the WA can be used to  
147 emphasize one class during evaluation.

148 When the decision criterion of the agent can be influenced, the receiver  
149 operating characteristic (ROC) curve [Green and Swets, 1988, Macmillan and  
150 Creelman, 2004] is a good starting point for evaluation. It shows the perfor-  
151 mance under a varying decision criterion (Fig. 1B). As a performance metric,  
152 the area under the ROC curve (AUC) is used [Swets, 1988, Bradley, 1997].  
153 Instead of comparing a single measure from a confusion matrix like the other  
154 metrics discussed here, it captures the trade-off between correct responses to  
155 both classes with the disadvantage that some decision criterion has to be var-  
156 ied. Calculation of this multi-point AUC is therefore not straightforward and  
157 has to be solved by numerical integration or interpolation. Two simplifications  
158 have been suggested to infer the AUC from a single data point: the interpola-  
159 tion of the ROC is either performed linearly which results in the same formula  
160 as the BA [Sokolova et al., 2006, Sokolova and Lapalme, 2009, Powers, 2011],  
161 or by assuming underlying normal distributions with equal standard deviations  
162 [Macmillan and Creelman, 2004]. The latter approach is often used in signal  
163 detection theory and psychophysics by rating detection performance with the  
164 sensitivity measure  $d'$  [Green and Swets, 1988, Stanislaw and Todorov, 1999,  
165 Macmillan and Creelman, 2004]. Each value of  $d'$  corresponds to one specific  
166 ROC curve with area  $AUC_z$  (see Fig. 1B).

167 In contrast to ROC analysis, computation of the F-Measure [Rijsbergen,  
168 1979, Powers, 2011] only requires three numbers from the confusion matrix  
169 (TP, FN and FP), because with the F-Measure one is solely interested in the  
170 performance on the positive class. It is often used in information retrieval when  
171 the negative class is not of interest, e.g., because the TNs cannot be determined  
172 easily. In this respect, it has been suggested as a metric for imbalanced classes.  
173 As indicated in Fig. 1B, the F-Measure combines the TPR with the proportion  
174 of all positive classifications that are correct, called precision (PR) or positive  
175 predictive value, using the harmonic mean of the two. Similar to the geometric  
176 mean, the harmonic mean is sensitive to differences of its entities.

177 An attempt to infer the goodness of performance from the correlation be-  
178 tween the true class labels and the agent's decisions is provided by Matthews  
179 Correlation Coefficient (MCC). The MCC (also known as phi correlation coeffi-  
180 cient) comes from the field of bioinformatics [Matthews, 1975, Gorodkin, 2004,  
181 Powers, 2011] and evaluates the Pearson product-moment correlation between  
182 the true labels and the classification outcome. For computation of the MCC,  
183 the two classes are not handled independently, as one can see from the equation  
184 in Fig. 1B.

185 Finally, the quantification of mutual information (MI) is, like the MCC, an  
186 attempt to compare the true world with the agent's decision. The difference is  
187 in the concept: MI, denoted by  $I(X;Y)$ , is based on the comparison of informa-  
188 tion content measured in terms of entropy. The entropy of the true world is the

189 prior entropy  $H(X)$  which is solely computed from the ratio between the two  
190 classes. The agent predicts  $H(X|Y)$  (calculated from the confusion matrix) us-  
191 ing his own entropy  $H(Y)$ . MI is a measure of what the classification result and  
192 the true class distribution have in common (compare Fig. 1B). It is often used  
193 in neuroscience to characterize the quality of neural responses [Pola et al., 2003,  
194 Smith and Dhingra, 2009, Quiroga and Panzeri, 2009] or has been suggested for  
195 the prediction of time series [Bialek et al., 2001]. As a performance measure, MI  
196 has been suggested for discrimination tasks as a tool to complement classical  
197 ideal observer analysis [Thomson and Kristan, 2005] and to evaluate classifica-  
198 tion performance [Metzen et al., 2011]. Since the raw value obtained for MI  
199 is depending on the prior entropy  $H(X)$  (determined from the class ratio), it  
200 is straightforward that MI values for different class ratios should be compared  
201 using a normalized MI (nMI) [Forbes, 1995].

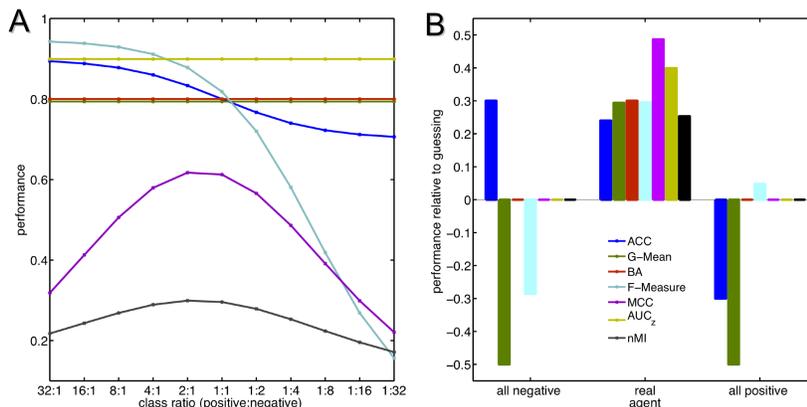
## 202 4 Different Metric – Different Result

203 The outcome of a study should not be affected by an improper choice of the  
204 metric. Here, the sensitivity of the described metrics to class imbalance is illus-  
205 trated with two examples that can be easily reproduced. In the first example,  
206 it is mimicked that a task has been performed and the investigator ends up  
207 with a confusion matrix and has to judge a performance. It is assumed that  
208 the agent performs with the same proportion of correct and incorrect responses  
209 irrespective of the ratio between the classes (TPR=0.9; TNR=0.7). Therefore,  
210 the agent would obtain twice as many TPs and FNs, when, the occurrence of  
211 the positive class is doubled. The metrics introduced in Section 3 were used to  
212 estimate the performance for each of the different class ratios applied. Sensi-  
213 tivities of these metrics to changes in the underlying class ratio are depicted in  
214 Figure 2A. ACC, F-Measure, MCC and MI behave sensitive to the introduced  
215 imbalance, because they are not built from a separate evaluation of the two  
216 classes. By contrast, G-Mean, BA (WA) and AUC ( $d'$ ) stay constant revealing  
217 what actually happened: the agent did not change its behaviour. This example  
218 illustrates how important it is to carefully select the metric with respect to the  
219 data.

220 The second example illustrated in Figure 2B takes a different perspective.  
221 What happens to the value of the respective metric when the class ratio is fixed,  
222 but the agent changes its strategy to the extreme case of responding solely with  
223 one class no matter which data it received? To illustrate this, the same confusion  
224 matrix as in the first example was used and the class ratio fixed to 1:4. The  
225 performance changes relative to pure guessing (TPR=TNR=0.5) are computed  
226 for an agent labeling all instances as negative or positive, respectively. Most  
227 metrics show what should be revealed: the modified agent is not better than  
228 guessing. However, the values obtained for ACC, F-Measure and G-Mean show  
229 a deviation from guessing. Most misleading is the obtained ACC of 0.8 for the  
230 case where all instances were classified as negative. This indicates a meaningful  
231 decision of the agent, and, yet, the ACC is purely based on the fact that the

Figure 2 about here

Figure 2:



232 negative instances are four times more frequent. Even worse, the estimated  
233 performance of this failing agent is better than the one of the real agent (0.74).

## 234 5 Conclusions: Metrics Insensitive to Imbalanced 235 Classes

236 Many treatments to the imbalance problem have been suggested, but only some  
237 of them are applicable when one wants to evaluate the behaviour of an agent  
238 that cannot be changed and comes *as is*, like it is often the case in neuroscientific  
239 studies. Then, the influence of different class ratios can be minimized by two  
240 approaches: either one can re-balance the data afterwards with the drawback  
241 of neglecting the true distributions in the task, or a metric can be chosen which  
242 is largely insensitive to the imbalance problem. The variety of used metrics  
243 makes this choice not straightforward. As has been illustrated, some metrics  
244 like the ACC are highly sensitive to class imbalance, while others like the BA  
245 are not. More generally, it appears that a reliable choice for imbalanced classes  
246 is a metric that separately treats positive and negative class as TPR and TNR,  
247 like WA, BA, G-Mean,  $d'$ , and AUC. Out of these, the BA is probably the most  
248 intuitive, because it can be interpreted similar to the ACC as a *balanced* percent  
249 correct measure. For the more general WA the respective weights have to be  
250 fairly determined, so if the two classes are equally important the BA is a proper  
251 choice.

252 Despite the fact that the situation is more complicated when more than  
253 two classes are considered, some of the principles illustrated here remain useful.  
254 Although the transfer of the suggested metrics to a multi-class scenario is not  
255 straightforward, it still holds that metrics that equally treat the existing classes

256 as performance rates are robust to changes in the individual class ratios. In  
257 addition, it would be favourable if the value of the metric is independent of the  
258 number of classes, such that, e.g., the same metric value in two experiments  
259 with different numbers of classes refers to the same performance. For the BA  
260 in an experiment with  $m$  classes, this could be achieved by summing up all  $m$   
261 rates and dividing them again by  $m$ . As an alternative approach, many multi-  
262 class problems can be boiled down to a two-class problem for evaluation, e.g.,  
263 by dividing the individual class examples into relevant and irrelevant before  
264 evaluation.

265 Finally, it should be stressed that the purpose of this review is to outline  
266 the implications when using imbalanced classes, and not to render metrics as  
267 generally inappropriate. Finding an appropriate metric for a particular question  
268 is complicated and often multiply constrained. Sometimes it may be necessary  
269 to use multiple metrics to complete the picture. When choosing a metric, one  
270 has to be aware of its particular drawbacks to know the weaknesses of one's  
271 own analysis. This is of critical importance, because the applied metric is the  
272 basis for all performance judgements in the respective task. Therefore, it should  
273 be informative, comparable and concurrently give an intuitive access for better  
274 interpretability. For imbalanced classes it is difficult to compare values of a  
275 metric where the guessing probability is depending on the class ratio, like is  
276 the case for the F-Measure. To generally improve the comparability between  
277 studies, the confusion matrix and an estimate of the class distribution could be  
278 supplementarily reported to the metric used. Many performance metrics can  
279 be computed from these numbers, so reporting these numbers could serve as a  
280 common ground to compare one's own results to existing ones even if a different  
281 metric was chosen. This information could be provided in a compressed way,  
282 e.g., the BA and the TPR alone can be used to compute a confusion matrix  
283 (containing rates).

## 284 **Disclosure/Conflict-of-Interest Statement**

285 The authors declare that the research was conducted in the absence of any  
286 commercial or financial relationships that could be construed as a potential  
287 conflict of interest.

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293 **Figure Legends**

294 **Figure 1: Confusion matrix and metrics.** (A) The performance of an  
 295 agent discriminating between two classes (positives and negatives) is described  
 296 by a confusion matrix. Top: The probabilities of the two classes are overlapping  
 297 in the discrimination space as illustrated by class distributions. The agent deals  
 298 with this using a decision boundary to make a prediction. Middle: The resulting  
 299 confusion matrix shows how the prediction by the agent (columns) is related to  
 300 the actual class (rows). Bottom: The true positive rate (TPR) and the true  
 301 negative rate (TNR) quantify the proportion of correctly predicted elements of  
 302 the respective class. The TPR is also called *Sensitivity* or *Recall*. The TNR  
 303 is equal to the *Specificity*. (B) Metrics based on the confusion matrix (see  
 304 text) grouped into sensitive and non-sensitive metrics for class imbalance when  
 305 both classes are considered. When the two classes are balanced, the ACC and  
 306 the BA are equal with the WA being a more general version introducing a class  
 307 weight  $w$  (for BA:  $w=0.5$ ). The BA is sometimes also referred to as the *balanced*  
 308 *classification rate* [Lannoy et al., 2011], *classwise balanced binary classification*  
 309 *accuracy* [Hohne and Tangermann, 2012], or as a simplified version of the *AUC*  
 310 [Sokolova et al., 2006, Sokolova and Lapalme, 2009]. Another simplification of  
 311 the AUC is to assume standard normal distributions so that each value of the  
 312 AUC corresponds to a particular shape of the ROC curve. This simplification  
 313 is denoted  $AUC_z$  and it is the shape of the AUC that is assumed when using  
 314 the performance measure  $d'$ . This measure is the distance between the means of  
 315 signal and noise distributions in standard deviation units given by the z-score.  
 316 The two are related by  $AUC_z = \Theta(d'/\sqrt{2})$  where  $\Theta$  is the normal distribution  
 317 function. An exceptional metric is the illustrated MI, because it is based on  
 318 the calculation of entropies from the confusion matrix. It can be used as a  
 319 metric by computing the difference between the prior entropy  $H(X)$  determined  
 320 by the class ratios and the entropy of the agent’s result  $H(X|Y)$  (calculated from  
 321 the confusion matrix). The boxes and connecting lines indicate the respective  
 322 entropy subsets. The MI  $I(X;Y)$  is a measure of what these two quantities share.

323 **Figure 2: Performance, Class Ratios and Guessing.** Examples of metric  
 324 sensitivities to class ratios (A) and agents that guess (B). Effect of the metrics  
 325 AUC and  $d'$  are represented by  $AUC_z$  using the simplification of assumed under-  
 326 lying normal distributions. The value for  $d'$  in this scenario is 0.81. Similarly,  
 327 the BA also represents the effect on the WA. (A) The agent responds with  
 328 the same proportion of correct and incorrect responses, no matter how frequent  
 329 positive and negative targets are. For the balanced case (ratio 1:1) the obtained  
 330 confusion matrix is [TP 90; FN 10; TN 70; FP 30]. (B) Hypothetical agent that  
 331 guesses either all instances as positive (right) or as negative (left) in comparison  
 332 to the true agent used in (A). Class ratio is 1:4, colours are the same as in (A).  
 333 The performance values are reported as difference to the performance obtained  
 334 from a classifier guessing each class with probability 0.5, i.e., respective perfor-  
 335 mances for guessing are: [ACC 0.5; G-Mean 0.5; BA 0.5; F-Measure 0.29; MCC  
 336 0;  $AUC_z$  0.5; nMI 0].

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