Abstract

No consistent conclusions have been drawn from existing studies regarding the effectiveness of different approaches to learning from imbalanced data. In this paper we apply bias-variance analysis to study the utility of different strategies for imbalanced learning. We conduct experiments on 15 real-world imbalanced datasets of applying various re-sampling and induction bias adjustment strategies to the standard decision tree, naïve bayes and k-nearest neighbour (k-NN) learning algorithms. Our main findings include: Imbalanced class distribution is primarily a high bias problem, which partly explains why it impedes the performance of many standard learning algorithms. Compared to the re-sampling strategies, adjusting induction bias can more significantly vary the bias and variance components of classification errors. Especially the inverse distance weighting strategy can significantly reduce the variance errors for k-NN. Based on these findings we offer practical advice on applying the re-sampling and induction bias adjustment strategies to improve imbalanced learning.

Keywords: Bias-Variance Analysis, Imbalanced Learning

1 Introduction

In many applications class distribution is imbalanced, and the minority class is by far the primary interest. In these applications, typically the purpose of classification learning is to correctly predict the minority class. For example predicting defects in source code is of utmost importance in software development projects, but defects only occur at a modest ratio of 5-10%. Accurate prediction of software defects can significantly reduce costs for software development.

Class imbalance has been reported to hamper the performance of standard classification models, whose aim is usually to optimize the overall accuracy. For example, the standard decision tree model tends to be overwhelmed by the majority class and ignore the minority class when making a decision about class labels.

Re-sampling and adjusting induction biases have been popular approaches to combating class imbalance. Changing the prevalence of positive and negative examples by sampling is a widely used method for addressing class imbalance. Strategies include random under-sampling of the majority class, random over-sampling of the minority class and more advanced intelligent over-sampling techniques (Kubat & Matwin 1997, Chawla et al. 2002). Adjusting the induction bias to favour the minority class is another method to achieve accurate classification on the minority class.

A natural question is what effect these imbalanced learning strategies have on the behaviour of standard learning algorithms. In particular, how well a model fits the problem under consideration and to what extent a model is affected by variation in class distribution. To this end we employ the bias and variance analysis of classification errors (Kohavi & Wolpert 1996) to improve our understanding of the behaviour of different learning algorithms in the presence of class imbalance, and the effectiveness of sampling and imbalance induction bias adjustment on different learning models.

With the bias-variance decomposition, three types of classification errors are distinguished: the bias errors are the systematic errors associated with the learning algorithm and the problem domain, the variance errors are caused by variations in samples and the intrinsic errors are associated with the inherent uncertainty of the problem domain. Generally high bias errors indicate that a model is not correct for the problem domain and high variance errors indicate unstable classification by the model. Intrinsic errors are associated with noise of the problem domain and is independent of the learning algorithm.

We employ the bias and variance decomposition of classification errors to study the behaviour of three representative learning algorithms, the C4.5 decision tree algorithm (Quinlan 1993), the naïve bayes (NB) (Good 1965, Duda & Hart 1973, Langley et al. 1992), and the k-nearest neighbour (k-NN) (Aha & Kibler 1991). We also study how random under- and over-sampling and advanced sampling techniques (See Section 3) vary the bias and variance components of errors for learning algorithms. We conduct a large-scale empirical study on 15 imbalanced datasets from the UCI repository and other disciplines.

Our main findings include: Imbalanced class distribution impedes the performance of standard learning algorithms in general, but depending on the learning algorithm, having varying effects on the bias and variance components of errors. The re-sampling strategies have varying effects on the bias or variance of learning algorithms. On the other hand adjusting the induction bias can significantly reduce the bias or variance components of errors, depending on learning algorithms. Based on these analysis we offer practical advice on applying the various re-sampling and induction bias adjustment strategies to combat the
imbalanced learning problem.

1.1 Related Work

A few empirical studies have studied and compared different sampling techniques (Japkowicz & Stephen 2002, Drummond & Holte 2003, Hulse et al. 2007). However, no consistent conclusions have been drawn from these studies. Most of these studies use a few datasets for experiments and so the conclusion is hard to generalize. A large scale experimental study was conducted in (Hulse et al. 2007), but datasets used in the study are not publicly available. It was found in (Hulse et al. 2007) that the effectiveness of re-sampling for imbalanced learning depends on the evaluation metrics and base learning algorithms. All these previous studies have examined the effectiveness of imbalanced learning strategies on classification accuracy. In this paper we focus on explaining the behaviour of imbalanced learning strategies with the bias and variance decomposition of classification errors. Our bias and variance analysis relates the inconsistent behaviour of re-sampling to that it does not generally have consistent effect on the bias or variance errors of learning algorithms. Importantly, we offer practical advice on how to combine re-sampling strategies for effective imbalanced learning.

When classification errors (misclassification costs) of different classes are distinguished, accuracy maximization is replaced with cost minimization – high cost is associated with misclassifying minority samples. Cost-sensitive learning methods (Domingos 1999) have been proposed to learn from imbalanced class distribution. In (Elkan 2001) the problem of optimal learning with different misclassification cost is studied. It is shown that in theory that rebalancing the positive and negative distribution has little effect on the decision tree and Bayesian methods. However this general theoretical result does not necessarily suggest that re-sampling strategies do not work in specific applications.

In an excellent survey by Weiss (Weiss 2004), techniques for imbalanced learning were reviewed. Sampling and adjusting decision bias are recognized as a commonly used technique for dealing with rarity, but no conclusion was drawn regarding their effectiveness. With some recent developments, advanced sampling techniques were proposed (Liu et al. 2006) for specific imbalanced learning applications. However, the general utility of these techniques is yet to be studied. The bias and variance analysis of classification errors (Kohavi & Wolpert 1996) is a widely used approach to provide insight into the error performance of classifiers. It has been used in various studies to compare the relative performance of different learning models, for example (Bauer & Kohavi 1999, Webb 2000, Putten & Someren 2004). To the best of our knowledge, it has not been used to study the problem of imbalanced classification.

2 Re-Sampling Strategies for Imbalanced Learning

Based on the assumption that standard learning methods perform better with equal class distribution, re-sampling training instances has been proposed for imbalanced learning.

2.1 Random Under-sampling and Over-sampling

Random under-sampling and over-sampling training instances are two basic methods of re-sampling for imbalanced learning. With under-sampling, examples of the majority class are randomly eliminated so as to achieve balanced class distribution. With over-sampling, examples of the minority class are randomly duplicated to achieve even class distribution. In essence, random over-sampling does not introduce new examples to directly bias the induction process. Some studies have shown that, compared with under-sampling, simple over-sampling is less effective at improving recognition of the minority class (Drummond & Holte 2003). However, another study that used artificial domains came to the opposite conclusion (Japkowicz & Stephen 2002).

2.2 Advanced Sampling Methods

A more advanced sampling method is to combine under-sampling and over-sampling to achieve balanced class distribution. This potentially can remedy the drawbacks when under-sampling and over-sampling are used separately. The Synthetic Minority Oversampling Technique (SMOTE) (Chawla et al. 2002) generates minority-class examples by adding examples from the line segments that join the $k$ minority-class nearest neighbours. This presumably leads to better generalization compared with random over-sampling. It was shown that a combination of over-sampling the minority class using SMOTE and under-sampling the majority class can achieve better classifier performance than only under-sampling the majority class. However, the effect of SMOTE alone on imbalanced learning has not been extensively studied.

3 Adjusting Induction Bias for Imbalanced Learning

In this section we discuss three popular base learning algorithms and where applicable, strategies adjusting their induction bias for imbalanced learning.

3.1 The Decision Tree

Some strategies have been proposed adjusting the decision tree induction to be more sensitive to imbalanced class distribution (Hulse et al. 2007):

- For imbalanced class distribution, pruning a decision tree can over generalize and completely ignore the positive class, and so decision trees are fully grown without pruning.

- Based on similar consideration, the minimal number of instances for leaves of a decision tree is set to one rather than a number > 1.

- With Laplace smoothing (Good 1965) the probability for the positive class at a leaf node is estimated as $\frac{L_p + 1}{L_p + L_n + 2}$, where $L_p$ and $L_n$ are respectively the number of positive and negative samples at the leaf. It has been shown that Laplace smoothing improves the tree performance for skewed class distribution.

3.2 The Naive Bayes

The Naive Bayes (NB) is a simple probabilistic induction model based on the Bayes Theorem (Duda &
In practical experiments it is impossible to estimate the intrinsic noise. The algorithm proposed in (Kohavi & Wolpert 1996) generates a bias term that includes the intrinsic noise. In their method, the training dataset is divided into a training pool and a test pool randomly. Each pool contains 50% of the training instances. Fifty training sets are generated from the training pool by random sampling. Classifiers are trained on each of the 50 training set, and bias and variance errors are estimated from the classifiers on the test set.

Generally there is a bias-variance tradeoff (Kohavi & Wolpert 1996). When adjusting a learning algorithm so that it is more sensitive to the training samples, its bias errors shrink but the variance errors increase. Learning models that overfit the given training data often have high variance errors — their results depend closely on the given training data and thus vary for different training datasets. On the contrary learning models with a strong induction bias are less likely to overfit and bias is a source of prediction errors if the induction bias of the model is not correct for a domain.

General description of the C4.5 decision tree, k-nearest neighbour and Naive Bayes learning algorithms in terms of their effect on the bias and variance components of classification errors is presented in Table 1. With the strong attribute-value independence assumption during classification, Naive Bayes has a strong induction bias. If the induction bias of NB is correct for the problem domain, then NB demonstrates low bias errors otherwise high bias errors. Without any representation model, the classification decision of k-NN does not have induction bias and its classification errors mainly come from variations in the distribution of training data. With a decision tree as the representation model, C4.5 has a medium level of induction bias. As a result the classification errors of C4.5 can come from the bias, variance or both components.

We can now characterise performance of the three base learning algorithms for imbalanced learning in terms of bias-variance decomposition. We can also characterise the effect of various re-sampling and induction bias adjustment strategies on the bias and variance components of errors.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Induction bias</th>
<th>Correct bias error</th>
<th>Correct variance error</th>
<th>Incorrect bias error</th>
<th>Incorrect variance error</th>
</tr>
</thead>
<tbody>
<tr>
<td>C4.5</td>
<td>medium</td>
<td>varying</td>
<td>varying</td>
<td>varying</td>
<td>varying</td>
</tr>
<tr>
<td>k-NN</td>
<td>weak</td>
<td>low</td>
<td>high</td>
<td>low</td>
<td>high</td>
</tr>
<tr>
<td>NB</td>
<td>strong</td>
<td>low</td>
<td>low</td>
<td>high</td>
<td>low</td>
</tr>
</tbody>
</table>

Table 1: The bias-variance relationship for C4.5, k-NN and NB

Hart 1973). NB estimates probabilities based on the attribute independence assumption. Although this assumption does not hold for many problems, NB often exhibits competitive classification accuracy compared with other learning algorithms. NB has a very strong induction bias and does not have any parameters that can be adjusted for imbalanced class distribution.

### 3.3 The k-Nearest Neighbour

With the k-nearest neighbour (k-NN) (Aha & Kibler 1991) algorithm, class labels of the k training instances closest to a test instance help determine the class label of the test instance. Inverse distance weighting is to weigh the vote of each neighbour according to the inverse of its distance from the test instance (Mitchell 1997). By taking the weighted average of the k nearest instances to the test instance, smooths out the impact of isolated noisy training instances. Furthermore it lifts the weight of instances from the minority class closest to the test instance — a point that has been largely overlooked by existing studies.

### 4 The Bias-Variance Analysis

The bias-variance analysis of classification errors is a useful tool for analysing classifier behaviour. This analysis decomposes classification errors into three terms, derived with reference to the performance of a learning algorithm when trained with different training sets drawn from some reference distribution of training sets:

- **Squared bias** denotes the systematic component of classification errors — how closely a learner describes the decision surfaces for a domain.
- **Variance** describes the component of classification errors from sampling — how sensitively a learner responds to variations in the training sample.
- **Intrinsic noise** measures the degree to which the target quantity is inherently unpredictable, which equals the expected cost of the Bayes optimal classifier.

There have been several proposals for the definition of the three terms for classification learning. The definition by Kohavi and Wolpert (Kohavi & Wolpert 1996) is widely used and is the definition we will use in this study. Given that an error has cost 1 and a correct prediction has cost 0, the expected error rate for a target function \( f \) and a training dataset of size \( m \) is

\[
err = \sum_x P(x)(\text{noise}_x^2 + \text{bias}_x^2 + \text{variance}_x)
\]

where \( x \) ranges over the instance space, and \( P(x) \) is the prior probability of \( x \).

In practical experiments it is impossible to estimate the intrinsic noise. The algorithm proposed
### Table 2: Fifteen datasets for experiments, ordered in decreasing level of skewedness.

<table>
<thead>
<tr>
<th>ID</th>
<th>Dataset</th>
<th>#instances</th>
<th>#attr (numerical, nominal)</th>
<th>Class (minority, majority)</th>
<th>Minority %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Oil*</td>
<td>990</td>
<td>47 (47, 0)</td>
<td>(true, false)</td>
<td>4.35%</td>
</tr>
<tr>
<td>2</td>
<td>Hypo-thyroid</td>
<td>3163</td>
<td>25 (7, 18)</td>
<td>(hypothyroid, negative)</td>
<td>4.77%</td>
</tr>
<tr>
<td>3</td>
<td>PC1*</td>
<td>1109</td>
<td>21 (21, 0)</td>
<td>(true, false)</td>
<td>6.94%</td>
</tr>
<tr>
<td>4</td>
<td>Glass</td>
<td>214</td>
<td>9 (9, 0)</td>
<td>(3, remainder)</td>
<td>7.94%</td>
</tr>
<tr>
<td>5</td>
<td>Flag</td>
<td>194</td>
<td>28 (10, 18)</td>
<td>(white, remainder)</td>
<td>8.76%</td>
</tr>
<tr>
<td>6</td>
<td>Satimage</td>
<td>6435</td>
<td>36 (36, 0)</td>
<td>(4, remainder)</td>
<td>9.73%</td>
</tr>
<tr>
<td>7</td>
<td>CM1*</td>
<td>498</td>
<td>21 (21, 0)</td>
<td>(true, false)</td>
<td>9.84%</td>
</tr>
<tr>
<td>8</td>
<td>New-thyroid</td>
<td>215</td>
<td>5 (5, 0)</td>
<td>(3, remainder)</td>
<td>13.95%</td>
</tr>
<tr>
<td>9</td>
<td>KC1*</td>
<td>2109</td>
<td>21 (21, 0)</td>
<td>(true, false)</td>
<td>15.46%</td>
</tr>
<tr>
<td>10</td>
<td>SPECT</td>
<td>267</td>
<td>22 (0, 22)</td>
<td>(0, 1)</td>
<td>20.60%</td>
</tr>
<tr>
<td>11</td>
<td>Hepatitis</td>
<td>155</td>
<td>19 (6, 13)</td>
<td>(1, 2)</td>
<td>20.65%</td>
</tr>
<tr>
<td>12</td>
<td>Vehicle</td>
<td>846</td>
<td>18 (18, 0)</td>
<td>(van, remainder)</td>
<td>23.52%</td>
</tr>
<tr>
<td>13</td>
<td>Splice-ei</td>
<td>3190</td>
<td>60 (60, 0)</td>
<td>(EI, remainder)</td>
<td>24.04%</td>
</tr>
<tr>
<td>14</td>
<td>Haberman</td>
<td>306</td>
<td>3 (3, 0)</td>
<td>(2, 1)</td>
<td>26.47%</td>
</tr>
<tr>
<td>15</td>
<td>German</td>
<td>1000</td>
<td>20 (7, 13)</td>
<td>(2, 1)</td>
<td>30.00%</td>
</tr>
</tbody>
</table>

In our experiments, we use classifiers J48, NB and IBk of the WEKA (Witten & Frank 2005) data mining software for the base algorithms C4.5 (Quinlan 1993) decision tree, NB and k-NN. The base algorithms with default settings, which usually are designed for uniform class distribution, are compared against their settings for adjusting induction bias for skewed class distribution. Specifically, for J48 the imbalance-favourable settings are without pruning, with Laplace-smoothing and that minimum one instance is allowed for a leaf node. For IBk, the imbalance-favourable settings are k=3, and inverse-distance weighted voting. There are not any parameter settings for adjusting bias for imbalanced distribution.

We use the instance re-sampling filters in WEKA to implement the re-sampling strategies in Section 3. For under-sampling, the majority class is randomly under-sampled with replacement so that it has the same number of instances as the minority class. For over-sampling, the minority class is randomly over-sampled so that it has the same number of instances as the majority class. The SMOTE filter in WEKA is used for the SMOTE over-sampling strategy.

### 6 The Bias-Variance Analysis of Imbalanced Learning

In our experiments we employ the bias and variance decomposition software in the WEKA toolkit to provide a measure of the squared bias and intrinsic noise combined error and the variance error component for classification algorithms. The bias and variance decomposition algorithm in WEKA precisely follows the approach of (Kohavi & Wolpert 1996), as described in Section 4.

#### 6.1 The bias-variance decomposition for base learning algorithms

Fig. 1 shows the bias and variance decomposition of expected errors for the base algorithms C4.5, k-NN and NB on 15 datasets in our experiments. Generally for all three base algorithms, the bias component is the dominant source of errors. Not surprisingly NB has the highest bias component of errors — except on Oil where bias comprises 43.94% of errors, on all other datasets bias is the bigger proportion of errors, comprising on average 81.02% of errors. C4.5 and k-NN demonstrates varying bias-variance decomposition on 15 datasets, with the bias portion of errors ranging from 43.82% (C4.5 on Vehicle) to 98.10% (C4.5 on Flag).

The BVD profile for base algorithms differ on each dataset. For example on the most imbalanced Oil dataset, the bias component of errors for C4.5, k-NN and NB are dramatically different, 57.89% for C4.5, 79.79% for k-NN and 43.94% for NB respectively. On the Vehicle dataset, the bias component is respectively 43.82% for C4.5, 51% for k-NN and 92.94% for NB.

Our analysis suggests that imbalanced class distribution has different effect on the base learning algorithms and it varies significantly for different problems. This complex profile of bias-variance component suggests that learning from imbalanced class distribution is a challenging problem.

#### 6.2 The bias-variance decomposition for sampling techniques

A relatively large number of instances in the training dataset is needed to ensure accurate estimation of errors. In our experiments the smallest dataset (Hepatitis) contains 155 instances, which we consider sufficiently large. Undersampling the majority class to match the minority can result in some datasets have a very small number of instances. We chose datasets whose total number of instances is at least 100 after undersampling. As a result only 10 datasets are included in our experiments of the bias-variance decomposition for the random under-sampling strategy, as is shown in Fig. 2. To compare under-sampling against other sampling techniques, the same datasets were used for the experiments of the other sampling strategies.

From Fig. 2 it can be seen that generally random under-sampling increases both the bias and variance errors for all three base learning algorithms, and the increase in variance errors is more pronounced than that in the bias errors. k-NN demonstrates the most consistent and significant response to under-sampling – on all 10 datasets both its bias and variance components of errors significantly increase, and the increase in variance is more pronounced. C4.5 is also very sensitive to under-sampling, and shows increment in both bias and variance errors on all 10 datasets. In contrast NB is not so sensitive to the under-sampling strategy. On KC1 the bias errors for under-sampling
Figure 1: The bias-variance decomposition for base algorithms C4.5 (J48), k-NN (IBk) and NB

Figure 2: The bias-variance decomposition for the under-sampling strategy
Figure 3: The bias-variance decomposition for the over-sampling strategy

Figure 4: The bias-variance decomposition for the SMOTE over-sampling strategy
Figure 5: The bias-variance decomposition for base C4.5 and imbalanced C4.5

Figure 6: The bias-variance decomposition for base $k$-NN and imbalanced $k$-NN
remain the same as that of the standard NB.

In Fig. 3, generally for random over-sampling, the three base learning algorithms do not show significant changes in the bias errors on most datasets. On the other hand random over-sampling has different effects on the variance of the three base learning algorithms — C4.5 and $k$-NN show increase in variance, while NB does not demonstrate change in variance errors on most datasets.

In Fig. 4 generally SMOTE over-sampling does not show significant changes in either the bias or variance errors on most datasets (except for the bias component of C4.5 on Haberman), and this is universally true for all three learning algorithms.

As a summary, our experiments have demonstrated that either random over-sampling or SMOTE intelligent over-sampling does not significantly change the bias errors of the three base learning algorithms. This can be explained by that the generated new samples are either replicates or near replicates of existing positive samples and they do not produce effect on the decision boundary for classes. Over sampling generally can also negatively affect the variance errors of the decision tree and $k$-nearest neighbour models, and it does not change the variance of NB.

In contrast, under-sampling significantly changes the bias and variance of base algorithms, due to the fact that some “important” samples affecting the decision for class boundary may have been removed. However, generally the effect is “negative”, that is the bias and variance errors of all algorithms are exacerbated rather than reduced.

6.3 The bias-variance decomposition of induction bias adjustment techniques

Fig. 5 and Fig. 6 show the bias and variance decomposition of expected errors for C4.5 and $k$-NN respectively on 15 datasets. It can be seen from Fig. 5 that for C4.5 the imbalance-favourable induction adjustment strategies, namely no pruning, minimal one instance for leaf nodes and Laplace smoothing, do not change the bias errors of the decision tree model on most datasets, but they significantly increase the variance errors on many datasets ($p$-value=0.00055 in the Wilcoxon signed rank test). Given that these strategies mainly affect the decisions towards the leaves of a decision tree, it is not surprising that the variance of the decision tree algorithm increases significantly on most datasets — most variance errors come from leaves at the bottom of the tree. In contrast branches towards the root of the tree are mostly unaffected by these bias adjustment strategies and therefore the bias errors of the algorithm do not change on most datasets.

In Fig. 6 the “inverse distance weighting” heuristic significantly reduces the variance component of $k$-NN significantly on all 15 datasets, with $p$-value = 0.00083. It is also noteworthy that the strategy has never exacerbated the bias errors on any dataset. Furthermore on CM1, SPECT, Hepatitis, Splice, Haberman and German, bias errors are significantly reduced.

Comparing the imbalance bias adjustment strategies of C4.5 and $k$-NN, the strategies in the decision tree algorithm has focused on modifying the representation tree for classification, especially towards the leaves at the bottom of the decision tree. Such strategies exacerbate the variance errors of the decision tree model. As a learning algorithm without explicit model representation, the imbalance induction bias adjustment of $k$-NN reduces both the bias and variance errors of the learning algorithm. This shows that the strategy has improved both the generality and stability of the $k$-NN algorithm.

7 Discussions and Conclusions

In this paper we have studied the re-sampling approach and the adjusting induction bias approach for employing standard learning algorithms for imbalanced classification. The re-sampling strategies we consider include random over-sampling, random under-sampling and SMOTE intelligent over-sampling. We employ bias-variance analysis to study the behaviour of re-sampling and imbalance bias adjustment on 15 real-world imbalanced datasets for popular algorithms, including the decision tree, Naive Bayes and $k$-nearest neighbour.

We have found that imbalanced class distribution impedes the performance of standard learning algorithms in general, but depending on the learning algorithm, having varying effects on the bias and variance components of errors. For the naive bayes algorithm, class imbalance mainly presents as a high bias problem, whereas for the decision tree and $k$-nearest neighbour models, errors can come from either the bias or variance component, depending on the application domain.

Over-sampling alone, either randomly or intelligent like SMOTE, does not have significant impact on the bias of any of the three learning algorithms. It exacerbates the variance errors of the decision tree model and $k$-NN to different degrees but does not change the variance of the Naive Bayes. Random under-sampling on the other hand, exacerbates the bias and variance errors of all three learning algorithms. Our practical advice in this regard is therefore to apply the sampling strategies on problems with low bias errors and to intelligently combine the over-sampling with under-sampling to reduce the variance errors. More research is needed to investigate how to best combine under-sampling and over-sampling.

Our experiments on C4.5 has shown that the strategies adjusting the imbalance induction bias for the decision tree model as described in Section 3 can exacerbate the variance errors, while such strategy for the $k$-NN model can reduce the variance as well as bias errors. So for the decision tree model the imbalance bias adjustment strategies should be executed with care. Specifically they should be applied to problems with low variance errors. In contrast the imbalance induction bias adjustment strategy for the $k$-NN algorithm is strongly recommended.

The simple Naive Bayes model, with a strong induction bias, presents as a high bias problem with the imbalanced class distribution. It is noteworthy that our experiments show that the Naive Bayes model is a stable model whose bias and variance are not sensitive to the various sampling techniques. An alternative promising approach to improving the Naive Bayes model for imbalanced learning may be to reduce the bias component by relaxing the “naïvety” of the induction process.

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