Representing Classification Problems in Genetic Programming

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Abstract - In this paper five alternative methods are proposed to perform multi-class classification tasks using genetic programming. These methods are: Binary decomposition, in which the problem is decomposed into a set of binary problems and standard genetic programming methods are applied; Static range selection, where the set of real values returned by a genetic program is divided into class boundaries using arbitrarily chosen division points; Dynamic range selection in which a subset of training examples are used to determine where, over the set of reals, class boundaries lie; Class enumeration which constructs programs similar in syntactic structure to a decision tree; and evidence accumulation which allows separate branches of the program to add to the certainty of any given class.

Results showed that the dynamic range selection method was well suited to the task of multi-class classification and was capable of producing classifiers more accurate than the other methods tried when comparable training times were allowed. Accuracy of the generated classifiers was comparable to alternative approaches over several datasets.

1 Introduction

Genetic programming (GP) is a way of automatically constructing computer programs using a process analogous to biological evolution [6]. As a relatively new approach to problem solving, GP has been applied to a range of tasks including that of classification [3, 4, 5].

Due to the extremely flexible nature of computer programs to represent solutions to problems, GP methods of problem solving have a great advantage in their power to represent solutions to complex problems, and this advantage remains true in the domain of classification. This flexibility of representation gives genetic programs the capacity to represent classification problems with means unavailable to other commonly used classification techniques such as decision trees, statistical classifiers and neural networks. Because of this it is possible that GP methods could be more suited to some classification problems than other classification methods.

One advantage of using the GP methodology for classification tasks is that the more training time that is allowed the more accurate (to the point where over-fitting begins to occur) the classifier can be trained. If large amounts of time are available to train classifiers then this time can be utilised to better train genetic classifiers. This is an advantage over some other methods for performing classification (eg. C4.5), which will always produce the same classifier regardless of the amount of time available for training. Another advantage for GP is that each run is probabilistic and different runs attempting to solve the same problem will virtually never produce the same result. Such variability of the final solution lends GP classifiers well to a voting strategy, which is often able to produce more accurate classification results.

Of great importance to any programming language’s capacity to represent a solution to a problem are the syntactic rules of the language and the set of primitive functions, types and operators in the language. This remains true for genetic programs, and when formulating such rules and primitives for a GP system for classification, the choice as to which rules and primitives to employ is one of uncertainty.

The aim of the research is to explore methods by which multi-class classification can be implemented within the GP paradigm and to identify which of these methods are most suited to the task of classification in terms of accuracy of classification and the amount of time needed to arrive at accurate solutions. Five alternative program representation methods, comprised of different syntactic rules, language primitives and decision strategies are developed and tested against a set of classification tasks.

1.1 Genetic Programming and Classification Tasks

Generally GP trees can perform classification by returning numeric (real) values and then translating these values into class labels [12, 13]. For binary classification problems the division between negative and non-negative numbers acts as a natural boundary for a division between two classes. This means that genetic programs can easily represent binary class problems. Unfortunately, when more than two classes are involved, finding meaningful division points over the set of reals the genetic programs return is more difficult. If boundary regions are chosen at arbitrary points over the set of reals then genetic programs face the problem of not only containing the necessary elements to distinguish between classes, but also must perform a translation task to provide output in the necessary range pre-specified for a given class.

Several investigations have previously employed a GP search strategy to generate a decision tree classifier [2, 9]. These investigations have shown the method to be capable...
of producing accurate classifiers. Such classifiers do however limit the produced programs to decision tree structures, which are more constrained (and thus less able to express certain problems) than standard genetic programs returning real values.

Previous investigations into classification using GP have produced accurate classifiers for binary class problems [3, 4]. GP employed for classification tasks do however have a requirement for long training times when compared to many other classification methods. It is also often quite difficult to extract a meaningful reason as to why a given class was chosen. Because of these factors the GP method is seen to be applicable to tasks where accuracy is the most important factor in classification, and training times and understandability are seen as relatively unimportant.

2 The Datasets

A set of six datasets were chosen from the UCI Machine Learning repository [1]. These datasets were chosen because they show variety in their domain, size and in the difficulty of classification. They also vary in the number of target classes for classification. All datasets were comprised of numeric or binary attributes. These datasets were also used in [7] and therefore allow direct comparison of results of GP classifiers to results of well known classification methods. The data sets are as follows:

1. Wisconsin Breast Cancer [8] (W.B.C): Consists of 2 classes and 10 numerical attributes with 699 instances. Sixteen instances containing missing values were removed for the purposes of classification in this investigation. Error rates were estimated using ten fold cross validation.

2. BUPA Liver Disorders (BUPA): Consists of 2 classes and 6 numerical attributes with 345 instances. Error rates were estimated using ten fold cross validation.

3. Pima Indians Diabetes (Pima): Consists of 2 classes and 8 numerical attributes with 768 instances. Error rates were estimated using ten fold cross validation.

4. Satlog Pixel (Pixel): Consists of 6 classes and 36 numerical attributes with 4435 instances. Error rates were estimated using an independent test set of 2000 instances.

5. Thyroid disease (Thyroid): Consists of 3 classes with 15 binary attributes (considered to be numerical for this investigation) and 6 numerical attributes. There were 3772 instances in the training set. Error rates were estimated using an independent test set of 3428 instances.

6. Vehicle silhouette (Vehicle): Consists of 4 classes and 18 numerical attributes with 846 instances. Error rates were estimated using ten fold cross validation.

3 Classifier Representation

Five alternative representation methods were implemented to produce solutions for the classification problems listed above. In each case strongly typed genetic programming [10] was used to construct genetic programs. For each method the terminal and function sets were kept as similar as possible so that the different GP methodologies had the same elements to construct solutions for the classification tasks. It was necessary to make some changes to the function and terminal set for the implementation of each representation method.

The five representation methods used were:

3.1 Binary Decomposition of Classification Problem

Standard methods of genetic program representation are able to perform binary classification tasks with a high degree of accuracy [4, 12]. Unfortunately, when more than two classes are involved, finding meaningful division points over the set of reals the genetic programs return, which then allow the output of a program to be interpreted as more than two classes, is more difficult. The problem of choosing arbitrary values can be avoided however by decomposing a multi-class problem into a set of binary classification problems [3, 4]. Given a problem set of $n$ classes $P = \{e_1, e_2, \ldots, e_n\}$, the problem can be decomposed into $n-1$ binary classification problems. The first binary problem will be to distinguish between classes $\{e_1, x\}$ where $x$ is an amalgamation of all other classes in the problem set. Ie: $P = \{e_1\}$. The second problem will be to classify $\{e_2, y\}$ where $y$ is all remaining classes $P - \{e_1, e_2\}$. This decomposition will continue until problem $n-1$, which will consist of only $\{cn-1, cn\}$, itself a binary classification problem.

Once solutions to all binary classification problems can be found, the amalgamation of these solutions forms a solution to the problem as a whole. The error rate of such a classifier would normally be found by applying the amalgamation of solutions to a test set. Due to the difficulty of attaining such an amalgamation initially in the GP methodology, in this implementation the error rate of the solution is calculated by adding the error rate of each component. Each binary solution was therefore weighted to account for only the section of the problem that it attempted to solve. The calculation of the error rate for the overall problem was:

$$E = \sum_{i=1}^{n-1} E(i) \times \frac{|i|}{|P|}$$

where $i$ is a binary decomposition, $P$ is the overall problem set, $E(i)$ is the error rate of the solution for decomposition $i$, and $n$ is the number of distinct classes in the problem. This means that for the first binary decomposition the error rate is simply added to the overall error rate as $|i|$ will be equal to $|P|$. The second decomposition will add only a proportion of its error rate to the overall error rate as all ele-
Table 1: Standard Function Set

<table>
<thead>
<tr>
<th>Name</th>
<th>Return Type</th>
<th>Arguments</th>
<th>Argument Types</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plus</td>
<td>Double</td>
<td>2</td>
<td>Double, Double</td>
<td>Arithmetic addition</td>
</tr>
<tr>
<td>Minus</td>
<td>Double</td>
<td>2</td>
<td>Double, Double</td>
<td>Arithmetic subtraction</td>
</tr>
<tr>
<td>Mult</td>
<td>Double</td>
<td>2</td>
<td>Double, Double</td>
<td>Arithmetic multiplication</td>
</tr>
<tr>
<td>Div</td>
<td>Double</td>
<td>2</td>
<td>Double, Double</td>
<td>Protected arithmetic division</td>
</tr>
<tr>
<td>IF</td>
<td>Double</td>
<td>3</td>
<td>Boolean, Double, Double</td>
<td>Conditional. If arg1 is true, then return arg2, otherwise return arg3</td>
</tr>
<tr>
<td>&lt;=</td>
<td>Boolean</td>
<td>2</td>
<td>Double, Double</td>
<td>True if arg1 is less than or equal to arg2</td>
</tr>
<tr>
<td>&gt;=</td>
<td>Boolean</td>
<td>2</td>
<td>Double, Double</td>
<td>True if arg1 is greater than or equal to arg2</td>
</tr>
<tr>
<td>=</td>
<td>Boolean</td>
<td>2</td>
<td>Double, Double</td>
<td>True if arg1 is equal to arg2</td>
</tr>
<tr>
<td>Between</td>
<td>Boolean</td>
<td>3</td>
<td>Double, Double, Double</td>
<td>True if the value of arg1 is between the values of arg2 and arg3</td>
</tr>
</tbody>
</table>

Table 2: Standard Terminal Set

<table>
<thead>
<tr>
<th>Name</th>
<th>Return Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Random(-1, 1)</td>
<td>Double</td>
<td>Randomly assigned constant with value between -1 and 1</td>
</tr>
<tr>
<td>Attribute[x]</td>
<td>Double</td>
<td>Value of attribute x</td>
</tr>
</tbody>
</table>

This method of calculation of the error rate will lead to a slight over-estimation of error in multi-class problems. For each decomposition errors will fall into two categories. These are either classifying an item of the target class as a class belonging to the remaining set of classes, or classifying an item from the remaining set of classes as an item of the target class. Over-estimation of the error occurs because of the second type of error. In a real classification system built using this method, an item of data that was misclassified at a higher level of decomposition but which actually belonged to a lower level of decomposition would not then be passed on to a lower level of decomposition for classification. In this investigation any item that is misclassified at a higher level of decomposition can still be misclassified at lower levels of decomposition. In this scenario however the true rate of error cannot be any higher than the recorded error rate and the amount of over-estimation is predicted to be minor. This is because, for most problems, error rates are small, meaning few items are misclassified, and thus the number of additional items that would be considered by classifiers at lower levels of decomposition is seen to be relatively small.

This approach uses the standard function and terminal sets shown in Table 1 and 2 respectively.

An example program built using this representation method can be seen in Figure 1. In this example the output of the tree is a real number. Due to the conditional node “IF”, the output of the tree will either be the value of attribute 5 multiplied by: the constant -0.5; or attribute 2 added to attribute 7. If the constant value 0.23 is less than or equal to the value of attribute 2 then it will be the former case, otherwise the latter.

![Figure 1: An example program tree for Binary Decomposition, Static Range Selection or Dynamic Range Selection](image)

### 3.2 Static Range Selection

Genetic programs performing classification tasks generally return real values and, as stated above, it is difficult to find meaningful points over the set of real values to choose as division points for class boundaries, particularly for multi-class classification problems. In this approach we attempt to choose boundary regions based on intuitive guesses about the problem and likely points over the set of reals that class boundaries might occur.

For binary problems (W.B.C, BUPA and Pima) the choice for division is identical to that of the binary decomposition method, as the split between negative and non-negative numbers is used to distinguish between class boundaries. The Pixel dataset (6 classes) used the following ranges: Class1 = [-inf, -5], Class2 = [-5, -1], Class3 = [-1, 0], Class4 = [0, 1], Class5 = [1, 5], Class6 = [5, inf].

For the Thyroid dataset (3 classes) the ranges used were:
which is an enumerated type. The set of values that this type
is used to determine the fitness of the given individual.

It is highly possible that the ranges chosen are not opti-
mal for each problem, but it is intuitive that programs will be
more readily able to produce results in these ranges because
all randomly assigned constants are within the range [-1, 1]
and all attributes are scaled between [0, 1]. Because it is not
possible to know the optimal ranges however these selected
values are as likely to perform well as any other values arbi-
trarily chosen.

This approach uses the standard function and terminal sets
shown in Table 1 and 2 respectively.

3.3 Dynamic Range Selection

An alternative approach to static range selection, where
ranges are arbitrarily chosen to correspond to class bound-
aries that all programs for the run must adhere to, is to allow
each program to use a separate set of ranges for class bound-
aries that are dynamically determined for each individual pro-
gram.

Given a classification problem with many training exam-
amples and an individual from a GP population it is possible to
use a subset of the training examples and record the values
that are returned when attributes for specific classes are used
as inputs. Based upon these outputs the effectively infinite
range of the reals can then be segmented into regions corre-
sponding to class boundaries based upon areas the program
has returned values for each class in the subset of training
examples.

There would be many possible methods of segmenting the
range of reals based on program outputs from a subset of
training examples. For the purpose of practicality this in-
vestigation limited the range for segmentation to that of [-250,250].
This range is seen to be sufficiently large to allow
programs to distinguish between all possible classes in the
problem sets used in this investigation. The algorithm used
in this investigation for dynamically determining the ranges
for each program in the population is given in Figure 2. Note
that the output value for each training example is rounded to
the nearest integer. This rounding is performed to again limit
the effectively infinite space of the real numbers, but is seen
to still allow programs a necessary level of granularity over
this range to distinguish between class boundaries.

Once segmentation of the output ranges has been per-
formed the remainder of the training examples can then be
used to determine the fitness of the given individual.

This approach uses the standard function and terminal sets
shown in Table 1 and 2 respectively.

3.4 Class Enumeration

In this method a new data type is introduced called ClassType,
which is an enumerated type. The set of values that this type
can store is limited to the number of different class types for
the given problem. A new terminal, ClassNum is also intro-
duced which returns a value of type ClassType, correspond-
ing to one of the possible classes in the problem. Properties
of this terminal can be seen in Table 4.

The program trees generated using this method of con-
struction will always return a value of type ClassType. To
facilitate the introduction of this new type, the “IF” function
is modified (as per Table 3) to return a ClassType value, and
the second and third argument are changed to accept only this
type. This means that child sub-trees stemming from the sec-
ond two arguments of an “IF” function can only hold another
“IF” function, or a ClassNum terminal.

An example program can be seen in Figure 3 (where Cx
refers to a ClassType terminal representing class x). Analy-
sis of the structure of programs resulting from this method
of construction shows a degree of similarity to the structure
of decision tree classifiers such as C4.5 [11]. Execution of
the program (in GP) or evaluation of the tree (in decision tree
algorithms) will follow from the root node, through a series
of conditional branches until a single leaf node, containing a
class label, is reached. The major difference in the structure
of the program trees produced by this GP approach to that
of decision trees produced by C4.5 is that at each conditional
branch of the tree the GP approach can consider almost any
arithmetic expression that is possible given the function and
terminal set. In contrast, conditional nodes of a C4.5 deci-

Class1 = [-inf, -1], Class2 = [-1, 0], Class3 = [0, 1], Class4 = [1, inf].

The Vehicle dataset (4 classes) used the following ranges:
Class1 = [-inf, -1], Class2 = [-1, 0], Class3 = [0, 1], Class4 = [1, inf].
Table 3: Class Enumeration: Alteration to the Standard Function Set

<table>
<thead>
<tr>
<th>Name</th>
<th>Return Type</th>
<th>Arguments</th>
<th>Argument Types</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>IF</td>
<td>ClassType</td>
<td>3</td>
<td>Boolean, ClassType, ClassType</td>
<td>Conditional. If arg1 is true, then return arg2, otherwise return arg3.</td>
</tr>
</tbody>
</table>

Table 4: Class Enumeration: Addition to the Standard Terminal Set

<table>
<thead>
<tr>
<th>Name</th>
<th>Return Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ClassNum</td>
<td>Classtype</td>
<td>One, out of the possible set of classes for the given problem</td>
</tr>
</tbody>
</table>

The program trees are only able to consider a single attribute value in comparison to a fixed constant value. This gives the GP program trees more freedom in their expressive capabilities, but also increases the search space to be considered by the genetic search.

3.5 Evidence Accumulation

This method allows many different branches of the program trees to contribute to the decision to choose a certain class. Aside from the program tree each genetic program also contains a vector data storage area, termed the certainty vector. This vector contains one element for each possible class within the program. Before program execution all elements of the certainty vector are initialized to zero. As the program executes values are added (or subtracted) from certain elements of the vector through the operation of a new terminal “AddToClass[x][c](-1, 1)" shown in Table 6. This terminal will add a value in the range -1 through 1, to one of the elements of the certainty vector.

When program execution halts, the certainty vector is examined and the element with the highest value in the vector is declared to be the most certain outcome for classification. In the event that two or more elements share the highest value, the results are inconclusive, and the outcome of classification is considered to be an error.

Because the outcome of the classification lies within the certainty vector it is not necessary for the program itself to return a value. This change in requirements for the program output means that an alteration to the conditional “IF" function must be made and an addition to the function set is also needed as shown in Table 5. The “BLOCK" function will accept from two to four arguments (this value is randomly chosen when programs are first generated) and simply evaluates each argument in a sequential order. This function is required so that it is possible for multiple additions (or subtractions) to the certainty vector are possible (with only conditional functions only one addition per program would be possible).

An example program can be seen if Figure 4 (terminals of the form \[\text{AddToClass}[x][c](-1, 1)\]) indicates an AddToClass function which will add to class \(n\) the certainty value of \(x\). In this example the program will automatically add the value 0.3 to the class 1 element of the certainty vector. Then, depending on whether attribute 3 is greater than or equal, or less than the value 0.6, it will either subtract 0.3, or add 0.7 to the certainty vector of class 3. The final classification will be the class with the greatest certainty value after execution.

3.6 System Parameters

Due to the probabilistic nature of GPs, it is not certain that the outcome of one run will be the same as the output of any other run over the same training data. To help ensure valid results, each method was run ten times over each data set and the recorded error rates were then averaged over the ten runs.
All numeric attributes across the datasets were scaled to a range of 0 through 1. Each run consisted of a population size of 500 individuals, except for those against datasets with independent test sets for error evaluation. Population size for these two datasets (Pixel and Thyroid) was 1000 individuals. The termination criteria for each run was either perfect classification on the training set, or after 50 generations had been processed. When moving to a new generation elitist reproduction was used (10%), whilst the remaining 90% of individuals were selected for crossover using roulette wheel selection. No individuals were selected for mutation. Programs were generated with an initial maximum depth of 6, with overall program depth limited to 17.

Runs were conducted on a 4 processor ULTRA-SPARC4 and training times are given as a combination of user and system CPU time for the runs.

### 4 Summary and Analysis of Results

Tables 7 and 8 show the results obtained from the GP runs for test error rates and training times respectively. Classification error rates and times are given as an average of ten runs.

For the first three datasets (all binary classification problems: W.B.C., BUPA and Pima) there appeared to be little difference between the four methods of program representation. Dynamic range selection performed slightly better than any other method in terms of accuracy of classification, while class evaluation took slightly less time. The consistency of each method (shown in the standard deviation of error) varied only slightly over each dataset. Over all three datasets the evidence accumulation method required a great deal more run time. This is understandable, due to the “BLOCK” function leading to broader (and thus larger) programs and more evaluations of tree branches.

When the three multi-class problems were considered (Pixel, Thyroid and Vehicle) the variation in training time, accuracy, and consistency became much more distinct. The binary decomposition and dynamic range selection classifiers were far more accurate than the other three methods of classification, while the dynamic range selection method was more consistent (lower standard deviation of error). The binary decomposition method used a much longer period of time to produce the classifiers in these problems when compared to other methods, particularly in the case of the Vehicle and Pixel datasets (the Thyroid dataset can possibly be seen as a rare case amongst multi-class classification problems as 91% of instances belong to a single class). The large amount of time required for training the binary decomposition classifiers for these multi-class problems is understandable, as several GP runs must occur to produce a single classifier, where methods like class evaluation and dynamic range selection can produce a classifier for the problem in a single run.

Results for the Pixel and Vehicle datasets indicated that dynamic range selection and class enumeration methods resulted in classifiers of relatively high accuracy in multi-class problems, but took less time to train than binary decomposition methods. Because of this it was of interest to know whether, given a greater amount of training time, such methods could exceed the classification accuracy of binary decomposition. Figure 5 shows the progression of test error rate as generations increased for the Pixel dataset for both the dynamic range selection and class enumeration methods. It can be seen that while dynamic range selection is able to immediately produce more accurate classifiers in the initial generation, it is slow to improve upon this fitness as generations progress. The class enumeration method begins with a less accurate starting point, but is able to utilise the genetic search process to improve fitness over time. However it can be seen that in the last ten generations the rate of improvement for the class enumeration and the dynamic range selection is very small, suggesting class enumeration would be unable to improve over the dynamic range selection method were more time allowed for training this method. To determine whether this was the case, and to determine whether, given comparable run time to the binary decomposition methods, these methods could outperform binary decomposition, the dynamic range selection and class enumeration methods were trialed again on the pixel and vehicle datasets. For the pixel dataset population sizes of 2000 were used, whilst for the vehicle dataset population sizes of 1000 were used. Runs were processed for 80 generations. The results of these runs showed that, when able to utilise the additional available run time, the dynamic range selection method was able to equal or surpass the binary decomposition method in terms of accuracy of classification on both datasets (error rate of 0.161 for the pixel dataset in 8:21:15, and error rate of 0.371 for the vehicle dataset in 6:18:53). The class enumeration method was however unable to surpass either binary decomposition methods.
or dynamic range selection methods (error rate of 0.236 for the pixel dataset in 7:13:31, and error rate of 0.382 for the vehicle dataset in 6:56:53). These results indicate that the dynamic range selection method was more readily able to perform both multi-class and binary classification than any other method tried.

![Image](image.png)

**Figure 5: Error Rate for Best of Generation Individuals for the Pixel Dataset: Mean values over 10 Runs**

The rank values given in Table 9 relate the results attained by the GP classifiers to thirty-three alternative methods of classification trained against these datasets in [7]. The rank values given are that of the classifier that would be displaced in rank (out of a possible of 33) by the genetic classifier. From these rank values it can be seen that for the W.B.C and BUPA datasets GP methods (and in particular dynamic range selection) are quite comparable to other contemporary methods of classification used in [7]. For other datasets, particularly the multi-class vehicle and pixel sets, it can be seen that the GP approaches tried here rank poorly in the set of thirty-three classifiers. However, in no case was a genetic classifier the worst performer out of the thirty-three (this would have resulted in a ranking of 34).

### 5 Conclusion and Future Work

The aim of this investigation was to explore alternative representations and implementations of multi-class classification problems within the GP paradigm, and determine which, out of five representation methods developed and tested, was better able to perform classification tasks. Each of the five methods resulted in classifiers that were competitive with the thirty-three classifiers examined in [7]. Of the five methods developed, results indicate that dynamic range selection is more appropriate for both binary and multi-class problems as it is capable of producing classifiers of a higher degree of accuracy when comparable training times are allowed.

Results indicate that for some datasets GP classifiers are capable of producing competitive results, and in other datasets these classifiers perform relatively poorly when compared to other classification methodologies.

Future work, involving the use of subset selection techniques used in [4], dynamic selection of subsets used for the evaluation of ranges for the dynamic range selection method, larger populations and longer run times and the inclusion of automatically defined functions to GP classifiers, could substantially improve the performance of such GP classifiers when compared with other classification techniques. It is also possible to use the dynamic range selection method on multi-class datasets after these datasets have been decomposed into a set of binary datasets, as was performed in the binary decomposition method used in this paper. This could further improve the applicability of the dynamic range selection method to multi-class problems.

Another future adaptation to the GP approach to classifi-
cation will be the inclusion of symbolic attribute information into GP classifiers.

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**Bibliography**


<table>
<thead>
<tr>
<th>Method</th>
<th>W.B.C.</th>
<th>BUPA</th>
<th>PIMA</th>
<th>Pixel</th>
<th>Thyroid</th>
<th>Vehicle</th>
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<tr>
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<td>8</td>
<td>14</td>
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<td>25</td>
<td>31</td>
<td>33</td>
<td>27</td>
<td>33</td>
</tr>
</tbody>
</table>

Table 9: Associated Ranks For Mean Error Rate Over 10 Runs