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Advanced Review

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Generating ensembles of heterogeneous classifiers using Stacked Generalization



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Over the last two decades, the machine learning and related communities have conducted numerous studies to improve the performance of a single classifier by combining several classifiers generated from one or more learning algorithms. Bagging and Boosting are the most representative examples of algorithms for generating homogeneous ensembles of classifiers. However, Stacking has become a commonly used technique for generating ensembles of heterogeneous classifiers since Wolpert presented his study entitled Stacked Generalization in 1992. Studies that have addressed the Stacking issue demonstrated that when selecting base learning algorithms for generating classifiers that are members of the ensemble, their learning parameters and the learning algorithm for generating the meta-classifier were critical issues. Most studies on this topic manually select the appropriate combination of base learning algorithms and their learning parameters. However, some other methods use automatic methods to determine good Stacking configurations instead of starting from these strong initial assumptions. In this paper, we describe Stacking and its variants and present several examples of application domains. © 2015 John Wiley & Sons, Ltd.

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INTRODUCTION

classifier is a system that takes instances from a Adataset and assigns a class or category to each of them. To perform this task, the classifier must have some type of knowledge. The classifiers can be created by using various forms of learning (e.g., deduction, analogy, or memorization), but the most common way of acquiring this knowledge is to infer it from a set of previously classified instances. This form of learning is called *supervised learning*.

Most research in *machine learning* has been devoted to developing methods that automate the classification tasks. Despite the variety and number of models that have been proposed, including artificial neural networks,¹ decision trees,² inductive logic programming,³ and Bayesian learning algorithms,⁴

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task remains unobtainable.⁵ Furthermore, no single approach can claim to be superior to any other.⁶ Thus, the combination of different classification models is considered a viable alternative for obtaining more accurate classification systems. The strategy in ensemble systems is to create a set of classifiers and combine their outputs such that the combination outperforms all of the single classifiers. To achieve this goal, it is necessary to guarantee that (1) the individual classifiers are both accurate and diverse and (2) the output combination amplifies the correct decisions and cancels out the incorrect decisions.⁷

the construction of a perfect classifier for any given

Studies in the ensemble field have typically focused on generating the ensemble members by applying a single learning algorithm and combining their outputs using a mathematical function. In con-trast, Stacking generates the members of the Stacking ensemble using several learning algorithms and subse-quently uses another algorithm to learn how to com-bine their outputs.

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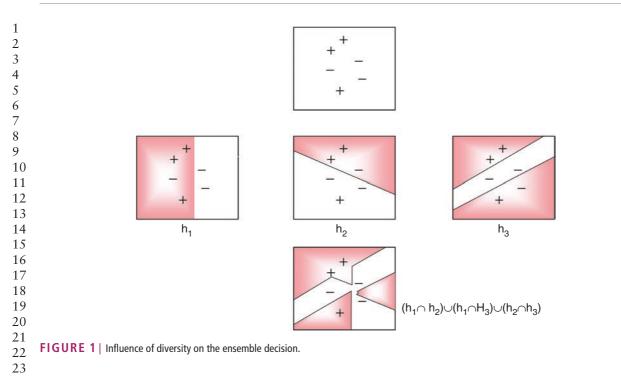
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The remainder of this paper is organized as follows. First, some background on ensemble classifiers is given. Then, we present the main features of and a review of some of its variants, related approaches and recent applications. Finally, we draw some conclusions and discuss important topics about Stacking.

32 ENSEMBLES OF CLASSIFIERS

An ensemble of classifiers is a set of classifiers whose
 individual decisions are combined to obtain a system
 that hopefully outperforms all of its members.⁸

36 _ENREF_2Similar to what occurs with other 37 systems in the field of artificial intelligence, the ensem-38 bles of classifiers respond to an attempt to emulate 39 human behavior. Specifically, these systems try to repli-40 cate the performance of a human being when it faces 41 an important decision. For example, it is common to 42 ask the opinion of different doctors before having a 43 surgery, performed or read reviews before buying a 44 product. In other words, a decision is considered more 45 reliable if it is made based on the opinion of different 46 experts. Extrapolation of this proposition to the field 47 of machine learning leads to the development of sys-48 tems composed of several classifiers, in which the final 49 decision is made collectively. This line of research in 50 the machine learning field is known as the study of 51 ensembles of classifiers.9

52 The strategy in ensemble systems is to create a 53 set of accurate and diverse classifiers and combine 54 their outputs such that the combination outperforms

24 all the single classifiers. Therefore, classifier ensembles 25 are built in two phases: generation and combination. 26 In the generation phase, the individual components of 27 the ensemble, known as base classifiers, are generated. 28 In the combination phase, the decisions made by the 29 members of the ensemble are combined to obtain 30 one decision. A detailed description of these phases is 31 provided in the following subsection. 32

Generating Base Classifiers

To obtain an ensemble of classifiers that outperforms 35 all its members, the base learners must be both 36 accurate and diverse. A classifier is accurate when its 37 classification error is lower than that obtained when 38 the classes are randomly assigned. Two classifiers are 39 diverse if they make errors at different instances. 40

41 Demanding accurate classifiers appears to be 42 a logical requirement; the combination of a set of 43 incorrect decisions cannot easily generate a correct 44 hypothesis. To illustrate why diversity is a necessary 45 condition, consider, in a two classes domain, an 46 ensemble of three classifiers, h_1 , h_2 , and h_3 , and a 47 new example x that must be classified. If the three 48 classifiers are not diverse, then when the decision given 49 by h_1 is wrong, the decisions given by h_2 and h_3 will 50 also be wrong. Therefore, the final ensemble decision 51 will be wrong. However, if the base classifiers are 52 diverse, the decisions given by both h_2 and h_3 will be 53 correct even when the decision given by h_1 is wrong. Therefore, the ensemble decision will be correct if 54

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Name	Symbol	Definition	\uparrow/\downarrow^1	Pairwise
Q statistic	Q	$\frac{N^{11}N^{00} - N^{01}N^{10}}{N^{11}N^{00} + N^{01}N^{10}}$	Ļ	Y
Correlation coefficient	ρ	$\frac{\sqrt{N^{11} N^{00} - N^{01} N^{10}}}{\sqrt{(N^{11} + N^{10})(N^{01} + N^{00})(N^{11} + N^{01})(N^{10} + N^{00})}}$	\downarrow	Y
Fail/non-fail disagreement measure	dis	$\frac{N^{01} + N^{10}}{N^{11} + N^{10} + N^{01} + N^{00}}$	↑	Y
Double-fault measure	DF	$\frac{\frac{1}{N^{00}} + \frac{1}{N^{00}}}{\frac{N^{11} + N^{10} + N^{01} + N^{00}}{K}}$	\downarrow	Y
		$\frac{\sum_{i=1}^{N_{ii}}}{N} - \sum_{i=1}^{K} \left(\frac{N_{i*}}{N} \frac{N_{*i}}{N}\right)$		
Kappa degree-of- agreement statistic	K	$\frac{1}{1-\sum_{i=1}^{K} \left(\frac{N_{i*}}{N} \frac{N_{*i}}{N}\right)}$	Ţ	Y
Plain disagreement measure	Div_plain	$\frac{1}{N}\sum_{k=1}^{N} ls\left(C_{i}\left(x_{k}\right),=C_{j}\left(x_{k}\right)\right)$	1	Y
Ambiguity	Amb	$\frac{1}{LKN} \sum_{\substack{l=1\\N}}^{L} \sum_{n=1}^{N} \sum_{k=1}^{K} \left(ls \left(C_{l} \left(x_{k} \right) = k \right) - \frac{N_{k}^{0}}{L} \right)$	1	Ν
Entropy	Ε	$\frac{1}{N}\sum_{n=1}^{N}\frac{1}{\left(l-\frac{1}{2}\right)}\min\left(l\left(x_{k}\right), L-l\left(x_{k}\right)\right)$	↑	N

22 N, cardinality of the test set; K, number of classes; L, the number of base classifiers; N^{ab} is the number of instances in the dataset, classified correctly (a = 1) or 23 incorrectly (a = 0) by the classifier *i*, and correctly (b = 1) or incorrectly (b = 0) by the classifier *j*; N_{ij} , number of instances in the dataset, labeled as class *i* by the first classifier and as class *j* by the second classifier; $C_i(x_k)$, class assigned by classifier *i* to instance *k*; Is(c), a Boolean function. Its value is 1 if c is true and 0 if c 24 is false; $N_{l,i}^n$, number of base classifiers that assign instance n to class k; and $l(x_k)$, number of classifiers that correctly classified instance k. 25 ¹Monotonically increasing/decreasing measures are identified with an ascending/descending arrow, respectively.

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27 all the decisions have the same relevance. Figure 1 28 illustrates this example graphically.

29 Diversity is a necessary condition for obtaining 30 a good ensemble. However, measuring diversity is not 31 straightforward because there is no formal definition 32 of diversity and no consensus on how to quantify 33 this magnitude.¹⁰ Some of the more common ways to 34 quantify ensemble diversity are shown in Table 1. 35

We have analyzed the relevancy of diversity 36 among the base classifiers and how to quantify it. 37 It is now necessary to review the most well-known 38 techniques for generating diverse classifiers. 39

The techniques used to generate diverse classi-40 fiers are based on the idea that the hypothesis of a 41 classifier depends on both the learning algorithm and 42 the subset used to generate these classifiers. Therefore, 43 it is possible to generate classifiers whose decisions are 44 dissimilar from each other by varying the training set 45 and/or learning algorithm. 46

Three different approaches can be used to gener-47 ate an ensemble of classifiers⁹: 48

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50 • Resampling the training examples: This 51 approach includes two of the most widely known methods for constructing classifier ensembles: *Bagging*¹¹ and *Boosting*.¹² *Bagging* builds dif-52 53 54 ferent versions of the training set by sampling with replacement. In contrast, •Boosting obtains the different training sets by focusing on the instances that are misclassified by the previously trained classifiers.

- Manipulating the input features. Another way to achieve diversity between classifiers is by modifying the set of attributes used to describe the instances.^{13–17}
- Manipulating the output target: Another 36 approach for generating a pool of diverse 37 classifiers is having each classifier solve a dif-38 ferent classification problem. This category 39 includes methods that solve multiclass problems 40 by converting them into several binary subprob-41 lems. Among the strategies for decomposing 42 a multi-class problem into two-class problems 43 are one-against-one (OAO),18 one-against-all 44 (OAA),¹⁹ one-against-higher-order (OAHO)²⁰ 45 and error correcting output codes (ECOC).²¹ 46 Other systems that decompose the multiclass 47 problem into several pairwise subproblems, such 48 as binary-complementary-ensemble (BCE)^{22,23} 49 and complementary-complementary ensemble 50 $(CCE)^{24}$ can be grouped into this approach. 51

Methods that vary the learning algorithm can be subdivided in two groups:

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• Approaches that use different versions of the same learning algorithm. Kolen and Pollak²⁵ demonstrated that a pool of artificial neural networks starting from different initial weights can be trained to generate diverse classifiers and thus a good ensemble. Alternatively, a pool of diverse decision trees can be obtained by varying the criterion used to expand a C4.5. node.²⁶

9 • Approaches where diversity is obtained using 10 different learning algorithms. According to 11 Wolpert,²⁷ ensembles with base classifiers trained 12 from different learning algorithms (heteroge-13 neous ensembles) exploit the different biases of 14 each learning algorithm. Therefore, most studies 15 in the field of ensembles have focused on the 16 combination of different inducers, such as arti-17 ficial neural networks, decision trees, Bayesian 18 models, nearest neighbor, and support vector 19 machines. As will be shown below, Stacking²⁷ 20 and most of its variants achieve diversity by 21 applying this approach. 22

Integrating Decisions 24

25 Once the base classifiers that comprise the ensem-26 ble have been built, the next step is to establish a 27 procedure through which the individual decisions are combined to obtain a final hypothesis. There are two 28 main strategies for combining classifiers: fusion and 29 selection.^{6,28} Classifier selection presupposes that each 30 31 classifier is an expert in some local region of the space. 32 Therefore, when an instance is submitted for classification, the ensemble decision coincides with the deci-33 sion given by the classifier responsible for the region of 34 the space to which the instance belongs.²⁹ In classifier 35 fusion, the decisions from all members of the ensemble 36 37 are combined in some manner to make the ensemble decision. Classifier fusion algorithms include combin-38 ing rules, such as the average, majority vote, weighted 39 majority vote, and the Borda Count, and more com-40 plex integration models, such as meta-classifiers. A 41 meta-classifier is a second-level classifier generated 42 from the outputs given by the base learners. According 43 to Rokach,³⁰ Stacking, arbiter tree,³¹ combiner tree³² 44 and the Grading approaches³³ are considered integra-45 tion methods based on meta-learning. 46

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48 STACKED GENERALIZATION 49

50 Stacking is short for Stacked Generalization.²⁷ As 51 noted above, unlike other ensemble generation algo-52 rithms, such as *Bagging* or *Boosting*, which generate

53 an ensemble of classifiers using the same learning algo-

54 rithm (homogeneous ensembles), Stacking generates

1 an ensemble composed of heterogeneous classifiers. 2 Because each learning algorithm uses different meth-3 ods to represent the knowledge and different learning 4 biases, the hypothesis space will be explored from dif-5 ferent perspectives with the aim of generating a pool 6 of diverse classifiers. Therefore, when their predictions 7 are combined, the resultant model is expected to be 8 more accurate than each individual member.

9 To combine the individual predictions of the 10 ensemble members, Stacking uses the concept of 11 meta-classifiers or meta-learners. The meta-classifier 12 or level-1 model is generated using a learning algo-13 rithm following a cross-validation-like process. This 14 classifier attempts to model how the outputs of the base classifiers or level-0 models should be combined 15 to generate the final output. Figure 2 provides a gen-16 eral overview of the Stacking process. 17

Stacking is an ensemble of classifiers in which (1) 18 the base learners are trained using different training 19 parameters (generally different learning algorithms) 20 and (2) the outputs of the base learners are combined 21 by using a meta-classifier. One of the issues in *Stacking* 22 is obtaining the appropriate combination of base-level 23 classifiers and the meta-classifier, especially in relation 24 to each specific dataset. If only a small number of 25 classifiers and algorithms will be used, this problem 26 can be solved by a simple method, namely, exhaustive 27 search, in a reasonable amount of time. However, it is 28 difficult to determine the best Stacking configuration 29 when the search space is large.

Formal Definition

33 Given a dataset S, Stacking first generates randomly 34 a subset of equal size datasets S_1, \ldots, S_T and 35 subsequently follows a process similar to a J-fold 36 cross-validation process: it omits one of the subsets 37 (e.g., S_i) to be used later. The remaining instances 38 $S^{(-j)} = S - S_j$ are used to generate the level-0 classifiers 39 by applying K learning algorithms, $k = 1, \ldots, K$, to 40 obtain K classifiers. $S^{(-j)}$ and S_i are the training and test 41 sets respectively of the *j*-th fold in the cross-validation. 42 After the level-0 models have been generated, the S_i set 43 will be used to generate the level-1 instances. Level-1 44 training data are generated from the predictions of the 45 level-0 models over the instances in S_i , which were 46 omitted for this purpose (Figure 3a). Level-1 data have 47 *K* attributes, whose values are the predictions of each 48 one of the K level-0 classifiers for every instance in S_i . 49 At the end of the cross-validation process, each level-1 50 training example will be composed for K attributes 51 (the K predictions) and the target class, which is the 52 real class value for every instance in S. Once the level-1 data have been built from all instances in S, any learn-53 54 ing algorithm can be used to generate the level-1 model

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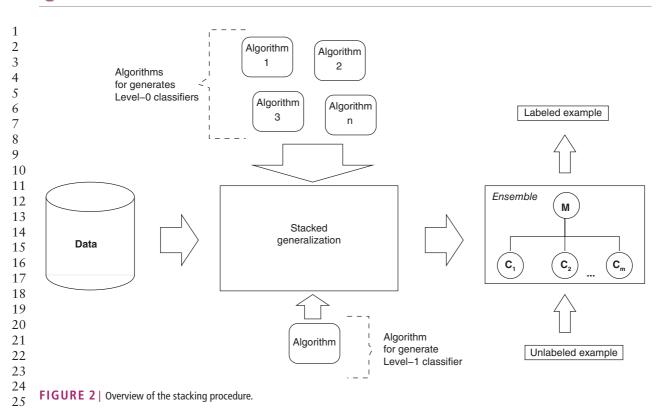
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27 (Figure 3b). To complete the process, the level-0 mod-28 els are re-generated from the entire dataset S (it is 29 expected that this process improves the accuracy of the 30 classifiers slightly) (Figure 3c). In Figure 3d the final 31 ensemble structure generated by Stacking is shown. To 32 classify a new instance, the level-0 models produce a 33 vector of predictions that is the input to the level-1 model, which in turn predicts the class. 34

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36 37 STACKING VARIANTS AND RELATED 38 APPROACHES

Since Wolpert first proposed *Stacking* in 1992, several
related studies have been published. In general terms,
these studies can be grouped into two categories: those
that address the *Stacking* parameter selection and
those that present approaches similar to *Stacking*. We
provide a brief review of these two types of studies in
the following subsections.

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48 Stacking Variants

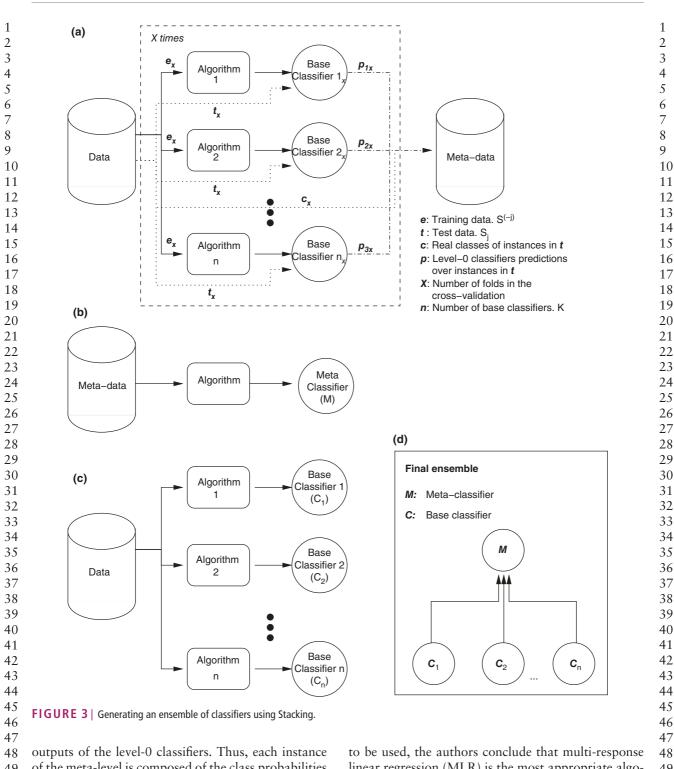
- 49 As initially noted by Wolpert,²⁷ some issues of *Stack*-
- 50 ing are considered black art, such as the selection of
- 51 base classifiers, the type of meta-data and the classi-
- 52 fier to be used in level-1. Some studies that address
- 53 these issues and other related topics are presented
- 54 below.

Skalak³⁴ proposed the use of instance-based 27 28 learning classifiers that store a few prototypes per 29 class as level-0 classifiers. They also proposed to use 30 a decision tree as a meta-classifier or level-1 classifier. Fan et al.³⁵ proposed to determine the overall 31 32 accuracy of the ensemble generated by Stacking using 33 conflict-based accuracy estimates. The authors use two 34 tree-based classifiers and one rule-based classifier as 35 base-level classifiers. In contrast, for the meta-level, 36 they use a rote table that behaves as a decision tree 37 without pruning in this case. This Stacking configuration is evaluated using four datasets (including two 38 artificial datasets). Although the authors claim that 39 the proposed measure is superior to all existing mea-40 sures, their results do not clearly demonstrate that this 41 42 estimate can be generalized to more datasets or other 43 meta-classifiers.

Merz³⁶ proposed a variant of *Stacking* that uses correspondence analysis to detect correlations between base-level classifiers. Once dependencies have been removed from the original meta-level space, a nearest neighbor method (meta-level algorithm) is applied over the resulting feature space. This approach is called *SCANN*.

Ting and Witten³⁷ address two Stacking configuration issues: level-1 classifier types and the data types of the meta-level. They propose the use of class probabilities rather than a single class prediction as 54 Advanced Review

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outputs of the level-0 classifiers. Thus, each instance
of the meta-level is composed of the class probabilities
given for each level-0 classifier, followed by the actual
class of the instance. The authors argue that by using
the class probabilities as meta-data, Stacking uses
both the prediction and confidence of the base-level
classifiers. Regarding the type of meta-level classifier

to be used, the authors conclude that multi-response48linear regression (MLR) is the most appropriate algo-49rithm for generating the meta-level model, at least50when using class probabilities as meta-level data.51Moreover, Ting and Witten studied the necessity of52non-negative constraints for the attribute weights in53linear models because both Breiman³⁸ and LeBlanc54

and Tibshirani³⁹ report the need to use nonnegative constraints when using *Stacking* in a regression task.
They concluded that non-negative restrictions are not necessary in *Stacking* to improve the overall accuracy of the ensemble when performing a classification task. However, these restrictions are useful for improving the interpretability of the level-1 model.

8 Based on work of Ting and Witten,³⁷ Seewald⁴⁰ 9 used MLR as the level-1 classifier but with a differ-10 ent set of attributes in the meta-level to overcome a 11 weakness of Stacking with MLR (SMLR) in domains 12 with more than two classes. This weakness was not 13 present in the original version of Stacking, and See-14 wald argues that this new weakness may be due to 15 the dimensionality of the meta-data. When MLR is 16 used as the meta-classifier, a linear equation for each 17 class is constructed using the class probability distribu-18 tions given by the base classifiers. StackingC, as this 19 variant is known, is proposed to use only the class 20 probabilities associated with the class to which the lin-21 ear model is built, thus reducing the dimensionality 22 of the attributes of the meta-level by a factor equal 23 to the number of classes. The results of this research 24 indicate an improvement over SMLR when used with 25 the full set of probability distributions. Furthermore, 26 Seewald argues that the observed improvement is due 27 to not only the reduction of the dimensionality of the 28 meta-data but also the high diversity of class models 29 generated at the meta-level. 30

Todorovski and Džeroski41 proposed a variant 31 of Stacking that uses a decision tree approach as the 32 learning method in the meta-level. This method, called 33 meta decision trees (MDTs), replaces class-value pre-34 dictions in its leaf nodes by the name of the base-level 35 classifier that should be used to obtain the class for 36 a specific example. The meta-level data are com-37 posed of properties of the probability distributions 38 that reflect the confidence of the base-level classifiers 39 (e.g., entropy and maximum probability) rather than 40 41 the distributions themselves. These properties are used to generate small MDTs. 42

Džeroski and Ženko42 proposed two additional 43 variants of Stacking. The first variant addresses the 44 45 issue of the type of meta-data based on SMLR proposed by Ting and Witten.³⁷ The authors propose an 46 47 extension of meta-data, adding two additional sets 48 of attributes: the probability distributions multiplied 49 by the maximum probability and the entropies of 50 the probability distributions. Moreover, Džeroski and 51 Żenko proposed another extension of SMLR in which 52 they replace the linear regression approach by a tree 53 induction approach as the meta-level model. They 54 called this method Stacking with multi-response model

1 trees (SMRMT). According to the authors, compar-2 ing different Stacking approaches, SCANN, SMDTs, 3 SMLR, and the SelectBest scheme (selecting the best 4 classifier with cross-validation) appear to perform at 5 approximately the same level. Moreover, Džeroski and 6 Żenko concluded that SMRMT outperforms previous 7 Stacking variants, including StackingC, and selects the 8 best classifier from the ensemble by cross-validation.

9 Menahem et al.43 proposed a new variant of 10 Stacking called Troika, whose main feature is that 11 the meta-level is composed of three layers. In the first 12 layer, the outputs of the base classifiers are combined 13 using a OAO ensemble, whose members are called 14 specialist classifiers. The goal of each specialist is to 15 predict the probability that an instance belongs to one 16 of the two classes that it distinguishes. In the second 17 stage, the outputs of the specialists are combined again 18 using a OAA schema. The task of the level-2 classifiers 19 is to learn the behavior patterns of the specialist 20 classifiers and to predict whether the output given by a 21 specialist is correct. The third layer contains a classifier 22 and produces the ensemble final decision. Moreover, 23 the authors analyze three arrangements to train the 24 base classifiers (OAO, OAA, and all-against-all) and 25 determine that Troika is more accurate than Stacking 26 and *StackingC* in all cases. Regarding the runtime, the 27 authors conclude than Troika outperforms Stacking 28 and StackingC only when the base classifiers are 29 trained using the OAO architecture.

30 Ledezma et al.44 proposed an approach to deter-31 mine good Stacking configurations by a genetic search. 32 Their approach, called GA-Stacking, not only deter-33 mines which meta-level and which (and how many) 34 base classifiers must be present but also their learning 35 parameters. Moreover, GA-Stacking provides flexibil-36 ity and extensibility compared to previous Stacking 37 variants because it can easily incorporate new learning algorithms and is not restricted by 'a priori' assump-38 tions. Moreover, GA-Stacking adapts the Stacking 39 40 configuration to the domain biases and characteris-41 tics so that the Stacking configurations determined 42 by GA-Stacking are domain dependent. However, 43 GA-Stacking requires a longer execution time than the 44 other approaches to obtain a specific Stacking config-45 uration.

46 Following a similar approach to the work of Ledezma et al.44 and posing the Stacking configura-47 48 tion as an optimization problem, Chen and Wong⁴⁵ 49 proposed the use of ant colony optimization (ACO) 50 to determine domain-dependent Stacking configura-51 tions. They use the meta-heuristic ACO to determine 52 the level-0 Stacking classifiers with a predefined level-1 classifier⁴⁵ as well as the entire Stacking system config-53 54 uration (level-0 and level-1).46

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Recently, Shunmugapriya and Kanmani⁴⁷ proposed the use of another meta-heuristic search algorithm to determine which and how many base classifiers to use and what meta-classifier to use based on the domain. Therefore, they have proposed to use an artificial bee colony (ABC) method. The authors compared their results with the studies of Ledezma et al.44 and Chen and Wong,45 and they conclude that the results of the Stacking configurations determined 10 by ABC are comparable to those obtained in the 11 previous study.

12 The approaches introduced above are compared 13 in Table 2 with regard to the focus area, number of 14 base classifiers, algorithms for base-classifier genera-15 tion, type of meta-data, and meta-level classifier. In 16 addition, some observations are included. 17

19 **Related Approaches**

20 In addition to the Stacking variants already discussed, 21 there are studies that can be viewed as either Stack-22 ing-based implementations or studies that hold many 23 similarities with Stacking.

24 Chan and Stolfo⁴⁸ proposed a strategy similar 25 to Stacking, which they called Combiner. The main 26 idea behind the Combiner, as the authors claim, is to 27 merge the predictions of base classifiers by learning 28 the relation between the predictions of base classifiers 29 and the correct prediction. Moreover, they propose 30 a variant of the combiner strategy called *attributes* 31 combiner, in which the attributes of the meta-level 32 are composed of not only the predictions of a class 33 but also the original attributes of the instance. As 34 shown in Schaffer's study of Stacking bi-level,49 this 35 approach can reduce the performance of the ensemble. 36 In contrast, Chan and Stolfo⁴⁸ proposed an approach 37 that uses what they call an Arbiter, which is a classifier 38 independent from the remaining base classifiers that 39 is trained on a subset of the original dataset. This 40 subset of the data consists of the instances in which 41 the base classifiers present diverse predictions. The 42 purpose of an arbiter is to provide an alternative 43 and more elaborate prediction when base classifiers 44 present contradictions. In addition, Chan and Stolfo 45 proposed what they call an arbiter tree, in which 46 arbiters that specialize in resolving conflicts between 47 pairs of classifiers are arranged in a binary decision 48 tree. To carry out the classification of an instance, 49 the method starts from the leaf nodes formed by base 50 classifiers and goes up through the tree to the root 51 node that provides the final classification.

52 Ting⁵⁰ proposed a composite learner framework 53 that selects the classification that is estimated to have 54 the higher accuracy as the final prediction of the

1 ensemble. This framework uses the predictions of the 2 base classifiers to learn a function that reflects the 3 inner measure of confidence of the algorithm on an 4 estimate of their accuracy on the output. This function 5 can be used to combine the expertise of the classifier.

6 Gama and Brazdil⁵¹ proposed a method closely 7 related to Stacking that they called Cascade Gener-8 alization. In this method, the classifiers are applied 9 sequentially, and there is no meta-classifier. When each 10 base classifier is applied to the data, it increases the 11 number of attributes of the dataset by adding the class 12 probability distribution. The following classifier then 13 uses this new dataset so that the order in which clas-14 sifiers are used becomes an important factor.

15 Seewald and Fürnkranz³³ proposed a scheme 16 known as Grading. This scheme creates a meta-level 17 classifier for each level-0 classifier. The learning 18 task for each level-1 classifier is to predict whether 19 the level-0 classifier prediction will be correct. The 20 meta-level data are composed of base-level attributes, 21 and the class values are correct or incorrect. The final 22 prediction of the ensemble is calculated through a 23 weighted voting mechanism over the predictions of 24 the base classifiers. The weight assigned to the vote of 25 each base classifier is the confidence that his predic-26 tion will be correct. This weight is estimated by the 27 meta-classifier associated with the base classifier. This 28 work has some similarities with the work performed 29 by Ting.50

Torres-Sospedra et al.⁵² proposed a combination 30 31 strategy based on ANN in which the predictions 32 of the level-0 classifiers for the entire training set 33 are used to train the meta-classifier. Based on this 34 idea, they propose two different combination schemes: 35 Stacked and Stacked+. In both schemes, the outputs 36 provided by the base learners are used as inputs to the 37 meta-level, but in Stacked+, the original input data are also used as inputs to the meta-classifier. 38

Inspired by the work of Wolpert²⁷, Cohen 39 and Carvalho53 proposed a stacked of classifiers 40 41 to be applied in sequential partitioning tasks. This 42 meta-learning method, called stacked sequential 43 *learning*, SSL, that seeks to augment an arbitrary 44 base learner in sequential learning problems.⁵⁴ 45 In this approach, during the training phase, a 46 cross-validation process is carried out in order to 47 obtain the predicted labels, which are joined with the 48 original input features vector, taking into account a 49 neighborhood around the examples. With this train-50 ing dataset-that they called extended dataset-a 51 metalearner is built and a base learner is obtained 52 from the original dataset. Then, in the inference phase, 53 when a new instance arrives, the base learner is used 54 to generate the prediction label for the instance. After

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Year	Authors	Focus Area	Base Classifiers	Algorithms for Base Classifiers	Type of Metadata	Meta Classifier	Observations
1997	Skalak ³⁴	Base classifier selection	2, 3 and more than 3 (3, 5, 11, 21)	Instance-based classifiers (simple nearest neighbor classifier)	Class predictions	Voting, Nearest Neighbor and ID3	Homogeneous ensemble
1999	Merz ³⁶	Meta-level	5 to 8	Back propagation neural network, CN2, C4.5, OC1, OC1 variant, PEBLS, 1-NN, naïve Bayes	Class predictions represented in a space of uncorrelated dimensions	Nearest neighbor	Correspondence analysis (errors)
1999	Fan et al. ³⁵	Overall accuracy of the ensemble	2 and 3	Ripper, Cart, ID3 and C4.5	Class predictions	A rote table (it functions as an un-pruned full decision tree)	New metrics: conflict-based accuracy estimate and conflict-based accuracy improvement estimate
1999	Ting and Witten ³⁷	Meta-level	ĸ	C4.5, naïve Bayes and IB1	Class probability distributions	Multi-response linear regression (MLR)	Represents meta-level data as a class probability vector
2002	Seewald ⁴⁰	Meta-level data	9	Decision table, C4.5, naïve Bayes, kernel density, MLR and K*	Reduced class probability distributions	MLR	A Stacking variant called StackingC
2000	Todorovski and Džeroski ⁷²	Meta-level data and learner	5	C4.5, LTree, CN2, k-NN and naïve Bayes	Class probability distribution properties (e.g., entropy and maximum probability)	Meta decision trees (MDTs)	A Stacking variant called Stacking with MDTs
2004	Džeroski and Ženko ⁷³	Meta-level data and learner	3 and 7	C4.5, k-NN, naïve Bayes, K*, kernel density estimation, decision table, MLR	Class probability distributions and class probability distribution augmented with two additional calculated attributes	Multi-response model trees (MRMT) and MLR	Two Stacking variants
2009	Menahem et al. ⁴³	Meta-level classifier	1, 3 and 6	C4.5, VFI, IBk, PART, Bayes-Net, SMO.	Class probability distributions	Three stages in logistic algorithm	A Stacking variant in which the meta-level is split into three layers. Base classifiers are trained using two different binarization methods (OAA, OAO) and the AAA scheme.
2010	Ledezma et al. ⁵⁵	Whole Stacking system	Variable. up to 10	C4.5, naïve Bayes, simple naïve Bayes, IBK, PART, DT, decision stump, random forest, random tree, MLR, MRMT, K*, VFI, conjunctive rule, JRip, Nnge, hyper-pipes	Probability distributions	Variable. Selected by a genetic algorithm	Uses genetic algorithms for the parameter settings of Stacking: GA-Stacking
2011	Chen and Wong ^{45,46}	Entire Stacking system	Variable	Naïve Bayes, logistic classifier, IB1, IBk, K*, OneR, PART, ZeroR, decision stump, C4.5	Probability distributions	C4.5 ⁴⁵ and selected by the ant colony ⁴⁶	Uses an ant colony optimization technique for the parameter settings of Stacking: ACO-Stacking
2013	Shunmugapriya and Kanmani ⁴⁷	Entire Stacking system	Variable. up to 10	Naïve Bayes, logistic classifier, IB1, IBk, K*, OneR, PART, ZeroR, decision stump, C4.5	Probability distributions	Variable. Selected by the artificial bee colony algorithm	Uses a bee colony algorithm for the parameter settings of Stacking: ABC-Stacking

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this label generation, the extended instance is created so that the metalearner can use it to produce the final prediction.

4 GA-Stacking^{44,55}_ENREF_55, Based on 5 Ordoñez et al.⁵⁶ proposed an approach that uses 6 genetic algorithms to determine which base classifiers 7 must be present in the ensemble as well as the method 8 used to combine these classifiers. Although the final 9 ensemble uses a meta-classifier as the decision com-10 bination method in some cases, in other cases, it uses 11 other methods of combining base classifier decisions. 12 Hence, it is considered a related work and not a 13 Stacking variant.

14 Based on work of Cohen and Carvalho,53 Gatta 15 et al.⁵⁷ proposed a new framework whose goal is to 16 capture the data interactions using a neighborhood 17 function. In this way, the meta-classifier is trained 18 using an extended training set that is composed by 19 the original data set and the output given by this 20 neighborhood function. To evaluate the performance 21 of this general framework, called MS-SSL, two imple-22 mentations of the neighborhood function were pro-23 posed. These implementations were based on the 24 combination of two different Multi-Scale Decompo-25 sition schemes (a pyramidal decomposition and a 26 multi-resolution decomposition) and a sampling pat-27 tern. Both models (Pvr-SSL and MR-SSL) were built 28 using AdaBoost, with a maximum of 100 decision 29 stumps, as classification algorithm. The proposed sys-30 tems were evaluated in two domains: a text categoriza-31 tion task and an image pixel classification problem. 32 According to the authors, experimental results proved 33 that, in both domains, MS-SSL outperforms classical 34 SSL, CRF58 and AdaBoost. A drawback presents in 35 MS-SSL is the impossibility of dealing with multiclass 36 problems. One way to address this difficulty is mod-37 ifying the neighborhood function and replacing the 38 base classifiers used in the original MS-SSL scheme by 39 others capable of dealing with data belonging to N 40 classes. This adaptation, called MMSSL, is presented 41 and applied for the resolution of several multi-class 42 sequential learning problems in.⁵⁹ In this study, the 43 authors concluded that MMSSL shows significant 44 performance improvement compared with classical 45 approaches. Moreover, authors note that MMSSL is 46 able to keep the relationship among classes at differ-47 ent scales. Therefore, from a qualitative point of view, 48 it is possible to state that the results of MMSSL are bet-49 ter than those obtained with the rest of the evaluated 50 models.

51 Trivedi and Kapadia⁶⁰ suggested improving the 52 ensemble accuracy by combining the philosophies of 53 both *Stacking* and *Boosting*. The proposed algorithm, 54 named '*sequential stacking*', trains the base classifier sequentially, giving more importance to instances that were misclassified by the previous classifiers. After the training, the outputs of the level-0 classifiers are used to train the meta-classifier. Therefore, the diversity among the base classifiers is achieved using a version of Boosting instead of cross-validation.

Applying Stacking

Most works related to Stacking have focused on determining an answer to what Wolpert called black art. However, there is a series of studies focused on the application of Stacking in real domains. We present some of the most representative examples below.

15 Doumpos and Zopounidis⁶¹ used Stacking to 16 distinguish potential defaulters from non-defaulters. 17 Their work is focused on the combination of seven 18 classification algorithms (linear discriminant func-19 tions, quadratic discriminant functions, logistic 20 functions, probabilistic neural networks, near-21 est neighbors, decision trees, and support vector 22 machines), which have been successfully used in pre-23 vious studies on credit risk assessment. The outputs 24 of the level-0 classifiers are transformed by applying 25 a principal component analysis and are subsequently 26 sent to the meta-classifier. To complete the study, 27 seven different meta-classifiers were implemented 28 (each using one of the seven above-mentioned clas-29 sification algorithms) and 54 different scenarios 30 (different combinations of the characteristic parame-31 ters of each classification algorithms) on three datasets 32 were analyzed. According to the authors, although the 33 experimental results are affected by the value of the 34 classification algorithm parameters, the models based 35 on Stacking are more efficient than the single-method 36 models. Moreover, they observed that the exclusion 37 of a level-0 classifier does not necessarily reduce the 38 Stacking performance.

Hu and Tsoukas⁶² applied a method based on 39 40 the Stacking methodology to identify the factors that 41 affect consumer choices. The main goal of this study 42 was to investigate the role of demographic and situ-43 ational factors on consumer choices. In their investi-44 gation, they use classifier ensembles composed only 45 of ANNs. According to the authors, all implemented 46 models benefited from stacked generalization, and the 47 best models are those that contain exclusively situa-48 tional variables.

Qian and Rasheed analyzed *Stacking* and *Voting* 49 as tools to predict the trend of the Dow Jones index⁶³ 50 and the trend of the exchange spot rate of the US dollar against the British pound trend.⁶⁴ In their investigation, they used artificial neural networks, decision 53 trees and k-nearest neighbors as level-0 classifiers but 54

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provided no information about the meta-classifier. In
both studies, they conclude that Stacking and Voting
have a similar performance, and in both cases, their
gain in relation to the best level-0 classifier is null. The
authors argue that this result is due to the lack of diversity among the level-0 classifiers.

7 The application of the main idea behind the 8 Stacked Generalization is known as blending of clas-9 sifiers in some domains.⁶⁵ Such is the case of the work 10 of Sill et.al⁶⁶ in which the authors present the applica-11 tion of Stacking as a key facet of the second place team 12 solution to the Netflix Prize Competition.⁶⁷ In this 13 work, the authors presented a meta-level linear tech-14 nique, known as Feature-Weighted Linear Stacking. 15 This technique combines the base classifiers predic-16 tions linearly through coefficients that are themselves 17 linear functions of some additional inputs known as 18 meta-features. This approach demonstrates an accu-19 racy improvement over the standard linear stacking. 20 However, as authors claim, the creation of useful 21 meta-features is an art, so it depends on the applica-22 tion domain.

Escalera et al.,68 applied Stacked Sequential 23 24 Learning⁵³(SSL)to a problem related with laughter 25 detection. In their study, they proposed the fusion of 26 both audio and video cues to deal with the laugh-27 ter recognition in face-to-face conversations. Once 28 the audio and the visual cues have been identified, 29 processed, and merged to obtain a unique feature 30 vector, a level-0 classifier is trained. Then, according 31 to the SSL scheme, an extended data set is created 32 which joins the original training data features with 33 the predicted labels produced by the level-0 classifier. 34 Finally, this extended data set is used as input to a sec-35 ond classifier. The experimental results demonstrated 36 that the proposed model outperforms AdaBoost. 37 Nevertheless, the use of both audio and visual cues 38 does not seem to improve the results obtained when 39 only audio features are used.

40 A study developed using work from computer 41 science, psychiatry, and nuclear medicine⁶⁹ analyzed 42 the use of Stacking to differentiate Alzheimer's dis-43 ease and mild cognitive impairment. Because medicine 44 offers a host of tools designed to help the physician 45 in his diagnostic process, in this study, Stacking is 46 viewed as not only a method for building hetero-47 gonous ensembles but also a method for integrating 48 the decisions from different diagnostic tools, includ-49 ing PET scans, Consortium to Establish a Registry 50 of Alzheimer's Disease, mini-mental state examination 51 and clock drawing tests. Therefore, each level-0 classi-52 fier is k-NN trained from data from one of the sources. 53 The experimental results demonstrated that the mean

54 accuracy of a simple k-NN including all of the features

was 76%, whereas the mean accuracy of Stacking was 83%. Thus, Stacking achieved an accuracy gain of 7%.

StackTIS⁷⁰ is a *Stacking*-based methodology whose objective is the detection of potential translation initiation sites (TISs). The proposed model is based on the combination of three different classifiers, where each classifier learns from data described by different attributes. The first classifier is an SVM that is trained to identify the coding potential of a cDNA sequence. This classifier uses the 64 codon frequencies as input. The second classifier is a first-order homogeneous Markov chain, whose inputs are the segment of cDNA that enclose an ATG codon (starting from position -7 and ending at position +5). The third classifier is a heuristic model that calculates the probabilities of an ATG to be the TIS based on its distance from the 5'. Finally, the predictions given by these three components are used as input to the meta-classifier. In this work, two different learning algorithms were considered as meta-classifiers, namely, MLR and M5',⁷¹ but the experimental results indicate than M5' outperforms MLR slightly. StackTIS was tested on two human datasets and one rice dataset. According to the authors, for the three evaluated domains, StackTIS outperforms other popular approaches that are common in the TIS prediction literature.

Razmara and Sarkar (•Razmara & Sarkar, 28 29 2013) applied an Stacking variant to the field of the 30 Statistical Machine Translation. In their investigation, the authors adopted the approach suggested by 31 Wolpert under which cross-validation can be used 32 to construct different weak classifiers. So, Razmara 33 and Sarkar propose building an homogeneous ensem-34 ble in which each base classifier-translation model 35 implemented using a statistical machine translation 36 system called Kriya (Sankaran, Razmara, & Sarkar, 37 2012) – is training using k-1 partitions of the data. 38 Then, the remaining data partition is used to tune the 39 base learner parameters. The hypothesis from these 40 base classifiers are combined in a second module called 41 *Ensemble Decoding.* To provide a greater flexibility in 42 its answer – scores –, the *Ensemble Decoding* module 43 is prepared to handle different mixture operations: 44 weighted sum, weighted max, model switching, and 45 product. Experimental evaluation on two language 46 pairs showed that the proposed model outperforms 47 Bayesian Model Averaging and, in most cases the 48 ensemble outperforms every one of its base translator. 49

CONCLUSION

Today, it is common to use algorithms, such as *Bagging* and *Boosting*, to generate ensembles of classifiers 54

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1 as a standard method in classification tasks. Such tech-2 niques are implemented in a large number of data 3 mining tools, which facilitates their use and evalua-4 tion. Thus, many studies have focused on the appli-5 cation of these techniques in a variety of domains. 6 However, after more than two decades since the pub-7 lication of Wolpert's paper, the use of Stacking in real 8 applications remains relatively rare, possibly due to 9 what Wolpert called black art. In other words, there 10 are several issues that could be considered when using 11 *Stacking*, such as the following:

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- - The algorithms that are used to create the base-level classifiers and their learning parameters,
 - The number of base classifiers,
- The algorithm used to generate the meta-classifier and its learning parameters, and
- The type of attributes that should be used to create the meta-data.

24 One of the conclusions of this study is that there are many contradictory results and that there 25 is no consensus on which Stacking configuration 26

is optimal. This conclusion corroborates Wolpert's 2 statement regarding the need for prior knowledge to configure these parameters.

4 Nevertheless, in recent years, there has been a 5 trend in the literature toward Stacked Generalization, 6 which is the use of meta-heuristics, such as genetic 7 algorithms, ant colonies or artificial bee colonies, to 8 automatically configure the Stacking system param-9 eters. Thus, the Stacking system that is generated is 10 domain dependent. However, this type of approach 11 has a higher computational cost than other Stack-12 ing approaches because several generations of indi-13 viduals must be evaluated to obtain the final system. 14 Even if this task is not crucial for a large number of 15 domains, given that most classification tasks do not 16 require real-time operation, it could be a relevant issue 17 in the era of big data. However, it would be interesting 18 to explore adding incremental capabilities to *Stacking* 19 in future research.

20 Although Stacking is applied to real-world prob-21 lems less frequently than other ensemble methods, such as Bagging or Boosting, the exponential growth 22 of data as well as the diversity of these data continues 23 24 to make Stacking an interesting alternative for gener-25 ating ensembles. 26

30 ACKNOWLEDGMENTS 31

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