A Game Theoretic Approach Based on Differential Evolution to Ensemble Learning for Classification

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Abstract: Aggregating results of several learners known to each perform well on different data types is a challenging task that requires finding intelligent, trade-off solutions. A simple game-theoretic approach to this problem is proposed. A non-cooperative game is used to aggregate the results of different classification methods. The Nash equilibrium of the game is approximated by using a Differential Evolution algorithm. Numerical experiments indicate the potential of the approach for a set of synthetic and real-world data.

1 INTRODUCTION

The evaluation and aggregation of the results of several classifiers continue to be a challenging task in machine learning. It is well-known that different methods produce different results on different data sets, making it difficult to decide which method to use for prediction purposes or how to aggregate results in an optimal manner. Stacking ensemble methods use another learner to aggregate results and make predictions (Polikar, 2012). The main goal of aggregating the results of different learners is to find a good trade-off between the results to reduce bias and variability (Mienye and Sun, 2022). The main goal of using another learner is to create an intelligent and explainable aggregation.

One of the fields that specialize in defining and computing different types of trade-offs is game theory (Maschler et al., 2020). In game-theoretic models, agents interact in strategic and conflicting situations, and equilibria are defined. The term equilibrium is used because, most of the time, the solution’s definitions include some notion of stability. One of the most popular solution concepts in game theory is the Nash equilibrium, which ensures stability against unilateral deviations.

In this paper, we propose using the Nash equilibrium as a solution for a meta-learner of a stacking ensemble method. In a stacking ensemble approach, several base learners are trained on the data set, and their results are aggregated by using another learner, called a meta learner. A game among base learners is defined, in which each of them aims to maximize its marginal contribution to the accuracy of the ensemble. The Nash equilibrium of the game is approximated using a differential evolution algorithm.

The proposed method is called Nash stacking differential evolution and is described in Section 3, after a short review of related work in Section 2. Numerical experiments performed on synthetic and real-world data are used to illustrate the behavior and potential of the approach in Section 4. The paper ends with conclusions.

2 RELATED WORK

The binary classification problem consists of finding a rule to assign one of two labels, or classes, to data instances, based on known information about the data. This means that we are given a data set \( X \subset \mathbb{R}^{n \times p} \) containing \( n \) instances \( x_i \in \mathbb{R}^p \) and their corresponding labels \( Y \in \{0, 1\}^n \) from which to learn the rule. The goal may be to use the rule to explore or explain the data or to make predictions about instances from the same distribution for which the labels are unknown.

The binary classification problem is one of the most studied in the literature, with many proposed methods varying in their approach (Hastie et al., 2016; Zaki and Meira Jr., 2014). One of the reasons so many approaches exist is that different methods perform well on different data sets, and it is a difficult task to predict which method will perform better on new data. Ensemble methods aim to provide ways to combine the results of several learners to overcome...
this shortcoming. There are two main categories of ensemble learning: homogeneous and heterogeneous (Mienye and Sun, 2022); homogeneous methods use the same learner several times on different instances of the data, while heterogeneous methods use different learners on the same data and aggregate results. Stacking generalization is a heterogeneous ensemble learning method that uses the results of several, and typically very different learners by further training another model to combine them (Wolpert, 1992; Pavlyshenko, 2018).

Stacking models use a set of base algorithms, called level-0 models, trained directly on the data set and (another) model, called meta-learner, or level-1 model to learn how to combine their predictions best (Polikar, 2012). They are widely used for various applications and settings. For example, a stacking model considering different feature combinations for the default risk of small enterprises is presented in (Chi et al., 2023). Medical applications include detecting heart irregularities and predicting cardiovascular disease in (Mohapatra et al., 2023). A variation of stacking, called A-stacking is used for spoof fingerprint detection in (Agarwal and Chowdary, 2020).

In (Dong et al., 2021) a stacking ensemble is used to predict wind power, and in (Sun and Trevor, 2018) it is used for annual river ice breakup dates. Rock deformation predictions are approached with stacking models in (Koopnialipoor et al., 2022). There are also multiple applications in sentiment analysis (Wang et al., 2014; AlGhamdi et al., 2022; Zhang et al., 2021; Chen et al., 2022; Agarwal and Chowdary, 2021).

3 NASH-STACKING CLASSIFICATION (NS)

Consider a set of $k$ base learners $ML_1, ML_2, \ldots, ML_k$. Each of them is trained using $X, Y$, resulting in a set of predictions $\hat{Y}_{ij}$, $j = 1, \ldots, k$, and the corresponding probabilities $P_{ij}$. Thus, $\hat{y}_{ij}$ is the class predicted by model $ML_j$ for the instance $x_i \in X$, and $p_{ij}$ is the probability that the instance $x_i$ is classified as $j$ by the learner $ML_j$. Predictions are made based on probabilities $p_{ij}$: if $p_{ij} > 0.5$, then instance $x_i$ is labeled as $j$, otherwise as $0$.

The goal of ensemble learning is to combine the results of the $k$ learners so that those that performed well are used, and those that performed poorly are discarded. A simple and effective meta-learner would be linear model, as it also provides a possible interpretation of the parameters. In this approach the goal is to find parameter $\alpha' = (\alpha'_1, \ldots, \alpha'_k)$ such that ensemble probabilities are computed as:

$$EP_i(\alpha', P) = \sum_{j=1}^{k} \alpha'_j p_{ij}, \forall i = \{1, \ldots, n\}, \quad (1)$$

with $\sum_{j=1}^{k} \alpha'_j = 1$, can be used to make reliable predictions.

3.1 Ensemble Learning Game

A new method for learning the parameter $\alpha$ as an equilibrium of a non-cooperative game is proposed. A non-cooperative game is defined by three elements: a set of players $K$, a set of actions available to them $A$, and a set of payoff functions $U$ that take into account the actions of all the players. The game $\Gamma(K,A,U)$ proposed in this paper consists of:

- The set of players $K$ is represented by the $k$ base learners:
- The set of actions $A$: each player $j$ chooses a $\alpha_j$ parameter to contribute to the ensemble model. Thus $A \subset \mathbb{R}^k$; an element $\alpha \in A$ is called the strategy profile or a situation of the game, in which player $j$ has chosen $\alpha_j$.
- The payoff functions $U = (u_j)_{j=1}^k$ are computed as a marginal contribution of each player to the accuracy of the model:

$$u_j(\alpha) = ACC(\alpha_j P, Y) - ACC(\alpha_{-j} P_{-j}, Y), \quad (2)$$

and

$$U(\alpha) = (u_1(\alpha), u_2(\alpha), \ldots, u_k(\alpha)), \quad (3)$$

where

$$ACC(\alpha_j P, Y) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(\mathbb{1}(EP_i > 0.5) = y_i). \quad (4)$$

$EP_i$ is given in Eq. (1) and $\mathbb{I}(\cdot)$ is the identity function taking the value one if the argument is true and zero otherwise. In Eq. (2), the index $-j$ in $\alpha_{-j}$ and $P_{-j}$ indicates that the $j^{th}$ component of $\alpha$ and $P$, respectively, is removed.

Thus, the payoff each player tries to maximize is represented by its contribution to the overall accuracy of the model. A higher payoff indicates that the learner contributes more to the overall accuracy of the ensemble. Non-cooperative game theory offers many solution concepts. Among the most popular is the Nash equilibrium, which can be described as a strategy profile of the game from which none of the players has a unilateral incentive for deviation, i.e. none of the players can improve their payoffs by changing their strategies while all others maintain theirs. For game $\Gamma$, the Nash equilibrium may indicate that none
of the methods can contribute more to the ensemble by unilaterally changing its parameter in $\alpha$. While at this stage it is not possible to assess if the game has an equilibrium, by using a stochastic search method that detects equilibria we can find solutions that may present equilibrium properties that may be of interest to a decision maker.

### 3.2 Differential Evolution for Nash Equilibria Detection

Differential evolution (DE) is a simple and efficient stochastic search and optimization method that evolves a population of potential solutions to the problem (Storn and Price, 1997). It has been adapted to approximate the Nash equilibria of a game using the Nash ascendancy relation in (Lung and Dumitrescu, 2008; Lung et al., 2010) during the selection phase. We further adapt the DE to approximate the NE of the game $\Gamma$, and we call this version the Nash Stacking Differential Evolution (NS-DE). The outline of NS-DE is presented in Algorithm 1.

**Algorithm 1: NS-DE: Nash Stacking - DE outline.**

1. Generate initial population $A = \{\alpha_1, \ldots, \alpha_{\text{popsize}}\}$ using the standard uniform distribution;
2. Evaluate population using payoffs $U$ in Eq. (3) and (5);
3. $nrgen = 0$;
4. while ($nrgen < \text{MaxGen}$) and (no changes in MaxGen/10 iterations) do
   5. for each $i = \{1, \ldots, \text{popsize}\}$ do
      6. create offspring $o_i$ from parent $\beta_i$ using the $\text{DE/rand/1/exp}$ scheme (Alg. 2);
      7. if ($o_i$ Nash ascends (Alg. 3) parent $\alpha_i$) then
         8. $o_i$ replaces parent $\alpha_i$;
      9. end if
   10. end for
11. end while
12. return non-dominated individuals;

Population and Initialization. The NS-DE population consists of individuals $\alpha \in \mathbb{R}^k$. In the first iteration, they are randomly generated following a standard uniform distribution.

Evaluation. The fitness of each individual is evaluated as the payoff function $U$ in Eq. (3). However, to ensure that the right side of equation (1) is a probability, only during the evaluation of the payoffs, the values of $\alpha_2$ are normalized to add to 1 by dividing them by their sum. Thus, when evaluating an individual $\alpha = (\alpha_1, \ldots, \alpha_k)$, its values are first modified to:

$$\alpha'_j = \frac{\alpha_j}{\alpha_1 + \alpha_2 + \ldots + \alpha_k}$$

$U(0, k)$ is a discrete uniform value between 0 and $k$.

**Algorithm 2: DE - the $\text{DE/rand/1/exp}$ scheme to create offspring $o_i$ from parent $\alpha_i$.**

1. $o_i = \alpha_i$;
2. randomly select parents $\alpha_1, \alpha_2, \alpha_3$, where $i_1 \neq i_2 \neq i_3 \neq i$;
3. $w = U(0, k)$$^1$;
4. for $j = 0$; $j < k \land U(0, 1) < \text{CR}$; $j = j + 1$ do
5. $o_{iw} = \alpha_{iw} + F(\alpha_{i2w} - \alpha_{i1w})$;
6. $w = (w + 1)\%k$;
7. end for

$^1U(0, k)$ is a discrete uniform value between 0 and $k$.

**Variation Operators.** NS-DE uses the $\text{DE/rand/1/exp}$ scheme, presented in Algorithm 2, to create an offspring (Thomsen, 2004). With a probability $\text{CR}$, some components of the offspring are modified using values from three different parents from the current population by adding the difference of two, multiplied by a scaling factor $F$, to the third. $\text{CR}$ and $F$ are parameters of the DE.

**Nash Ascendancy.** Each offspring replaces its parent if it is better than it. In the game-theoretic context, the concept of better is implemented by using a relation among strategy profiles that permits their comparisons for selection purposes. Thus, to guide the search of the DE population towards the equilibrium of game $\Gamma$, we use the Nash ascendancy relation from (Lung and Dumitrescu, 2008), described in Algorithm 3. The comparison is made by counting how many players can improve their strategies by unilaterally changing from one individual to the other. The individual with fewer such players is considered better from the Nash ascendancy point of view. If there is an equal number of players that can improve their payoffs from each side, then the two individuals are considered indifferent to each other.

**Output.** NS-DE provides the individual that is better than most other individuals in the population based on the Nash ascendancy relation.

**NS-DE Parameters.** NS-DE uses specific DE parameters: population size $\text{popsize}$, maximum number of iterations $\text{MaxGen}$, crossover rate $\text{CR}$, and scaling factor $F$. If 10% of the maximum number of iterations elapse without any replacements being made in the population, the search stops.

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Algorithm 3: Nash ascendancy test to compare offspring \( o \) to parent \( \beta \).

1: \( k_1 = k_2 = 0; \)
2: for \( j = 0; j < p; j = j + 1 \) do
3: \( \text{if } o_j \succ \beta_j \text{ then} \)
4: \( o'_j = O, \beta'_j = \beta; \)
5: \( o'_j = \beta_j, \beta'_j = o_j; \)
6: \( \text{if } u_j(o') > u_j(o) \text{ then} \)
7: \( k_1 + 1; \)
8: \( \text{end if} \)
9: \( \text{if } u_j(\beta'_j) > u_j(\beta) \text{ then} \)
10: \( k_2 + 1; \)
11: \( \text{end if} \)
12: \( \text{end for} \)
13: \( \text{if } k_1 < k_2 \text{ then} \)
14: \( \text{return } o \text{ Nash ascends } \beta \text{ is TRUE (1);} \)
15: \( \text{else} \)
16: \( \text{end if} \)
17: \( \text{if } k_1 > k_2 \text{ then} \)
18: \( \text{return } o \text{ Nash ascends } \beta \text{ is FALSE (-1);} \)
19: \( \text{else} \)
20: \( \text{return } o \text{ is INDIFFERENT to } \beta \text{ (0);} \)
21: \( \text{end if} \)
22: \( \text{end if} \)

4 NUMERICAL EXPERIMENTS

Numerical experiments are performed on a set of synthetic and real-world data to illustrate the behavior of the approach.

4.1 Experimental Set-up

Data. Synthetically generated datasets can be used to assess the behavior of a method for various parameters and degrees of difficulty. While good results on these datasets do not guarantee similar performance on real-world data, they do indicate the approach’s potential. In this paper, 36 datasets combining all of the following parameters were generated:

- number of instances: 100, 500, 1000;
- number of features: 3, 10, 20, 30;
- class separation: 0.1, 1, 10.

The data were generated by using the function \texttt{make\_classification} from the \texttt{sklearn} library (Pedregosa et al., 2011) available in Python. The class separation parameter controls the overlapping of the classes, with a smaller value indicating a larger overlap and a more difficult classification problem.

The following real-world data sets from the UCI machine learning repository (Dua and Graff, 2017) are used:

- R1 \textbf{arcene} , with 200 instances and 10001 attributes;
- R2 \textbf{banana} , with 5300 instances and 3 attributes;
- R3 \textbf{hill valley with noise} , with 1212 instances and 101 attributes;
- R4 \textbf{hill valley without noise} , with 1212 instances and 101 attributes;
- R5 \textbf{Kr vs kp} , with 3196 instances and 37 attributes;
- R6 \textbf{LSVT Voice Rehabilitation} , with 126 instances and 311 attributes;
- R7 \textbf{Madelon} , with 2600 instances and 501 attributes;
- R8 \textbf{Monks3} , with 554 instances and 7 attributes;
- R9 \textbf{Phoneme} , with 5404 instances and 6 attributes;
- R10 \textbf{Ringnorm} , with 7400 instances and 21 attributes;
- R11 \textbf{Thyroid Sick Euthyroid} , with 3163 instances and 26 attributes;
- R12 \textbf{Wilt} , with 4839 instances and 6 attributes.

Base Learners. The following base learners (Zaki and Meira Jr., 2014) are used for numerical experiments:

- \textbf{ML1}: Logit - logistic regression,
- \textbf{ML2}: RF - random forests,
- \textbf{ML3}: KNN - k Nearest neighbor,
- \textbf{ML4}: NaiveB - Naive Bayes,
- \textbf{ML5}: SVM - Support Vector Machine.

For each method, we used their implementation from the \texttt{sklearn} (Pedregosa et al., 2011) library, with default parameters. The results provided by the five methods were used to construct the five-player game \( \Gamma \), whose equilibrium is approximated by using NS-DE.

Performance Evaluation. For all synthetic and real-world data sets, 10-fold cross-validation is used to evaluate the performance of NS-DE. This means that each data set is divided into 10 equal-sized folds, and experiments are performed 10 times; each fold is used once for testing purposes and the other nine for training purposes. Three performance indicators are reported for test folds: the area under the curve AUC (Melo, 2013), the accuracy ACC (Zaki and Meira Jr., 2014), and log-loss LL (Vovk, 2015). AUC and ACC take values between 0 and 1; the higher, the better.
Figure 1: Synthetic datasets, box-plots of log-loss values reported by NS-DE, compared to the base approach. Lower values are considered better.

LL represents an error, and the smaller the value, the better the results can be considered.

For each data set, the ten values reported for each fold were compared between the two methods by using a non-parametric Mann Whitney U test (MWU), testing the null hypothesis that the NS-DE results were worse. Whenever the null hypothesis is rejected, for p-values smaller than 0.05 we can consider NS-DE results better.

Parameter Settings. NS-DE uses specific DE parameters. The experiments presented in this paper were carried out with a population size of 30 individuals, evolving for 30 iterations, with $F = 0.5$ and $CR = 0.8$. For each test data fold, 10 independent runs of NS-DE are performed, and the average of the performance indicators is reported.

4.2 Results and Discussions

Synthetic Data Sets. A total of 17 of the 108 comparisons performed indicated a significant difference in the results in favor of NS-DE. The rest of the results, although showing minor improvements, could not be considered significantly better, but also not worse. The most significant differences were in the values of the Log-loss indicator. Figure 1 presents box-plots of log loss results reported for each data set for the ten-folds. In the first row of plots, datasets with the smallest class separator value (with overlapping classes) are the most difficult, while in the last row, we have the datasets with best-separated data. The first column presents results for data sets with 100 instances, the second one data sets with 500 instances and the last one with 1000 instances. The boxes are grouped based on the number of attributes. We find that most significant differences appear for data-sets with lower class separator values and a higher number of instances. The number of attributes in the data set does not seem to influence the results, which is maybe due to the fact that both methods work with the results of the base learners and not directly with the data sets.

Example 4.1. As an example of a result, consider a synthetic dataset with 500 instances, 3 attributes, and class separation 0.1. Table 2 presents results reported by the base learners, the base ensemble, and NS-DE.
Table 1: Average and standard deviation values for the three indicators for the real-world datasets. Results marked with an (*) indicate that the difference between NS-DE and the base approach can be considered significant according to the MWU test.

<table>
<thead>
<tr>
<th>Data set</th>
<th>AUC mean</th>
<th>NS-DE std</th>
<th>ACC mean</th>
<th>NS-DE std</th>
<th>LL mean</th>
<th>NS-DE std</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>0.937</td>
<td>0.033</td>
<td>0.920</td>
<td>0.047</td>
<td>0.893</td>
<td>0.045</td>
</tr>
<tr>
<td>R2</td>
<td>0.955</td>
<td>0.009</td>
<td>0.952</td>
<td>0.010</td>
<td>0.891</td>
<td>0.015</td>
</tr>
<tr>
<td>R3</td>
<td>0.951*</td>
<td>0.009</td>
<td>0.831</td>
<td>0.044</td>
<td>0.892*</td>
<td>0.025</td>
</tr>
<tr>
<td>R4</td>
<td>0.983*</td>
<td>0.037</td>
<td>0.926</td>
<td>0.020</td>
<td>0.966*</td>
<td>0.063</td>
</tr>
<tr>
<td>R5</td>
<td>0.986</td>
<td>0.015</td>
<td>0.987</td>
<td>0.015</td>
<td>0.929</td>
<td>0.042</td>
</tr>
<tr>
<td>R6</td>
<td>0.794</td>
<td>0.191</td>
<td>0.762</td>
<td>0.216</td>
<td>0.768</td>
<td>0.095</td>
</tr>
<tr>
<td>R7</td>
<td>0.778*</td>
<td>0.024</td>
<td>0.728</td>
<td>0.022</td>
<td>0.707*</td>
<td>0.016</td>
</tr>
<tr>
<td>R8</td>
<td>0.792</td>
<td>0.011</td>
<td>0.981</td>
<td>0.025</td>
<td>0.967</td>
<td>0.025</td>
</tr>
<tr>
<td>R9</td>
<td>0.945*</td>
<td>0.010</td>
<td>0.917</td>
<td>0.012</td>
<td>0.892*</td>
<td>0.009</td>
</tr>
<tr>
<td>R10</td>
<td>0.996</td>
<td>0.002</td>
<td>0.995</td>
<td>0.010</td>
<td>0.955</td>
<td>0.021</td>
</tr>
<tr>
<td>R11</td>
<td>0.947</td>
<td>0.022</td>
<td>0.953</td>
<td>0.022</td>
<td>0.949</td>
<td>0.007</td>
</tr>
<tr>
<td>R12</td>
<td>0.989</td>
<td>0.009</td>
<td>0.987</td>
<td>0.012</td>
<td>0.983</td>
<td>0.010</td>
</tr>
</tbody>
</table>

Table 2: Example 4.1, results reported by the base learners, the base ensemble, and NS-DE.

<table>
<thead>
<tr>
<th></th>
<th>AUC</th>
<th>ACC</th>
<th>LL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Logit</td>
<td>0.429</td>
<td>0.460</td>
<td>0.725</td>
</tr>
<tr>
<td>RF</td>
<td>0.615</td>
<td>0.580</td>
<td>0.658</td>
</tr>
<tr>
<td>KNN</td>
<td>0.885</td>
<td>0.800</td>
<td>1.018</td>
</tr>
<tr>
<td>NaiveB</td>
<td>0.562</td>
<td>0.520</td>
<td>0.654</td>
</tr>
<tr>
<td>SVM</td>
<td>0.822</td>
<td>0.700</td>
<td>0.509</td>
</tr>
<tr>
<td>base</td>
<td>0.853</td>
<td>0.740</td>
<td>0.539</td>
</tr>
<tr>
<td>NS-DE</td>
<td>0.887</td>
<td>0.774</td>
<td>0.480</td>
</tr>
</tbody>
</table>

on one test fold. The solution provided by NS-DE (averaged over 10 DE runs) is

\[ \alpha = (0.4663, 0.6825, 1.2417, 0.1787, 1.1179). \]

\( \alpha \) reasonably identifies the contribution of the base learners to the ensemble, with the highest coefficient assigned to KNN and SVM. In this instance, KNN reports the best results when we look at AUC and ACC, but the worst log loss value.

As a remark, the sum of the coefficients is not one, but when used in the ensemble, the values are normalized, resulting in

\[ \alpha' = (0.1264, 0.1851, 0.3367, 0.0484, 0.3031). \]

Real-World Data. Table 1 presents the numerical results reported by NS-DE and the base method on the real world data for the three performance measures. Results for which the MWU test indicates a better performance than the base method are marked with an (*). In a similar manner to synthetic data, log loss values are significantly improved in most cases. In most cases, standard deviations reported by NS-DE are lower. For four datasets, AUC and ACC values are also significantly better.

5 CONCLUSIONS

A game-theoretic approach to evolving parameters of an ensemble meta-learner is proposed. As an initial attempt to use the Nash equilibrium to estimate parameters for a meta-learner, the marginal contribution to the accuracy of the training data is used as a pay-off function in a non-cooperative game. A differential evolution algorithm is adapted to approximate the Nash equilibrium of the game.

The preliminary results presented here show that the approach may be competitive, compared to a baseline model that averages the probabilities of the base models. Future models can explore existing stacking generalization models and the possibility of introducing the Nash equilibrium as a solution for different meta-learners in order to offer decision-makers different types of options.

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