**ORIGINAL ARTICLE**

**Machine collaboration**

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We propose a new ensemble framework for supervised learning, called **machine collaboration** (MaC), using a collection of possibly heterogeneous base learning methods (hereafter, base machines) for prediction tasks. Unlike bagging/stacking (a parallel and independent framework) and boosting (a sequential and top-down framework), MaC is a type of *circular* and *recursive* learning framework. The *circular* and *recursive* nature helps the base machines to transfer information circularly and update their structures and parameters accordingly. The theoretical result on the risk bound of the estimator from MaC reveals that the *circular* and *recursive* feature can help MaC reduce risk via a parsimonious ensemble. We conduct extensive experiments on MaC using both simulated data and 119 benchmark real datasets. The results demonstrate that in most cases, MaC performs significantly better than several other state-of-the-art methods, including classification and regression trees, neural networks, stacking, and boosting.

**KEYWORDS**
boosting, CART, deep neural network, ensemble learning, machine learning, regression

1 | **INTRODUCTION**

In recent decades, various learning methods, including deep neural networks (DNN), decision trees (DT, Breiman et al., 1984), support vector machines (Cortes and Vapnik, 1995), and k-nearest neighbours (kNN) have been developed for regression in supervised learning. As argued by Hastie et al. (2009), each of these methods may have advantages over the others in some respects, but not in others. For example, while DNN is effective at approximating complicated nonlinear functions, the problems of overfitting and vanishing gradients could harm their performances, especially when the sample size is small. As another popular learning method, DT is robust to irrelevant predictor variables and outliers and insensitive to monotone transformations of the input data. However, the lack of smoothness of the prediction surface is one limitation of DT. Another drawback of DT is that a slight change in data can result in quite different splits of the DT, leading to a potentially large variance of prediction. Ridge regression is also a popular learning method, being robust against the multicollinearity of the predictors. However, it can only capture the linear relationship between the response and predictors. There is no single learning method that will dominate all others in all scenarios. In this article, we propose a new ensemble learning framework to combine the strengths of these different learning methods through collaboration.

Ensemble learning has emerged and been extensively studied by many in the past few decades (e.g., Breiman, 1996; Dasarathy & Sheela, 1979; Ho, 1995; Schapire, 1990), with its popularity recently skyrocketing (e.g., Lu & Van Roy, 2017; Qi et al., 2019; Tian & Feng, 2021; Yu et al., 2018). Mendes-Moreira et al. (2012), Sagi and Rokach (2018), and Dong et al. (2020) are some recent comprehensive surveys. The general idea of ensemble learning is to combine the predictions obtained from different learning methods (hereafter, base machines), or predictions based on different subsamples or different feature spaces, in order to improve prediction performance. Bagging, stacking, and boosting are three prominent examples. In bagging (Breiman, 1996) and stacking, base machines are first run in parallel and independently, and then the final prediction is constructed as a simple/weighted average of the predictions from these base machines. In boosting (Schapire et al., 1998), the base machines work jointly in a top-down manner. In all three algorithms, the output from each base machine is fixed after being calculated. Like human collaboration, an idea that may yield potential improvement is to let different kinds of base machines communicate with each other and update their outputs after observing the predictions of the other base machines. Based on this idea, we propose the **Machine Collaboration** (MaC)
ensemble learning framework with heterogeneous base machines, where the word heterogeneous stands for that the base machines are of different types (e.g., DT, DNN, and Ridge Regression).

Compared with bagging, stacking, and boosting, MaC has the following desirable features. Figure 1 provides the schematic for bagging, stacking, and MaC. As illustrated, bagging and stacking are parallel and independent, boosting is sequential and top-down, while MaC is circular and recursive. In the framework of MaC, base machines work in a circular manner. Further, the circulation goes multiple rounds. Valuable information is passed recursively through base machines around a ‘round table’, but not top-down. In this process, the base machines update their structures and/or parameters once in each round, according to the information received from the other machines. We demonstrate that MaC can deliver competitive performance when compared with the base machines or other ensemble methods.

Three existing ensemble learning methods are closely related to MaC. One is the so-called super learner (hereafter, SL) proposed in van der Laan et al. (2007), which can be viewed as a stacking method. SL receives predictions from different kinds of base machines and then outputs a weighted average of these predictions as the final prediction, where the weights are obtained using cross-validation with some specified loss function. The second one is the LS-Boost proposed in Friedman (2001). LS-Boost works as a forward regression, using a particular base machine (e.g., tree) each time to fit the current residuals, and ensemble all machines in the end. LS-Boost is then a sequential and top-down method. While both ensemble methods work well in certain situations, we show that our newly proposed MaC performs better in our extensive simulation studies and real data analysis, partly due to its distinctive circular and recursive learning structure. The third one is the so-called additive groves which were proposed to train an additive ensemble of regression trees (see Sorokina et al., 2007, 2008). The main difference is that the additive groves are meant to build an ensemble of homogeneous models (regression trees), more in the spirit of LS-boost or bagging, while MaC focuses on heterogeneous ensembles in the spirit of stacking.

The main contributions of this work are fourfold. First, we propose a new type of ensemble learning framework, MaC, which is circular and recursive. The circular and recursive aspect could be a potential direction for exploring new methods of ensemble learning. Second, we present some desirable finite statistical properties of MaC. Third, we demonstrate via extensive simulations that MaC performs better than all individual base machines and the ensemble methods SL and LS-Boost. Lastly, in the real data analysis, we compare MaC with the competing methods on 119 benchmark datasets in the Penn Machine Learning Benchmarks (PMLB) (Olson et al., 2017), which demonstrate notable advantages of MaC over competing methods for most datasets.

2 | METHOD

We now introduce the details of the new ensemble learning framework, machine collaboration (MaC). In MaC, we consider a collection of base machines and allow them to collaborate to improve the prediction performance. The base machines could contain both hyperparameters and non-hyperparameters. Here, a hyperparameter is a parameter whose value controls the structure of the base machine and could be set using domain knowledge or selected by cross-validation or data-splitting. The remaining parameters, whose values are estimated by fitting the base machine with fixed hyperparameters on the training data, are non-hyperparameters. For example, in DNN, the learning rate, number of nodes, number of layers, and the activation function are hyperparameters, while for DT, the maximum depth is a hyperparameter. For DNN, the weights of each layer are non-hyperparameters, and for DT, the split variable and value for each split are non-hyperparameters. Hereafter, for the sake of
simplicity, we use ‘parameter’ instead of ‘non-hyperparameter’ unless confusion arises. First, we provide a simple sketch of MaC with two base machines in the next subsection. Then the general MaC framework is provided in Section 2.2.

### 2.1 Sketch of MaC with two base machines

Suppose we have a regression task and two base machines, $M_A$ and $M_B$ (e.g., a DT and a DNN). Denote the dataset as $D = \{\text{featureX}, \text{targetY}\}$. For two real-valued $n_t$-dimensional vectors $Z = (z_1, \ldots, z_n)$ and $\tilde{Z} = (\tilde{z}_1, \ldots, \tilde{z}_n)$, denote the loss function as $L(z, \tilde{z})$, the empirical risk function $R(Z, \tilde{Z}) = \frac{1}{n} \sum_{j=1}^{n_j} L(z_j, \tilde{z}_j)$. Let $\tilde{Y}_A$ and $\tilde{Y}_B$ denote the currently fitted values from machines $M_A$ and $M_B$, respectively. Note that the key idea of MaC is to update $\tilde{Y}_A$ and $\tilde{Y}_B$ alternately throughout the collaboration process. Figure 2 is a schematic of MaC with two base machines with the detailed steps as follows.

1. **Step 1** Randomly split data $D$ to training data $D^t = \{X^t, Y^t\}$ and validation data $D^v = \{X^v, Y^v\}$. Initialize $\tilde{Y} = \tilde{Y}_A = \tilde{Y}_B = 0$.
2. **Step 2** Update the working response for machine $M_A$ as $Y_A \equiv Y - \tilde{Y}_B$. Construct $D = \{X, Y_A\}$ and split it into $D^t$ and $D^v$ accordingly. Tune the hyperparameters and estimate the parameters of $M_A$ with the data $D$ and update the predicted value $\tilde{Y}_A$ of $Y_A$ using machine $M_A$. Then, update $\tilde{Y}_A = (\tilde{Y}_A', \tilde{Y}_A)$, where $\tilde{Y}_A'$ and $\tilde{Y}_A''$ denote the predictions of the training sample and the validation sample, respectively. Calculate the empirical risk of validation data $R^v = R(\tilde{Y}_A', \tilde{Y}_A'')$.
3. **Step 3** Update the working response for machine $M_B$ as $Y_B \equiv Y - \tilde{Y}_A$. Construct $D = \{X, Y_B\}$ split it into $D^t$ and $D^v$. Tune the hyperparameters and estimate the parameters of $M_B$ with the data $D$ and update the predicted value $\tilde{Y}_B$ of $Y_B$ using machine $M_B$. Then, calculate $\tilde{Y}_B = (\tilde{Y}_B', \tilde{Y}_B'') \equiv \tilde{Y}_A + \tilde{Y}_B$ and the empirical risk of validation data $R^v = R(\tilde{Y}_B', \tilde{Y}_B'')$.
4. **Step 4** Iterate Steps 2 and 3 with $M_A$ and $M_B$ up to $T > 0$ times. During each iteration, check the loss of validation data and stop the iteration if $R^v$ does not decrease any more.
5. **Step 5** The final prediction of $Y$ is the $\tilde{Y}$ from the iteration with the smallest $R^v$.

Note that we adopt a hold-out method to evaluate different machines. In theory, a cross-validation method (heuristically, CV), for example, $k$-fold CV scheme, could be adopted, for our experiments; however, Optuna, the hyperparameter optimization software framework taken by us, prevents us to adopt a CV method. Taking the $k$-fold CV as an example, Optuna will not give us the evaluation values for the same hyperparameters for all the $k$-folds so that we cannot take the average of the evaluation values across the $k$-fold. Developing a new optimization framework for $k$-fold is an interesting future work.

### 2.2 A general algorithm for MaC

We can easily extend the idea in the MaC for two machines to a situation with more machines. To describe the general algorithm (Algorithm 1) of MaC with more than two base machines, we need the following setup and notations. Suppose we have an independent and identically distributed sample of size $n$:

$$D = \{(D_1, \ldots, D_n) = ((X_1, Y_1), \ldots, (X_n, Y_n))\}$$

![Figure 2](image-url)  
**Figure 2** Machine collaboration.
generated from the true distribution \( P_0 \), which is an element of a statistical model \( P \). The support of \( P_0 \) is \( \mathcal{D} = \mathcal{X} \times \mathcal{Y} = \{ d \in \mathbb{R}^l \times R | P_0(d) \neq 0 \} \), where \( l \) is a positive integer denoting the dimension of \( \mathcal{X} \). MaC is constructed based on \( K_n \) different base machines \( \{ m_k, \lambda_k, \theta_k \} \), where \( \lambda_k \) and \( \theta_k \) are the vectors of hyperparameters and parameters of the \( k \)-th machine, respectively. Here, we use \( K_n \) to allow the number of base machines \( K \) to grow alongside sample size \( n \), as demonstrated in Section 3. We use the same loss function and risk function for tuning the parameters and hyperparameters of the base machines and the MaC throughout Algorithm 1. Moreover, assume the tuning and estimation algorithm for each base machine is given. Let \( \hat{Y}_k \) and \( \hat{Y}_v \) denote the predictions of the training sample and validation sample based on the \( k \)-th machine, respectively. For machine \( k = 1, \ldots, K_n \), define \( \hat{Y}_k \equiv (\hat{Y}_k^T, \hat{Y}_v^T) \), \( \hat{Y}_v \equiv \sum_{j \neq k} \hat{Y}_j \) and \( \hat{Y}_v \equiv \sum_{j=1}^{K_n} \hat{Y}_j^T \). Define the index pair of the outer and inner loops when the loop stops as \( \{ i^*, k^* \} \).

**Algorithm 1 Algorithm for Machine Collaboration (MaC)**

**Require**: \( K > 1 \) base machines \( \{ m_k, \lambda_k, \theta_k \} \). Maximum tolerance integers \( \tau > 0 \) and \( T > 0 \).

**Output**: The trained MaC, \( \hat{m}: \mathcal{X} \rightarrow \mathcal{Y} \); the prediction based on \( \mathcal{X}^* \), \( \hat{Y}^* \).

**Input**: \( D = \{ \text{feature data} \ X, \ \text{target data} \ Y \} \), a new feature data \( X^* \sim P_0 \).

1. Randomly split \( \mathcal{D} \) into training data \( \mathcal{D}' \equiv (X', Y') \) and validation data \( \mathcal{D}'' \equiv (X'', Y'') \) so that the proportion of the validation data is \( p \); 
2. Initialize \( t = 0 \), \( R_0 = \infty \), \( \hat{Y}_k = (\hat{Y}_k^T, \hat{Y}_v) = (0, 0) \) for \( k = 1, \ldots, K_n \); 
3. while \( i \leq T \) do 
   4. \hspace{1em} while \( k \leq K_n \) do 
   5. \hspace{2em} Construct \( \hat{D}' \) and \( \hat{D}'' \) by replacing \( Y \) in \( \mathcal{D}' \) and \( \mathcal{D}'' \) with \( Y_k \leftarrow (Y - \hat{Y}_k) \), where \( \hat{Y}_k = \sum_{j=1}^{K_n} \hat{Y}_j \); 
   6. \hspace{2em} For \( m_{k, \lambda_k, \theta_k} \), tune the hyperparameters and estimate the non-hyperparameters, obtain \( \hat{\lambda}_k^{(i)} \), \( \hat{\theta}_k^{(i)} \), using \( \hat{D}' \) and \( \hat{D}'' \) as training data and validation data, respectively. 
   7. \hspace{2em} \( \hat{Y}_k \leftarrow \left( m_{k, \lambda_k^{(i)}, \theta_k^{(i)}} (X'), m_{k, \lambda_k^{(i)}, \theta_k^{(i)}} (X'') \right) \); 
   8. \hspace{2em} \( \hat{Y}^v = \sum_{j=1}^{K_n} \hat{Y}_j^v \); 
   9. \hspace{2em} \( R_k^* \leftarrow R(Y^*, \hat{Y}^v) \); 
   10. \hspace{1em} end while 
11. \hspace{1em} \( \tilde{k} = \text{argmin}_k R_k^* \); 
12. \hspace{1em} if \( R_k^* < R_0 \) then 
13. \hspace{2em} \( R_0 \leftarrow R_k^* \); 
14. \hspace{2em} \( k^* \leftarrow \tilde{k} \); 
15. \hspace{2em} \( i^* = i; \ k^* = k \); 
16. \hspace{2em} \( \text{break} \); 
17. \hspace{1em} end if 
18. \hspace{1em} if \( t \geq \tau \) or \( i \geq T \) then 
19. \hspace{2em} \( i^* = i; \ k^* = k \); 
20. \hspace{2em} \( \text{break} \); 
21. end if 
22. end while 
23. \( \hat{m} = \left\{ m_1, \lambda_1^{(i^*)}, \theta_1^{(i^*)} + \cdots + m_{k^*}, \lambda_{k^*}^{(i^*)}, \theta_{k^*}^{(i^*)} \right\} + \left\{ m_{k^*+1}, \lambda_{k^*+1}^{(i^*)}, \theta_{k^*+1}^{(i^*)} + \cdots + m_{K_n}, \lambda_{K_n}^{(i^*)}, \theta_{K_n}^{(i^*)} \right\} \); 
24. return \( \hat{Y}^* = \hat{m} (X^*) \).
3 | THEORY FOR FINITE SAMPLE

Under the setting of Section 2.2, denote the cumulative distribution function of $X_1$ as $F_0$. Let $B_n \in (0, 1)^d$ be a random binary $n$-vector whose observed value defines a split of the data $D$ into a training sample $D'$ and a validation sample $D''$, with 1 for validation and 0 for training. Let $p$ denote the proportion of observations in the validation sample, and $P_n$, $P_{n,B_n}$ and $P_{n,B_n}$ denote the empirical distributions of $D$, $D'$, and $D''$, respectively.

Suppose we have a set of $K_n$ base machines $\{M_1, \ldots, M_{K_n}\}$. Assume the space of the hyperparameter $\lambda_j$ and the parameter vector $\theta_j$ of the $j$th base machine are $\Lambda_j \subseteq \mathbb{R}^{d_j}$ and $\Theta_j \subseteq \mathbb{R}^{d_j}$, respectively. Then, each base machine $M_j : \mathbb{P} \to \mathbb{P}(X_1 \mid X_j \times \Theta_j)$ is a space of real-valued parametric functions from $X' \to \mathbb{R}$, taking the values of the hyperparameters and parameters in the space $\Lambda_j \times \Theta_j$. For $j = 1, \ldots, K_n$, denote the realization of $M_j$ as $m_{j,\theta_j} : X' \to \mathbb{R}$, which is a function with hyperparameter vector $\lambda_j \in \Lambda_j$ and parameter vector $\theta_j \in \Theta_j$.

We consider candidate MaCs constructed by the sum of base machines with certain hyperparameters and parameters. In particular, we have $\mathcal{M} \equiv \{M_1(\cdot) + \cdots + M_{K_n}(\cdot) : \mathbb{P} \to \mathbb{P}(X' \mid \Lambda(n) \times \Theta(n))\}$, where $\Lambda(n) = \prod_{j=1}^{K_n} \Lambda_j$ and $\Theta(n) = \prod_{k=1}^{K_n} \Theta_k$ denotes the space of the hyperparameter vector $\lambda \equiv (\lambda_1, \lambda_2, \ldots, \lambda_{K_n})$ and parameter vector $\theta \equiv (\theta_1, \theta_2, \ldots, \theta_{K_n})$ of MaC, respectively.

Define the space of all candidate MaCs as $M \equiv \{\mathcal{M}(P) : P \in \mathbb{P}\} \subseteq \mathcal{S}(X, \Lambda)$, then each realization of $\mathcal{M}$, $m \equiv m_{j,\theta_j} : X' \to \mathbb{R}$ is an element of $M$ with hyperparameter vector $\lambda \equiv \Lambda(n)$ and parameter vector $\theta \in \Theta(n)$. Denote the loss function of $m$ by $L(D, m)$ and the risk of $m$ by $E_P [L(D, m)]$ for $D \in \mathcal{D}$ and $m$ denoting a base machine or a MaC. Endow the space $\mathcal{S}(X)$ a dissimilarity function $\delta : \mathcal{S}(X) \times \mathcal{S}(X) \to \mathbb{R}$, with the dissimilarity between $m_1$ and $m_2$ in $M$ defined as

$$\delta(m_1, m_2) \equiv \int |L(d, m_1) - L(d, m_2)| \text{d}P_0(d).$$

Define the pseudo-true MaC as

$$m_0 \equiv \mathcal{M}(P_0) = \arg\min_{m \in M} E_P [L(D, m)],$$

and the risk difference of $m$ as $\delta(m, m_0)$.

Denote the space of the hyperparameter vector in which the MaC algorithm searches by $\hat{\Lambda}(n) \subseteq \Lambda(n)$ with cardinality $|\hat{\Lambda}(n)| = j_n$. Indexing the elements of $\hat{\Lambda}(n)$ as $\{\lambda(j_1), \ldots, \lambda(j_{j_n})\}$, we construct a subspace $M_{k_n} \equiv \{m_{j,\theta_j} : \theta \in \Theta(n)\} \subseteq M$ according to the selection of hyperparameter vector for $k \in K_n \equiv \{1, \ldots, j_n\}$. For a particular subspace $M_{k_n}$ with fixed hyperparameter vector $\lambda_{k_n}$, the MaC algorithm searches for the optimal parameter vector on the parameter space $\Lambda_{k_n} \subseteq \Theta(n)$. After collecting MaCs whose hyperparameter vector is $\lambda_{k_n}$ and parameter vector $\theta \in \Theta_{k_n}(n)$, we create the space $M_{k_n} \equiv \{m_{j,\theta} : \theta \in \Theta(n)\} \subseteq M_{k_n}$. Define the risk approximation error of $M_{k_n}$ as $B_{k_n}(k) \equiv \min_{m \in M_{k_n}} \delta(m, m_0)$. Note that, in van der Laan et al. (2006), $M_{k_n}$ is called epsilon-net, which is a form of sieving net for the parameters.

For any empirical distribution $P_n$, define the estimated model with fixed $k$ based on our algorithm as

$$\hat{\mathcal{M}}_k(P_n) \equiv \arg\min_{m \in M_{k_n}} \int L(d, m) \text{d}P_n(d).$$

Then, the estimated MaC is $\hat{\mathcal{M}}(P_n) \equiv \hat{\mathcal{M}}(P_n, k_n)$, where $k_n \equiv \arg\min_{k \in K_n} \int L(d, \hat{\mathcal{M}}_k(P_n)) \text{d}P_n(d)$.

To introduce the following theorem, we need the following definition.

**Definition 1.** (Searching Number and Searching Resolution). Let $\hat{\Theta}_k(n) = \{\theta_{k,1}, \ldots, \theta_{k,n_k}\}$ with $n_k < \infty$. For a real number $\epsilon > 0$, define a sphere $B(m_{k,\epsilon}) \equiv \{m \in M_{k_n} : |m - m_{k,\epsilon}| < \epsilon\}$. We refer to $n_k$ as the searching number and $e_k \equiv \inf \left\{ \epsilon : M_{k_n} \subseteq \bigcup_{k=1}^{K_n} B(m_{k_n,\epsilon}) \right\}$ as the searching resolution of $M_{k_n}$ for the algorithm, where $m_{k,\epsilon}$ denotes the MaC in $M_{k_n}$ with the non-hyperparameter vector $\theta_{k,\epsilon}$.

Note that in the definition above, the space $\hat{\Theta}_k(n)$ is first fixed. If we first fix $e_k$ and then select a space $\hat{\Theta}_k(n)$ with minimum $n_k$ so that $\bigcup_{k=1}^{K_n} B(m_{k_n,\epsilon})$ can cover $M_{k_n}$, then $n_k$ is just what we would call a covering number.

Let us refer to the value of the parameter vector that results in the minimum of the empirical loss of estimation as the optimal parameter vector. In the theoretical analysis, following van der Laan et al. (2007), we only consider a MaC algorithm that searches the optimal parameter vector on a discrete set. For $\hat{\Theta}_k(n) = \{\theta_{k,1}, \ldots, \theta_{k,n_k}\}$ with $n_k < \infty$, we have the following finite sample result.
Theorem 1. Assume a constant $C_0 < \infty$ exists, $|Y| \leq C_0$ a.s. and $\sup_{m \in M} \sup_{X \in \mathcal{X}} |m(X)| \leq C_0$. Define $C_1 \equiv 4C_0^2$ and $C_2 \equiv 16C_0^2$. Let $L(D, m) \equiv (Y - m(X))^2$, $m_0(X) \equiv E_\delta |Y|$, $C(a) \equiv a(1 + a/2)^2 \left( \frac{2C_1}{a} + \frac{2C_2}{a^2} \right)$. Then, for any $a > 0$, the following inequality holds

$$E_\delta \delta \left( \mathcal{P}_{n,B}(x), m_0(x) \right) \leq (1 + a) \min_{k \in \kappa_k} \left( 1 + aB_0(k) \right) + C(a) \frac{1 + \log(J)}{n(1 - \rho)} + C(a) \frac{1 + \log(J)}{np},$$

where $B_0(k) = \min_{m \in M} \sum_{i \in \mathcal{X}} (m(x) - m_0(x))^2 dF_0(x)$. The proof of Theorem 1 is provided in Appendix A. Theorem 1 shows that the expectation of the risk difference of $\mathcal{P}_{n,B}(x)$ and $m_0(x)$ depends on the searching number $N_k$ and the cardinality $J_k$ of the searching space of the hyperparameters $\Lambda(n)$. Suppose we search for the optimal MaC on $M_k$. If the searching number $N_k$ of $M_k$ is small, the searching resolution $\kappa_k(N_k)$ may be large, and then $B_0(k)$ could be large too. As a result, a small $N_k$ could result in the risk bound increasing. Moreover, if $J_k$ is small, the value of $\min_{k \in \kappa_k} B_0(k)$ could be large. To reduce the prediction risk, we need to not only adjust $N_k$ to strike a balance between the term associated with $\log(N_k)$ and that associated with risk in the approximation error $B_0(k)$ but also adjust the balance between $\min_{k \in \kappa_k} B_0(k)$ and the term with $\log(J_k)$. Note that increasing the number of base machines, $K_n$, may reduce the first term of Equation (1), but cause the term with $\log(J_k)$ to increase; hence, a proper selection of the base machines and a moderate $K_n$ would also be helpful to reduce the risk.

Theorem 1 also illustrates a merit of the circular and recursive feature of MaC; that is, MaC only needs to add up the final $K_n$ machines during the loop of the algorithm without the need to record all single machines in the loop. Note that $K_n$ is ordinarily much smaller than the total number of all single machines of the algorithm. Using a circular and recursive type algorithm can reduce $J_n$ compared with a sequential and top-down type algorithm because a sequential and top-down type algorithm needs to add all single machines into its final estimate.

Remark 1. A related method of MaC is LS-Boost (Friedman, 2001), which essentially works via repeatedly fitting the residual on the predictors using one base machine at a time. Recall that we have $K_n$ base machines. For MaC, in Algorithm 1, the estimated machine in step $i$, $m_{\kappa_k(N_k)}$, is an updated version of $m_{\kappa_k(N_k)}$, for $i > 1$. In the MaC, the machines collaborate with each other by updating themselves after considering the actions of all others. Note that we only need to store one set of estimates for each machine at any given time. The final result of MaC is the summation of the $K_n$ machines with their most recent estimates. In contrast, for LS-Boost, if we expect to modify the result of the first round based on $K_n$ estimated base machines, we need to use a special version of LS-Boost, in which we fit the $K_n$ base machines, $r_n > 1$ times in a sequential fashion. In such an LS-Boost, late-coming machines complement earlier machines. The results of all single machines are kept and added to the final result. Finally, the estimated result of LS-Boost is the summation of the results from the $r_n \times K_n$ estimated base machines. As a result, the total number of single machines, $r_n \times K_n$, for LS-Boost could be much larger than that, $K_n$, for MaC. A large total number of single machines could increase the risk of LS-Boost. Admittedly, this is not decisive for a comparison between LS-Boost and MaC because there are additional factors such as the searching space of every single machine. As a result, LS-Boost and MaC may have their own advantages and disadvantages in different situations.

4 | EXPERIMENTS

4.1 | Artificial simulation experiments

We first generate data for 10 independent variables, $x_1, x_2, \ldots, x_{10}$, following a multivariate normal distribution $N(0, \Sigma)$, with a variance-covariance matrix $\Sigma = \Sigma_0 |_{10 \times 10}$, where $\Sigma_1 = \rho^{i+j}$ with $\rho = 0.1$. Then, generate the error term $\epsilon \sim N(0,1)$. We consider the following two data-generating processes (DGP).

- **DGP 1**: $y = c_0 + c_1 x_1 + x_2 + 0.5x_3 + 0.3x_4 + 0.2x_5 + c_2 I(x_4 > 0) + c_3 I(x_5 > 1) + c_4 I(x_1 x_2 > 0) + \epsilon$
  
- **DGP 2**: $y = c_0 + c_1 x_1 + x_2 + 0.5x_3 + 0.3x_4 + 0.2x_5 + c_2 I(x_1 > 0) \times x_2 - c_3 I(x_1 < 0) \times x_2 + c_4 I(x_1 > 0) \times \sin(x_5) + \epsilon$
where \( I(\cdot) \) stands for indicator function and the constants \( c_0 \) through \( c_5 \) are chosen to standardize each term (mean 0 and variance 1). It is clear to see that DGP 2 has stronger nonlinearity than DGP 1. Note that the variables \( x_6, \ldots, x_{10} \) are not included in either of the DGPs but are included as predictors for all methods. The sample size \( n \) and the number of replications for both are 1000. We set \( p = 0.25 \). The sample is randomly split into training data of 600 observations, validation data of 200 observations, and test data of 200 observations. We choose the mean squared prediction error \( \text{MSPE}_i = \frac{1}{n} \sum_{j=1}^{n} (\hat{y}_{ij} - y_j)^2 \) as the loss for both the artificial and real data experiments, where \( \hat{y}_{ij} \) is the prediction of \( y_j \) for the \( i \)th replication.

We use DT (CART, Breiman et al., 1984), DNN, and Ridge regression as base machines. The DNN used here has five dense layers. Each of the first four dense layers is associated with a dropout layer. We treat the number of nodes of the latent layers, the types of activation functions, the dropout ratio, the learning rate of optimization, the batch size, and the number of epochs as hyperparameters. The maximum depth of the DT is fixed as 10. The DT is pruned according to the cost complexity parameter, which is a hyperparameter. The tuning parameter that controls the strength of the penalty of Ridge is also a hyperparameter. The order of the base machines is also treated as a hyperparameter. As mentioned in

\[ \text{FIGURE 3} \quad \text{MaC versus alternatives.} \]
Section 2, all the hyperparameters are tuned with respect to the MSPE in the validation data. Using these three base machines for MaC, LS-boost, and SL, we compare the prediction performances on the test data between MaC, SL, and LS-Boost for both DGPs. For MaC, we set $T = 50$ and $r = 10$.

We conduct LS-boost with a similar setup of MaC. The three base machines are repeatedly used with a fixed order for at most $T = 50$ times. The order is selected according to the empirical risk of the validation data. The processes will be stopped if the empirical risk of the validation data does not decrease for $r = 10$ times. For LS-boost and SL, the hyperparameters of each base machine are tuned according to the empirical risk of the validation data, when we fit each base machine.

We use the Greene HPC Cluster of New York University to carry out all the experiments. All the experiments are carried out by CPU with a 2× Intel Xeon Platinum 8268 24C 205 W 2.9 GHz processor. For each simulation replication, the computing time of the artificial simulation is about 64 min, while that of the real data experiments with datasets of different sizes ranges from 42 min to 50 h.

The simulation results for DGP 1 are in Figure 3a,b, with that of DGP 2 in Figure 3c,d. We count the number of replications for which MaC wins; that is, it produces a smaller MSPE for the test data than its competitors, namely, a particular ensemble method or a base machine. As depicted in Figure 3a,c, for both DGPs, MaC generally outperforms all the other methods. The boxplots in Figure 3b,d show that MaC has a smaller mean and median of prediction errors on the test data than all the other methods, whose means and medians are marked by the blue rectangles and the orange lines, respectively. For the simulation and the real data experiment (in the next subsection), we calculate the mean and median of MSPE for each method, the paired $t$-statistic, and Cohen’s $d$ (Cohen, 1988) of the means of MSPEs for each pair, which consists of an alternative method and MaC. The results of the simulations are tabulated in the first two panels of Table 1. For both DGPs, all the paired $t$-statistics are large with values of at least 4.6, and most of Cohen’s $d$s are greater than 0.2, implying that the mean and median of MSPE for the MaC are significantly smaller than those of the other methods.

### 4.2 Real data experiment

We use the same base machines and the same setting as the simulations for our real data experiment. The real datasets are from PMLB, which is an open-source dataset collection for benchmarking machine learning methods. All the datasets do not contain personally identifiable information or offensive content. There are 122 datasets for regression in PMLB in total, including data about automobile prices, faculty salaries, pollution, and crime. The sample sizes of the datasets range from 47 to 1,025,010. We dropped three datasets with sample sizes greater than or equal to 1 million because of our limits in computing resources. As a result, the datasets used have sample sizes ranging from 47 to 177,147 with a mean of 5476.69, while the numbers of features are from 2 to 1000 with a mean of 26.05. To make the comparison between the different methods simpler, we standardize all variables in the datasets so they all have a mean of 0 and a variance of 1. We apply MaC, SL, LS-Boost, and the three individual base machines to predict the target variable in the test data for each dataset. We perform the experiment 20 times, in which for each time, each dataset is randomly split into training (64%), validation (16%), and test (20%). All the prediction results are in Figures 3e,f and 4. We count the number of datasets for which MaC outperforms its competitors in terms of MSPE on the test data. The results are in Figure 3e, which

| TABLE 1 | Results of simulation and real data experiment. | MaC | SL | LS-Boost | DNN | Tree | Ridge |
|---------|-----------------------------------------------|-----|----|----------|-----|------|-------|
| DGP 1   |                                              |     |    |          |     |      |       |
| Mean    | 1.92                                         | 2.21| 2.11| 2.48     | 2.53| 3.36 |
| Median  | 1.85                                         | 2.16| 2.06| 2.43     | 2.48| 3.31 |
| Paired $t$ | 23.62                                       | 15.45| 36.91| 47.10     | 104.45| |
| Cohen’s $d$ | 0.75                                         | 0.49| 1.17| 1.49     | 3.30| |
| DGP 2   |                                              |     |    |          |     |      |       |
| Mean    | 3.05                                         | 3.21| 3.27| 4.02     | 3.35| 6.25 |
| Median  | 2.73                                         | 2.96| 2.93| 3.60     | 3.11| 5.96 |
| Paired $t$ | 4.64                                       | 6.61| 23.61| 7.71     | 68.16| |
| Cohen’s $d$ | 0.15                                         | 0.21| 0.75| 0.24     | 2.16| |
| Real data |                                              |     |    |          |     |      |       |
| Mean    | 0.26                                         | 0.70| 0.28| 0.36     | 0.37| 0.52 |
| Median  | 0.20                                         | 0.27| 0.23| 0.32     | 0.32| 0.61 |
| Paired $t$ | 6.97                                       | 12.52| 33.02| 15.71     | 26.87| |
| Cohen’s $d$ | 0.22                                         | 0.40| 1.04| 0.50     | 0.85| |
shows that MaC wins for more than 60% datasets against all competitors. Moreover, as illustrated in Figure 3f, MaC has a smaller mean and median of MSPE than all the competing methods. To obtain a closer look at the settings where MaC has an advantage, we calculate the MSPE differences by subtracting the MSPEs of the other methods from that of MaC. The results of the MSPE differences are plotted in Figure 4 for all the methods. As shown, for each subfigure, there are more points with positive MSPE difference than with negative MSPE difference. It means that MaC has smaller MSPE than corresponding alternative methods. In Figure 4, we draw an orange cross when MaC outperforms others and a blue cross otherwise. MaC has superior performance across the entire range of sample sizes and the number of variables. Similar to the simulation, the paired t-statistics and Cohen’s $d$ for the real data in the third panel of Table 1 show that the mean and median of MSPE of the MaC are significantly smaller than those of the other methods.\footnote{\textsuperscript{5}}

5 | CONCLUSION

In this paper, we propose a new ensemble learning framework, MaC, for regression problems. The key feature of MaC being \textit{circular} and \textit{recursive} helps it to communicate among the base machines, yielding better performance in various scenarios. However, the framework of making an ensemble algorithm \textit{circular} and \textit{recursive} is not limited to supervised regression learning tasks. Some interesting extensions would be to apply this same MaC framework to other types of tasks such as classification and semisupervised learning. In our theoretical analysis, we derive the risk bound of MaC using a quadratic risk function. Deriving risk bounds for more general risk functions and comparing the risks of MaC with individual base machines, super learner, and boosting could also lead to a deeper understanding of MaC. We intend to address these extensions in future work. Similar to boosting methods, MaC has a limitation on the burden of computation, since the current version of the algorithm of MaC cannot be executed in parallel. It is another important future work to reduce the burden of computation.
AUTHOR CONTRIBUTIONS
The manuscript conceptualization, writing, reviewing and editing were shared by Qingfeng Liu and Yang Feng. The Python implementation and theoretical proofs were completed by Qingfeng Liu.

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CONFLICT OF INTEREST STATEMENT
The authors declare no potential conflict of interests.

DATA AVAILABILITY STATEMENT
The data that support the findings of this study are openly available in Penn Machine Learning Benchmarks at https://epistasislab.github.io/pmlb/.

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ENDNOTES
* As $N$ goes to infinity with $n$, Theorem 1 can be regarded as an approximate result for the MaC algorithm that searches the optimal parameter vector on the whole domain.
† Note that the MSPE of SL for one dataset is extremely large (42.48), which we ignore in some figures for better visibility (we calculate the paired $t$-statistic and Cohen's $d$ after deleting the pair corresponding to this dataset).

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APPENDIX A: PROOFS

The finite sample theoretical result in the main article is an application of the results of van der Laan et al. (2006). To prove Theorem 1, we require the following assumptions and proposition.

Assumptions

1. \( \sup_{m \in \mathbb{M} \in \mathbb{D}} | \mathbb{L}(D,m) - \mathbb{L}(D,m_0) | \leq C_1. \)

2. assume

\[
\sup_{m \in \mathbb{M}} \text{VAR}_E[\mathbb{L}(D,m) - \mathbb{L}(D,m_0)] \leq C_2.
\]

Proposition 1. Under Assumptions 1 and 2, the following finite sample inequality holds for some constant \( C(a) \)

\[
E_{P_n} \delta \left( \hat{\mathbb{L}} \left( \left( \frac{P_n}{k} \right), m_0 \right) \right) \leq (1 + a) \min_{k \in \mathbb{N}} \left\{ (1 + a)B_0(k) + C(a) \frac{1 + \log(N_k)}{n(1 - p)} \right\} + C(a) \frac{1 + \log(J_n)}{np}
\]

for any \( a > 0 \). Therein, \( N_k \) is the searching number of \( \mathbb{M}_k \) for the MaC algorithm,

\[
C(a) = 4(1 + a/2)^2 \left( \frac{2C_1}{3} + \frac{2C_2}{a} \right).
\]

Note that

\[
E_{P_n} \delta \left( \hat{\mathbb{L}} \left( \left( \frac{P_n}{k} \right), m_0 \right) \right) = E_{P_n} \delta \left( \hat{\mathbb{L}} \left( \left( \frac{P_n}{k} \right), m_0 \right) \right)
= E_{P_n} \left( \left( \frac{P_n}{k} \right)(x) - m_0(x) \right)^2 dF_0(x).
\]

Simply applying Theorem 3.1 (van der Laan et al., 2006) with fixed \( \varepsilon_k \), the conclusion of Proposition 1 is straightforward.
A.1 | Proof of Theorem 1

We provide a sketch of the proof using the results in (van der Laan et al., 2006) here.

Proof. To apply Proposition 1, we need only check Assumptions 1 and 2. First, Assumption 1 holds, given

\[
\sup_{m \in \mathcal{M}} \sup_{D \in D} |L(D, m) - L(D, m_0)| \\
= \sup_{m \in \mathcal{M}} \sup_{D \in D} \left| (Y - m(x))^2 - (Y - m_0(x))^2 \right| \\
\leq \sup_{m \in \mathcal{M}} \sup_{D \in D} \left| Y^2 + m^2(x) + 2Y^2 + m_0^2(x) \right| \\
= 4C_0^2 = C_1.
\]

For Assumption 2, note that using some simple algebra, we have

\[
\int (L(d, m) - L(d, m_0))dP_0(d) = \int (m(x) - m_0(x))^2dF_0(x).
\]

Then

\[
\text{VAR}_{P_0}[L(D, m) - L(D, m_0)] \\
\leq E_{P_0} \left( (L(D, m) - L(D, m_0))^2 \right) \\
= \int (m^2(x) - m_0^2(x) - 2ym(x) + 2ym_0(x))^2dP_0(d) \\
= \int (m(x) - m_0(x))(m(x) + m_0(x) - 2y)^2dP_0(d) \\
\leq 16C_0^2 \int (m(x) - m_0(x))^2dF_0(d) \\
= C_2E_{P_0}[L(D, m) - L(D, m_0)].
\]

Assumption 2 is satisfied. We complete the proof by applying Proposition 1. □