

A Genetic Algorithm with Tree-structured Mutation for Hyperparameter Optimisation of Graph Neural Networks

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Abstract—In recent years, graph neural networks (GNNs) have gained increasing attention, as they possess the excellent capability of processing graph-related problems. In practice, hyperparameter optimisation (HPO) is critical for GNNs to achieve satisfactory results, but this process is costly because the evaluations of different hyperparameter settings require excessively training many GNNs. Many approaches have been proposed for HPO, which aims to identify promising hyperparameters efficiently. In particular, the genetic algorithm (GA) for HPO has been explored, which treats GNNs as a black-box model, of which only the outputs can be observed given a set of hyperparameters. However, because GNN models are sophisticated and the evaluations of hyperparameters on GNNs are expensive, GA requires advanced techniques to balance the exploration and exploitation of the search and make the optimisation more effective given limited computational resources. **Therefore, we proposed a tree-structured mutation strategy for GA to alleviate this issue.** Meanwhile, we reviewed the recent HPO works, which gives room for the idea of tree-structure to develop, and we hope our approach can further improve these HPO methods in the future.

Index Terms—generic algorithm, tree-structured mutation, graph neural network, hyperparameter optimisation

I. INTRODUCTION

Graph is a data type used to describe the structured objects consisting of nodes and edges, such as citation networks, molecules, and road networks. In graph-related learning and prediction problems, traditional machine learning methods require using feature engineering to process graph data before training or prediction [1]. In contrast, graph neural networks (GNNs) are proposed to directly operate on graphs to solve graph-related problems in an end-to-end manner [1]. GNNs exploit neural networks to model graphs and perform representation learning, which requires that GNNs are set with appropriate hyperparameters (e.g., learning rate, the number of neural network layers) to control the learning process.

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From our perspective, more **sophisticated** neural architectures are required to process graph data, which may result in challenging HPO tasks for GNNs. Falkner et al. [2] pointed out that deep learning algorithms are very sensitive to many hyperparameters. The work presented in [3] demonstrated that HPO for GNNs is vital for achieving satisfactory results in practice. Therefore, research on effective HPO approaches for GNNs is critical and of great value for GNN applied to various real-world problems.

In brief, HPO is a trial-and-error process to obtain optimal solutions via iteratively generating and evaluating hyperparameter settings until the preset stopping condition(s) are satisfied. Commonly, the objective function of GNNs is selected as the fitness function of HPO to evaluate hyperparameters. However, the evaluation is often very expensive because training GNN models would take a lot of computational resources. On the other hand, with the development of deep learning, neural networks have an increasing number of layers or various other optional hyperparameters (e.g., activation functions, optimisation methods), which results in a large search space and increasing the difficulty of HPO. So, existing works of HPO have been conducted based on the issues of how to find the best solutions with fewer trials, reducing evaluation cost, and improving the capability of exploration. **In this paper, a trial denotes a complete process of evaluating a hyperparameter setting (solution) on the fitness function (objective function).**

There are many state-of-the-art HPO approaches with different search strategies. For example, TPE [4] and BOHB [2] are proposed based on Bayesian optimisation (BO) which are suitable for the functions that are expensive to evaluate. However, the former uses density functions to model two sets (good and bad) of hyperparameters, instead of using Gaussian process as in [5], [6] as a standard surrogate model to approximate the distribution over the objective function. **Furthermore, BOHB combines Bayesian optimisation and bandit-based methods to ensure good performance at anytime and speed up the process towards optimal solutions.** In general, BO-based methods balance the exploration and exploitation by acquisition function.

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On the contrary, CMA-ES [7] and HESGA [3] are evolutionary approaches that exploit high-quality individuals to guide the generation of promising offspring, while they rely on evolutionary operators to explore search space. CMA-ES employs an adaptive multivariate distribution to sample individuals, and HESGA uses a genetic algorithm that relies on crossover and mutation operators to generate better individuals. To deepen the work of HESGA [3], our research focuses on improving the exploration capability of the mutation operator.

Genetic algorithm with hierarchical evaluation strategy (HESGA) [3] utilises the elite archive to preserve excellent individuals, from which a parent can be selected to generate offspring. Meanwhile, the fast evaluation strategy has been introduced in HESGA to speed up optimisation and save computational resources. Furthermore, HSEGA uses the single point mutation as in [8]–[10] which is one factor for preventing GA from getting stuck in local optima and maintains the diversity of population [11]. However, we believe that the mutation operation in HSEGA can be further explored as only classical mutation operation was used in HSEGA. Therefore, in this research, we propose a tree-structured mutation (TSM) which employs the tree structure to store hierarchical historical information to guide mutation. In this way, GA can explore the whole search space more adaptively and effectively. Meanwhile, the idea of TSM is also compatible and scalable to other HPO algorithms that hierarchise historical information for future discovery.

Our contributions are summarised as follows:

- We have developed a tree-structured mutation operation for GA to adaptively maintain the balance between exploration and exploitation for searching the hyperparameter space of GNNs while retaining the randomness of mutation operator.
- We conducted a review of advanced HPO methods, and we found that the tree-structured approach has the potential to be integrated into other approaches.
- Our research contributes to the development of molecular machine learning [12] as well as HPO for GNNs in general.

The rest of this paper is organised as follows. Section II introduces relevant work on HPO. In Section III, the details of our tree-structured mutation are presented. The experiments are reported and the results are analysed in Section IV. Finally, Section V concludes the paper and explores some directions in future work.

II. RELATED WORK

In this section, we will first review some popular HPO methods. The genetic algorithm with hierarchical evaluation strategy (HESGA) [3] will then be introduced because our tree-structured mutation is proposed upon it. Finally, some mutation strategies will be reviewed. 分层评估策略

A. Hyperparameter Optimisation Methods

There have been a lot of state-of-the-art HPO methods, and these methods can be classified into *black-box optimisation*

and *multi-fidelity optimisation* approaches [13]. The former focus on the effectiveness of the search algorithms and the latter focuses on efficiently using computational resources in search algorithms [14]–[16].

Black-box optimisation [17], [18] implies that the details of the objective function and its gradient information is unknown during searching optimal solutions. In HPO, hyperparameters can be evaluated on the objective function, but we do not have access to any information about the model. Random search [19] and grid search are two simple and commonly used methods for HPO. Bergstra et al. [4] hold the point that random search is more efficient than grid search given a fixed limited computation budget for HPO. However, facing the problems with expensive evaluations, it is very challenging for random search and grid search to achieve satisfactory performance.

The use of *Bayesian optimisation* (BO) can alleviate the issue of high computational cost [14], [18]. The framework of BO is concluded in the sequential model-based algorithm [20] that iteratively exploits historical data to fit surrogate models or other transformations, while the most promising candidate is drawn according to a predefined criterion (i.e. acquisition function). The work presented in [4]–[6], [21] makes use of Gaussian processes (GPs) to approximate the distribution over the objective function, and the candidate is selected by the acquisition function: probability of improvement (PI) or expected improvement (EI). In contrast, TPE [4] employs Parzen estimators as a surrogate to directly model promising and unpromising hyperparameters, and the candidate solutions are drawn according to EI that is proportional to the ratio of two density functions. During searching optimal solutions, the acquisition function plays a significant role in balancing exploration and exploitation.

Furthermore, *evolutionary computation* has demonstrated the capability of solving HPO problems [3], [7], [22], [23]. CMA-ES [7] imitates the biological evolution, assuming that no matter what kind of gene changes, the results (traits) always follow a Gaussian distribution of a variance and zero-mean. Meanwhile, the generated population is evaluated on the objective function, and a portion of the individuals with excellent performance is selected to suggest evolution, moving to the area where better individuals would be drawn with higher probability.

Successive halving [24] is a bandit-based *multi-fidelity* method for efficiently allocating computational resource that gives the most budget to the most promising individuals. Meanwhile, successive halving is an iterative process in which the best half of individuals are retained, and half of the individuals with lower performance are discarded when a portion of the total computational resource runs out. Hyperband [25] and BOHB [2] are proposed based on the successive halving, but the former proposed a modification that frequently performs the successive halving method with different budget allocations to find the best solutions. Li et al. [25] pointed out that because the terminal losses are unknown, the trials of different allocations are helpful to recognise high-quality solutions. For example, two individuals might not have a significant

difference on fitness in the 30th epoch, but a greater difference may be observed in the 50th epoch if more computational resources (i.e., epochs) are allocated. Furthermore, BOHB combines Hyperband and BO to chase an ideal state in which performance and computational cost are both covered.

B. Genetic Algorithm

Genetic algorithm (GA) is a class of evolutionary computation has been applied to HPO [3], [26], [27]. GA evaluates the qualities of individuals in the population by using a fitness function. To search for high-quality individuals, GA relies on crossover, mutation, and selection operators. The selection is inspired by natural selection, which means GA selects individuals as parents according to the probabilities (e.g., roulette wheel) to generate next-generation by crossover and mutation, and the probabilities are proportional to their quality (fitness). There are many crossover techniques such as uniform crossover [28], single-point [29], and heuristic crossover [30]; they aim to recombine genes from the parents to generate offspring. In the evolutionary process, mutation operators as the last step are generally assigned with a low probability to be invoked. However, it plays a significant role for preventing GA from getting stuck in local optima. Similar to the probabilistic sampling of solutions in BO-based optimisation, the mutation is employed to **endue** GA with the exploration capability of solutions. **赋予**

Variable length genetic algorithm [31] has been proposed to solve neural network HPO problem by increasing the length of the chromosome (i.e., enlarge search space) if the fitness does not satisfy preset conditions. Moreover, HESGA [3] introduced the **elite archive mechanism** that stores some current optimal individuals. According to the roulette wheel, parents are selected from the elite archive and the population (Fig. 1). In this way, new offspring always own at least a portion of the strong genes from the parent in the elite archive if crossover occurs. Meanwhile, HESGA provides the strategy of using fast and full evaluation methods, to alleviate the expensive evaluations. Fast evaluation is applied to the whole population. **The individuals with the most difference of fitness in the early training stage (10% ~ 20% of the total epochs) are considered promising, and it assumes that individuals with a steeper learning curve have more significant potential to achieve satisfactory results. Meanwhile, the full evaluation is employed to measure a small portion of individuals selected by fast evaluation.** The fast and full evaluation can be considered *multi-fidelity optimisation*, which focuses on decreasing the evaluation cost by combining many low cost evaluations with low-fidelity and a small number of costly evaluation with high-fidelity.

C. Mutation

Many mutation strategies have been proposed for GA, and we only present some of them which are related to our research. **Random (uniform) mutation and non-uniform mutation** have been proposed in [32]. In random mutation, where a gene is replaced with a random value drawn from a defined range.

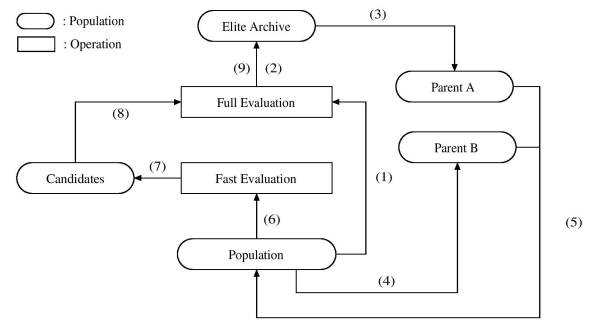


Fig. 1. Genetic Algorithm with Hierarchical Evaluation Strategy [3]

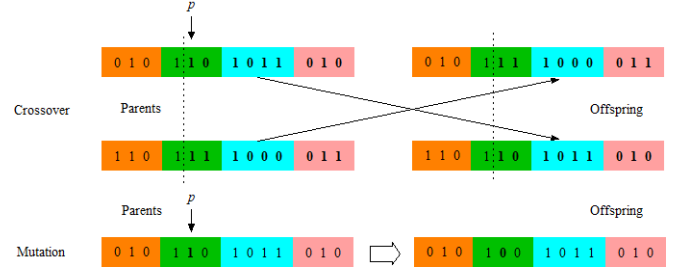


Fig. 2. Binary Crossover and Mutation [3]

On the other hand, in non-uniform mutation, the strength of mutation decreases along with the increasing number of generations. In adaptive mutation [33], [34], each solution is assigned with a mutation rate to maintain the diversity of the population without affecting algorithm performance. Based on Gaussian mutation, self-adaptive mutation [35] allows GA to vary the mutation strength during the evolution, while self-adaptive Gaussian mutation based adaptation of population size is proposed in [36]. In Pointed directed (PoD) mutation [37], each gene is tightly associated with a single bit that guides the direction of mutation which the gene may follow. Compared with Gaussian mutation, Deep et al. [38] reported that PoD mutation is more advantageous in unconstrained benchmark problems. The above mentioned mutation operators exploit the historical information which is generated during evolution to adjust the mutation strategy dynamically, which inspired **our TSM to improve the naive single point mutation used in [3].**

III. METHOD

In this section, the design of tree-structured mutation (TSM) will be described. Meanwhile, we will introduce the use of TSM in HESGA.

A. HESGA

The framework of HESGA [3] is shown in Fig. 1. The TSM is proposed as a further improvement of HESGA. The original HESGA uses the binary encoding scheme for hyperparameters on HPO: each hyperparameter is assigned with a fixed-length binary code with a step size (i.e., resolution). For example, if the batch size ranges from 8 to 512 with a step size of 8,

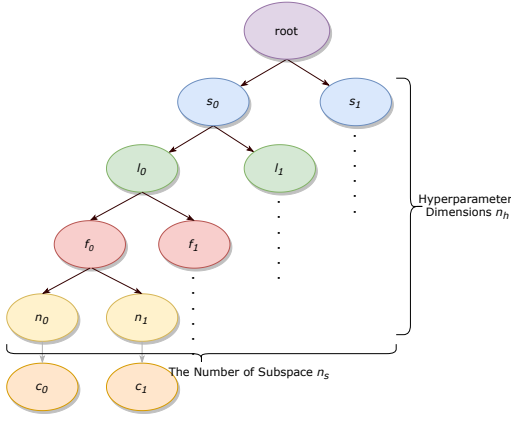


Fig. 3. Tree-structured hyperparameter space, the internal nodes of s, l, f, n represent the different hyperparameters and used to define their hyperparameter subspace with different subscripts, such as s_0 and s_1 respectively correspond to lower and upper portion of the hyperparameter s . n_s denotes the maximum width of the tree and n_h is the dimension of hyperparameter settings

and then a batch size of 16 is represented by $[0, 0, 0, 0, 0, 1]$. Single point crossover and mutation are employed in HESGA. Fig. 2 shows that both the mutation and crossover are implemented by a uniform distribution to randomly generate a position p at first. The bits on the right of the point p are swapped between the two parent chromosomes for the crossover, and the bit on the position p changes the value from 0 to 1, or vice versa for mutation. In initialisation, all randomly generated individuals are assessed by full evaluation, and some individuals with higher fitness values are selected to be included in the elite archive by Step (1) and (2) as shown in Fig. 1. To update the elite archive, the offspring is generated by operating crossover and mutation on the two parents that are respectively selected by roulette wheel from the elite archive and population in Steps (3), (4) and (5). Then, in Step (6), fast evaluation is operated to find a small number of individuals (candidates) which have better fitness values, and these individuals are further accessed by full evaluation in Step (8). The elite archive is updated if candidates are better than some of the individuals in the elite archive in Step (9). The work presented in [3] demonstrated that HESGA had achieved satisfactory performance on HPO for GNNs.

B. Tree-structured Mutation

In HPO using GA, the mutation operator is a way for GA to explore the hyperparameter search space. All mutation operators discussed in Section II-C are proposed based on the **core principle of effective mutation towards optimal solutions. Most of the black-box optimisation methods utilise historical information to carry out effective exploration.** Here, back to GA, we expect that the historical information can also be exploited with the tree to suggest mutations.

Considering that TPE [4] used tree structure to model the sampling of hyperparameter settings, we propose to employ a binary tree to build the hierarchical search space, as shown in Fig. 3. Each pathway from the root node to a leaf node

represents a subspace of the whole hyperparameter space. For example, from root to node c_0 , the child nodes (s_0, l_0, f_0, n_0) define the corresponding ranges of hyperparameters (*batch size, learning rate, the size of graph convolution layer, and the size of fully-connected layer*), which forms a subspace of the whole search space and can be represented by a binary string 0000. **Meanwhile, the left and right child nodes define the lower and higher ranges of hyperparameters by thresholds.** For example, if s ranges from 8 to 512, the median value 256 is chosen as the threshold to give two subspace with the same size. s_0 indicate a range from 8 to 255 and s_1 ranges from 256 to 512. In this way, the whole search space is divided into many subspaces, and the number of subspaces equals the total number of leaf nodes c (i.e., the maximum width n_s), or the square of the dimension of hyperparameter settings n_h^2 , where n_h is also the maximum depth of the tree without leaf nodes.

To use the tree to suggest mutations, the internal and leaf nodes take the responsibility to record historical information. **The internal nodes are used to store the times of mutation that occurred on different dimensions in a subspace. Concurrently,** a leaf node c is used to record the times of a subspace that has been visited. For example, when a hyperparameter setting λ **sampled from** the subspace (s_0, l_0, f_0, n_0) has been evaluated on an objective function, the value of node c_0 will increase by 1. **If λ underwent a mutation on batch size, then the counter in the s_0 node will increase by 1.** In this way, the whole search space is hierarchised which increase the ability of exploration for mutation.

In this research, based on the framework of HESGA, **we use TSM to replace the single point mutation, considering that a more sophisticated mutation may lead to better performance.** We observed that there might exist the same individuals in elite archive and populations that waste computational resources for evaluating them during the experiments. Many reasons may lead to this issue. For example, an extremely excellent individual in the population will be selected to be included in the elite archive while outperforms other individuals in the elite archive; it means this individual has a higher probability of being selected as both Parent A and B in the next generation. Two identical parents will invalid crossover by which the same individuals will be generated. To solve this issue, we set the condition in Step (5.2) (Fig. 4) to prohibit duplicates. **If the duplication is detected, the mutation is forcibly invoked.** Based on TSM, we use two strategies: TSM with a given individual and TSM without a given individual respectively for the situation: mutation is invoked with preset probability in Steps (5.1 and 5.2) and force mutation when duplicates are detected in Steps (5.3 and 5.4), as shown in Fig. 4.

1) *TSM with A Given Individual*: HESGA operates the single point mutation with the probability of 0.2, as indicated by Step (5) in Fig. 1. TSM is also invoked with the same probability in Step (5.1) in Fig. 4. **TSM uses historical information recorded in the tree to generate a probability distribution to guide the mutation compared with the change of a bit of binary encoding under a uniform distribution.** Specifically,

Algorithm 2 TSM without A Given Individual

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1: Input  $tree, t = []$ 
2: for  $c = 1 \rightarrow n_s$  do
3:    $t_{total} += f(t_c)$   $\triangleright t_c$  denotes the times recorded in
     node  $c$ ,  $f$  is reciprocal function
4:    $t.append(f(t_c))$ 
5: end for
6:  $t' \leftarrow$  each element in  $t$  is divided by  $t_{total}$ 
7:  $i = \text{roulette wheel}(n_s, t')$   $\triangleright$  subspace  $i$ 
8:  $v = []$ 
9: for  $j = 1 \rightarrow n_h$  do  $\triangleright$  in subspace  $i$ 
10:   $r_j \leftarrow$  the defined value range in node with depth  $j$ 
11:   $v_j = \text{uniform}(r_j)$   $\triangleright$  mutated value  $v_j$  by sampling
     from a uniform distribution given range  $r_j$ 
12:   $v.append(\text{binary}(v_j))$ 
13: end for
14:  $s = v$ 
15: Output individual  $s$ 

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Our experiments have been conducted on three benchmark datasets: ESOL, FreeSolv, and Lipophilicity from [12]. They are three molecular property prediction datasets that are used to assess the performance of GNNs. Meanwhile, there are many types of GNN algorithms, but the neural fingerprint graph model (GC) [39] has been selected because it was proposed to be used for molecular machine learning. GC exploits the neural architectures to model circular fingerprint [40] for learning the molecular representations for prediction tasks. There are four hyperparameters selected for HPO, including s_b (batch size), l_r (learning rate), s_g (the size of graph convolution layer), and s_f (the size of fully-connect layer); the search space is constructed as follows: the range of s_b is $8 \sim 512$ with step size 8, the range of l_r is $0.0001 \sim 0.0032$ with step size 0.0001, the range of s_g is $8 \sim 512$ with step size 8, and the range of s_f is $32 \sim 1024$ with step size 32. As mentioned in Section III-B, TSM requires thresholds to divide the whole search space into many subspace, and we uses the median values of s_b , l_r , s_g , and s_f , which are 256, 0.0016, 256, and 512, respectively to build the binary tree in experiments.

As in [3], the root mean square error (RMSE) of GC is used as the fitness function for HPO, and it is also used to measure the HPO performance. The best hyperparameter setting found by an HPO method (HESGA and HESGA+TMS) will be given to GC to run 30 times, and the mean of the 30 RMSEs are used to measure the performance of HPO. Meanwhile, in order to make the comparisons more convincing, t -test with a significance level of two tails 10% is employed to compare the performance of HESGA and HESGA + TSM and see if there exists a significant difference. In t -test, negative t value and the hypothesis $h = 1$ indicates that HESGA outperforms HESGA+TSM; positive t value and the hypothesis $h = 1$ indicates that HESGA+TSM significantly outperform HESGA; or $h = 0$ (the null hypothesis) means

that there is no significant difference between HESGA and HESGA+TSM.

In the experiments on ESOL (Table I), HESGA+TSM has a smaller mean and standard deviation of RMSEs than HESGA. However, there is no significant difference between HESGA and HESGA+TSM at the significance level $\alpha = 10\%$. We considered that the size of the ESOL dataset constrains the performance of HESGA+TSM, because a sufficient amount of data is a prerequisite for GC possessing better performance with a more complex architecture. In Table I, HESGA+TSM found larger s_g and s_f , which means the GC with more parameters, and they require more training data to tune them for better performance. Furthermore, if we set the significance level $\alpha = 20\%$, HESGA+TSM outperforms HESGA in the validation data set. Meanwhile, it is obvious that two hyperparameter settings are completely different and come from different two subspaces, which indicates the complex and multi-modal nature of the underlying hyperparameter search space, and the discovery in different subspaces is meaningful.

In the experiments on FreeSolv (Table II), HESGA presents better performance than HESGA+TSM. FreeSolv is the smallest dataset used in our experiments. The small size of the dataset is intrinsically challenging for GC to learn and keep a stable performance, which may lead to the underperformance of HESGA+TSM since its strength is exploration, stable and accurate feedback (i.e., the results of evaluation on GC) is essential for conducting efficient exploration.

Furthermore, when duplicates appear in the population, HESGA uses single-point mutation which retains most of the genes from parents, and relatively speaking the strength of the mutation is small, while HESGA+TMS is guided by the tree-based mutation, which explores the search space more broadly compared with HESGA. Therefore, we considered that when the size of a dataset is relatively small, global exploration may bring more fluctuation and unknown factors upon the instability of GC, which brings more difficulties to the problems. In contrast “local” exploration might be more effective since it reduces the underlying unknown risks from the global area.

In contrast, Lipophilicity is the largest dataset in our experiments, and as shown in Table III, HESGA+TSM outperforms HESGA in this dataset with a significant difference, and lower standard deviation means the result of HESGA+TSM is more stable. When the size of dataset increased, the full evaluation becomes more accurate, and it provides more helpful information for GA to generate strong offspring in terms of exploitation. Meanwhile, more effective exploration becomes necessary, and HESGA+TSM shows better performance because TSM uses historical information to search hyperparameter space rather than search each part of the hyperparameter space with equal probability.

V. CONCLUSION AND FUTURE WORK

In this paper, we proposed TSM for genetic algorithm as applied to HPO of GNNs, which improved the performance of HESGA on the largest dataset in our experiments. Compared

TABLE I
THE RESULTS ON ESOL DATASET

ESOL	Hyperparameters	Train	Validation	Test	
HESGA	$s_b=64$	0.2847	0.8843	0.8862	Mean RMSE
	$l_r=0.0028$				
	$s_g=304$	0.0424	0.0509	0.0506	Mean STD
	$s_f=64$				
HESGA + TSM	$s_b=48$	0.2734	0.86585	0.8743	Mean RMSE
	$l_r=0.0012$				
	$s_g=320$	0.0333	0.0357	0.0463	Mean STD
	$s_f=320$				
<i>t</i> -test on results with significance level of $\alpha = 10\%$		$t = 1.1249, h = 0$	$t = 1.5963, h = 0$	$t = 0.9311, h = 0$	

TABLE II
THE RESULTS ON FREESOLV DATASET

FreeSolv	Hyperparameters	Train	Validation	Test	
HESGA	$s_b=24$	0.5498	1.0970	1.0370	Mean RMSE
	$l_r=0.0030$				
	$s_g=208$	0.1251	0.1199	0.1246	Mean STD
	$s_f=224$				
HESGA + TSM	$s_b=8$	1.1181	1.4083	1.3508	Mean RMSE
	$l_r=0.0010$				
	$s_g=480$	0.2692	0.2408	0.2874	Mean STD
	$s_f=576$				
<i>t</i> -test on results with significance level of $\alpha = 10\%$		$t = -10.3063, h = 1$	$t = -6.2298, h = 1$	$t = -5.3940, h = 1$	

TABLE III
THE RESULTS ON LIPOPHILICITY DATASET

Lipophilicity	Hyperparameters	Train	Validation	Test	
HESGA	$s_b=136$	0.3656	0.7402	0.7293	Mean RMSE
	$l_r=0.0031$				
	$s_g=232$	0.0881	0.0476	0.0462	Mean STD
	$s_f=1024$				
HESGA + TSM	$s_b=168$	0.2390	0.6962	0.7021	Mean RMSE
	$l_r=0.0011$				
	$s_g=304$	0.0676	0.0284	0.0269	Mean STD
	$s_f=864$				
<i>t</i> -test on results with significance level of $\alpha = 10\%$		$t = 6.1358, h = 1$	$t = 4.2642, h = 1$	$t = 2.7381, h = 1$	

with operating HPO on a relatively small dataset, the achieved improvement of HPO performance on the larger dataset is more meaningful since the evaluations are more expensive. Meanwhile, the research of GA-based HPO for GNN is in an early stage; our work will help other researchers to better explore this area. On the other hand, our research contributes to the development of molecular machine learning, which may facilitate the research from the relevant domain such as materials science, biology and drug discovery. Furthermore, the idea of utilising tree structure to hierarchise search space and record the historical information can be applied to other HPO methods. Finally, in future, we believe more research can be done along further developing TSM for evolutionary HPO. We list some potential directions as follows.

A. Reward and Rejection Mechanism

Currently, the inner and leaf nodes are used to store the times of previous exploration. Inspired by reinforcement learning [41], the results of evaluations on fitness function can be recorded as rewards with the times together to affect

future discovery by reconstructing Eqs. (1) and (2), and in this way, TSM is not only for increasing the exploration ability, but also for improving the exploitation in the later stage by introducing a reward mechanism. Meanwhile, the times and rewards can also work together in a surrogate model to reject those unpromising trials according to historical information.

B. Adaptive Threshold

In TSM, the binary tree requires thresholds to be specified to generate child nodes. In our experiments, we choose median values as thresholds. However, it is easy to observe that s_b in all experiments are from the lower range (i.e. the left child node). If the thresholds are adaptive and can be updated by the rewards referring to the percentile in TPE [4], TSM may be further improved to better focus on adaptively adjusted subspace.

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DATA STATEMENT

All data used in our experiments are from MoleculeNet [12], which are publicly available in <http://moleculenet.ai/datasets-1>.

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