

# Solving Expensive Optimization Problems in Dynamic Environments with Meta-learning

## —Supplementary Material

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### I. APPENDIX A

In this section, we sequentially introduce the mathematical definitions of the benchmark problem, the working mechanisms of the peer algorithms, and the fundamental ideas of the statistical measurements.

#### A. Mathematical Definitions of Benchmark Problem

In our experiments, we choose the moving peaks benchmark (MPB) [1] as the benchmark test suite. The function of MPB has the following form:

$$f(\mathbf{x}, t) = \max_{i \in \{1, \dots, m\}} \{H_i(t) - W_i(t) \|\mathbf{x} - X_i(t)\|\}, \quad (1)$$

where  $m$  is the number of peaks,  $\|\cdot\|$  represents the Euclidean norm,  $H_i(t)$ ,  $W_i(t)$ , and  $X_i(t)$  denote the height, width, and location of the  $i$ -th peak at the  $t$ -th time step (or environment), respectively. To be specific, the height, width, and location of peaks change can be described as follows:

$$\begin{aligned} H_i(t) &= H_i(t-1) + h_{sev} \cdot \sigma, \\ W_i(t) &= W_i(t-1) + w_{sev} \cdot \sigma, \\ X_i(t) &= X_i(t-1) + \mathbf{v}_i(t),, \\ \mathbf{v}_i(t) &= x_{sev} \cdot \frac{(1-\lambda)\mathbf{r} + \lambda\mathbf{v}_i(t-1)}{\|(1-\lambda)\mathbf{r} + \lambda\mathbf{v}_i(t-1)\|}. \end{aligned} \quad (2)$$

where  $h_{sev}$ ,  $w_{sev}$ , and  $x_{sev}$  indicate height severity, width severity, and shift severity, respectively, and  $\sigma$  is a random number obeyed a Gaussian distribution with variance 1 and mean 0.  $\mathbf{v}_i(t)$  and  $\mathbf{v}_i(t-1)$  represent the current and previous shift vector of the  $i$ -th peak, respectively.  $\mathbf{r}$  is a random vector and  $\lambda$  is the correlation coefficient.  $\lambda = 0$  denotes that the peak relocations are in a random direction, whereas they depend on the previous direction for  $\lambda > 0$ .

TABLE I  
PARAMETERS FOR MPB

Parameter	Value	Parameter	Value
Peak shape	Cone	Correlation coefficient, $\lambda$	0.5
Number of peaks	5	Range of space for each dimension	[0, 100]
Shift severity, $x_{sev}$	5, 10	Range of height for each peak, $H_i$	[1, 12]
Height severity, $h_{sev}$	7, 10	Range of width for each peak, $W_i$	[30, 70]
Width severity, $w_{sev}$	1		

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### B. Peer Algorithms

A concise description of peer algorithms is provided as follows. More details can be referred to the corresponding original papers.

1) *Discounted information through noise sampling strategy* (DIN) [2]: The strategy represents the best variant for tracking the changing global optima in dynamic environments described in [2]. It discounts older samples by introducing artificial measurement noise, which is a function of the time step of the samples and is added to the covariance function.

2) *Model-based optimization* (MBO) [3]: This algorithm picks out the observations collected from the previous time steps within a sliding time window. In addition, the time is augmented as a covariate, allowing the surrogate to model the effect of the time directly.

3) *Transfer Bayesian optimization* (TBO) [4]: This algorithm develops a transfer learning strategy to empower BO for handling expensive DOPs. The basic idea is to employ an augmented covariance function to realize knowledge transfer among GPR models from different time steps. To save the computational cost for GPR modeling, a decay mechanism is proposed to remove less irrelevant samples.

4) *Data-driven evolutionary transfer optimization* (DETO) [5]: This algorithm builds upon TBO. It employs a hierarchical multi-output Gaussian process to facilitate knowledge transfer and optimize cost-efficiency. Additionally, it introduces an adaptive source task selection mechanism and a bespoke initialization strategy to further augment the efficacy of knowledge transfer. A differential evolution variant with local search is also proposed to optimize the acquisition function.

### C. Statistical Tests

In this paper, three statistical measures are adopted in our empirical study. Their basic ideas are introduced as follows.

- Wilcoxon rank sum test [6]: It is a non-parametric statistical hypothesis test. Particularly, the significance level is set to 0.05 in our experiments.
- Scott-Knott test [7]: This measure is used to rank the performance of peer algorithms over 20 runs on test problems. In a nutshell, it applies a statistical test and effect size to split the performance of all peer algorithms into several clusters. In the same cluster, the performance of peer algorithms is statistically equivalent. Note that the clustering procedure terminates until no split can be made. Finally, each cluster is assigned a rank according to the mean  $E_{BBC}$  values obtained by all peer algorithms within the cluster. Since a smaller  $E_{BBC}$  value is preferred, a smaller rank suggests a better performance of the algorithm achieves.
- $A_{12}$  effect size [8]: To make sure that the difference is not caused by a trivial effect,  $A_{12}$  is used as the effect size measure to assess the probability that one algorithm outperforms another. To be specific, given a pair of peer algorithms,  $A_{12} = 0.5$  denotes they are equivalent, whereas  $A_{12} > 0.5$  indicates that one obtains better results for more than 50% of the times.  $0.56 \leq A_{12} < 0.64$ ,  $0.64 \leq A_{12} < 0.71$ , and  $A_{12} \geq 0.71$  represent a small, a medium, and a large effect size, respectively.

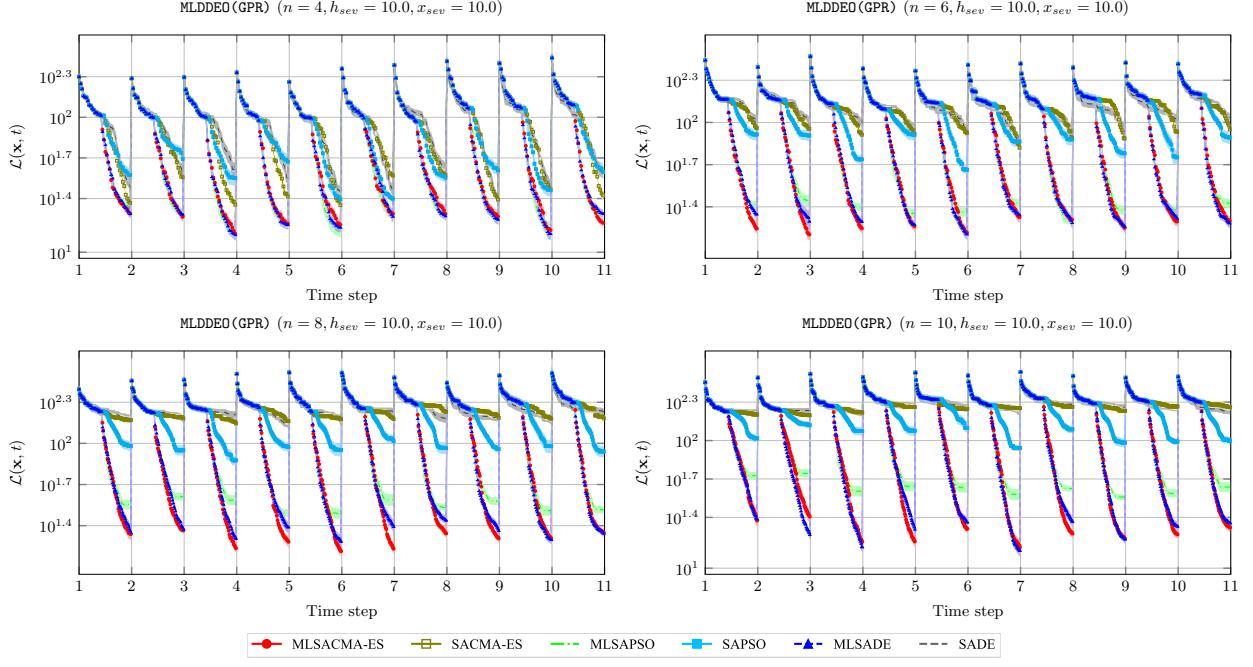
## II. APPENDIX B

In this section, we first analyze the remaining concerns: 4) the robustness of the proposed algorithm under varying degrees of environmental changes, 5) sensitivity study of the algorithm parameters, and 6) the investigation of the proposed framework applying different optimization solvers and surrogate models. Then, the experimental results (figures and tables) relevant to the main text are also presented.

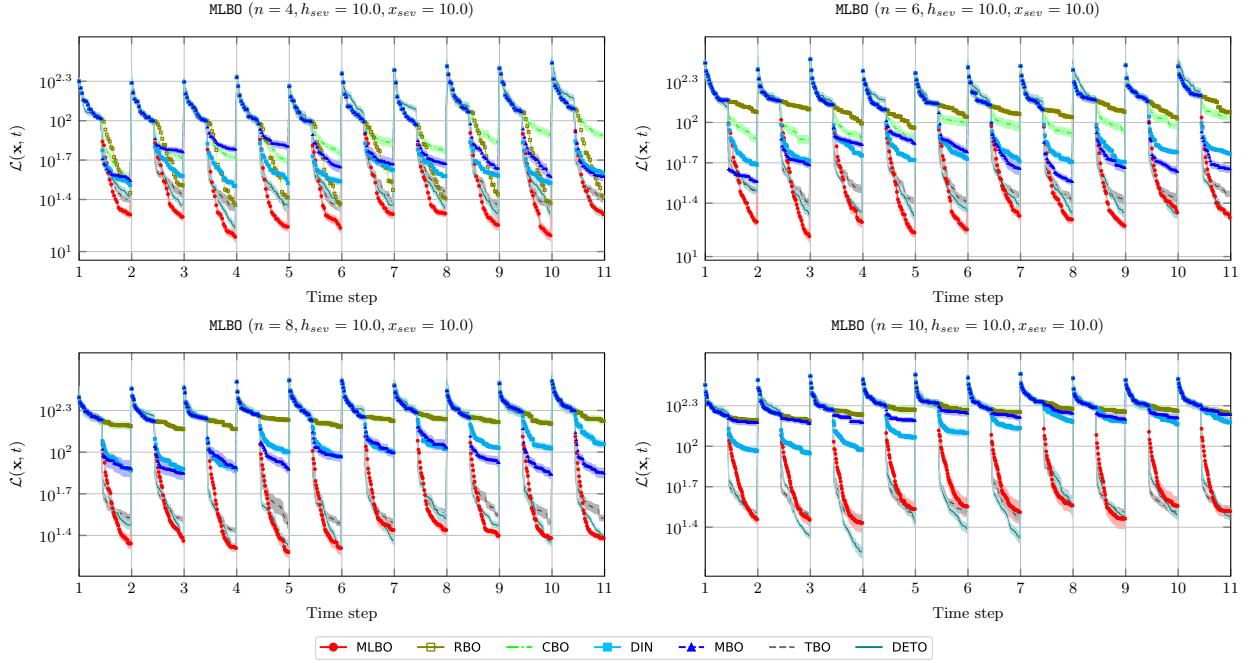
### A. Robustness of the proposed algorithm

To investigate the robustness of the proposed algorithm, experiments are carried out on different settings of  $h_{sev}$  and  $x_{sev}$ . In particular,  $(h_{sev}, x_{sev}) = (7.0, 5.0)$  denotes a slight change of the fitness landscape while  $(h_{sev}, x_{sev}) = (10.0, 10.0)$  indicates a severe change.

Again, we plot the loss function curves between different algorithms under the setting of  $(h_{sev}, x_{sev}) = (10.0, 10.0)$  during the evolutionary process as shown in Figs. 1 and Figs. 2. Based on the results shown in Table II and III, as well as Figs. 1 and Figs. 2, we observe that, even under a severe environmental change, the proposed algorithm instances can still obtain promising results with respective peer algorithms. To be specific, the proposed algorithm instances obtain the smallest  $E_{BBC}$  metric value as shown in Table II and III. In addition, the proposed algorithm instances can approximate the current global optimum more accurately than peer algorithms within the same function evaluations, as shown in Figs. 1 and Figs. 2. It is interesting to note that the metric values of our proposed algorithm instances are close under different environmental changes, indicating that the proposed instances are resilient and robust to different levels of environmental changes. SACMA-ES, SAPSO, SADE, and RBO perform similarly poorly under different environments due to random search after each change. In contrast, MBO and CBO are more sensitive to the levels of environmental changes. It can be seen from the improvement of the metric values when



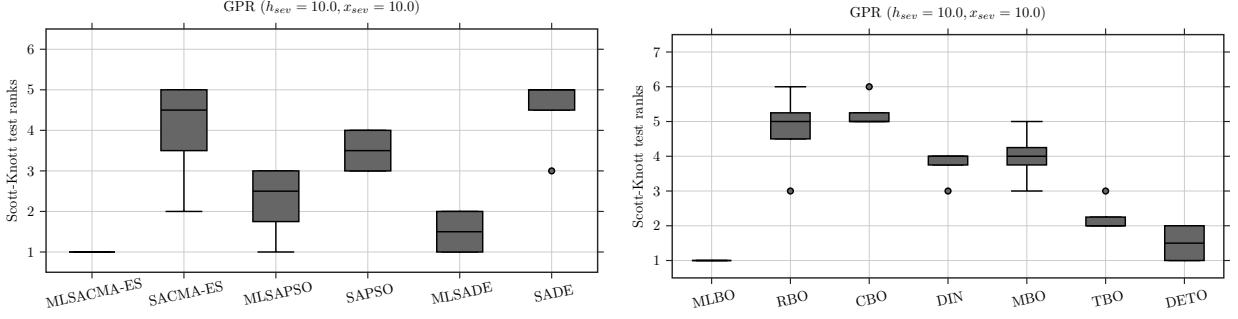
Figs. 1. Loss function of the mean errors between the true objective functions and the best objective values along with a confidence level over time at different dimensions with  $h_{sev} = 10.0$  and  $x_{sev} = 10.0$  when comparing MLDDEO by using GPR with other peer algorithms.



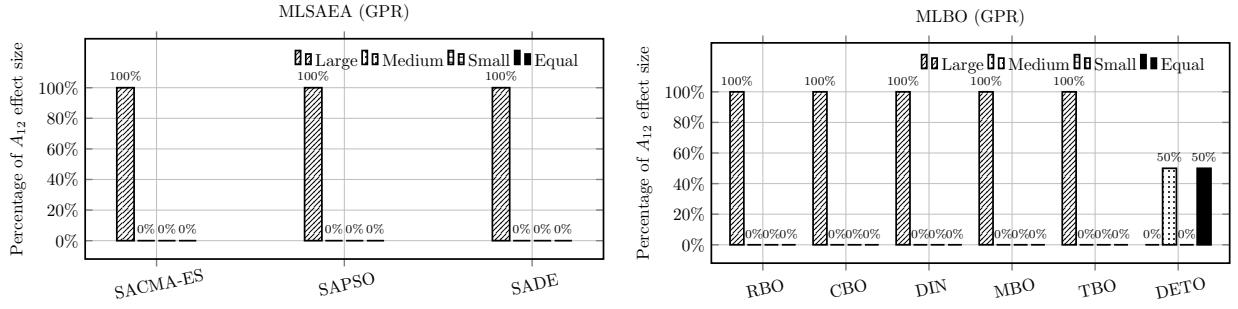
Figs. 2. Loss function of the mean errors between the true objective functions and the best objective values along with a confidence level over time at different dimensions with  $h_{sev} = 10.0$  and  $x_{sev} = 10.0$  when comparing MLBO with other peer algorithms.

increasing the value of  $h_{sev}$  and  $x_{sev}$ . The reason may be that the knowledge transfer approaches adopted in MBO and CBO might bring negative impacts when solving DOPs with severe changes.

We also apply the Scott-Knott test and the  $A_{12}$  effect size to evaluate the performance of our algorithm instances against the state-of-the-art peer algorithms on benchmark problems with  $(h_{sev}, x_{sev}) = (10.0, 10.0)$ . The distribution and median of the results are shown as box plots in Figs. 3 and the bar charts are shown in Figs. 4, respectively. From these results, it is obvious that our proposed algorithm instances consistently outperform other peer algorithms in the corresponding comparisons, although a severe change poses difficulties to the problem. Specifically, our proposed algorithm instances are consistently ranked in the smaller values, as the box plots shown in Figs. 3. Moreover, in all comparisons obtained from MLDDEO and MLBO, the large



Figs. 3. Box plots of Scott-Knott test ranks of  $E_{BBC}$  achieved by the proposed algorithm instances compared against the corresponding state-of-the-art peer algorithms with  $h_{sev} = 10.0$  and  $x_{sev} = 10.0$  (the smaller rank is, the better performance achieved).



Figs. 4. Percentage of  $A_{12}$  effect size of  $E_{BBC}$  with  $h_{sev} = 10.0$  and  $x_{sev} = 10.0$  when comparing MLDDEO or MLBO with corresponding state-of-the-art peer algorithms.

effect size is always 100% apart from the comparison with DETO, as shown in Figs. 4.

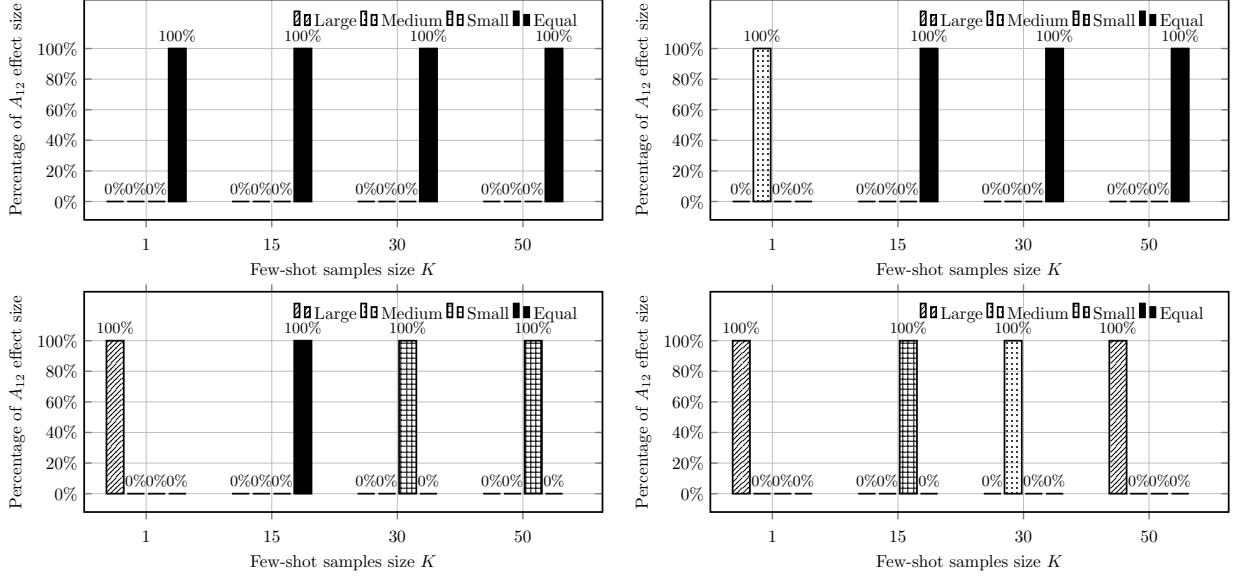
**Response to concern 4:** Increasing the levels of environmental changes usually makes the problem-solving process more difficult. However, when facing the different magnitude of environmental changes considered in this paper, the proposed algorithm instances can achieve promising results compared to respective peer algorithms under two optimization mechanisms. In short, the proposed framework has more robust performance to different levels of environmental changes.

## B. Parameter sensitivity study

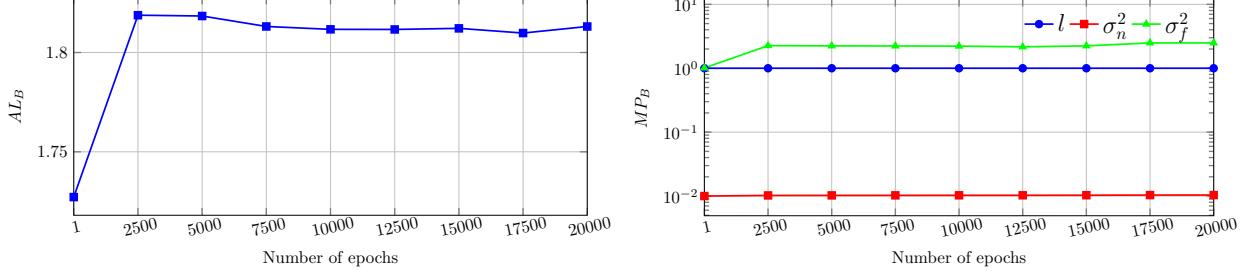
In the proposed framework, the user needs to specify parameters for the meta-learning component, including the few-shot sample size  $K$ , the number of epochs  $I_{ml}$ , the inner-loop learning rate  $\alpha$ , and the outer-loop learning rate  $\beta$ . Additionally, when utilizing NN, the batch size  $\xi$  for MLDDEO needs to be defined. To address concern 5, we choose MLBO and MLSACMA-ES using NN as the baseline, respectively. Their performance is empirically investigated under different settings of  $K = \{1, 5, 15, 30, 50\}$ ,  $I_{ml} = \{2000, 10000, 20000, 30000\}$ ,  $\alpha, \beta = \{0.001, 0.01, 0.1\}$ , and  $\xi = \{1, 5, 10\}$ , respectively.

1) *Sensitivity to the few-shot size  $K$ :* The statistical results of  $E_{BBC}$  values, based on the Wilcoxon rank sum test, are shown in Table IV. Additionally, the  $A_{12}$  effect size is shown in Figs. 5. These results indicate that in cases where the variable dimension is low, specifically when  $n \in \{4\}$ , the performance of MLBO with different  $K$  is classified as statistically equivalent. In other words, the proposed algorithm instance is not very sensitive to  $K$  in the lower dimensionality. In contrast, with the increase of dimensionality, especially when  $n \in \{8, 10\}$ , reducing  $K$  to 1 leads to a significant degradation in the  $E_{BBC}$  values and a large classification in effect sizes. Utilizing a small value for  $K$  may hinder the opportunity of exploiting previous information, thereby hindering the effectiveness of the meta-learning strategy. As an example depicted in Figs. 6, with  $K = 1$ , the model parameters in the GPR model (i.e., length-scale  $l$  and Gaussian noise  $\sigma_n^2$ ) hardly change during the meta-learning component. Meanwhile, the  $AL_B$  values increase beyond their initial value. In this case, meta-learning does not help the model learn good parameters for the new environment. On the other hand, it will obtain more information when selecting more samples in the meta-learning component by increasing the value of  $K$ . Nevertheless, a too large  $K$  will increase the risk of overfitting and lead to a degradation of the model's performance on new task. As the results shown in Table IV in the supplementary material and the  $A_{12}$  effect size given in Figs. 5, it is obvious that there is a performance degradation on the 10-th dimension when increasing  $K$  to 30 and 50. Based on the above findings, it is advisable to set  $K$  as 5.

2) *Sensitivity to the number of epochs  $I_{ml}$ :* The statistical results of  $E_{BBC}$  and the  $A_{12}$  effect size are shown in Table V



Figs. 5. Percentage of  $A_{12}$  effect size of  $E_{BBC}$ , when comparing MLBO with the recommended settings (i.e.,  $K = 5$ ) against others (i.e.,  $K = 1, 15, 30, 50$ ).

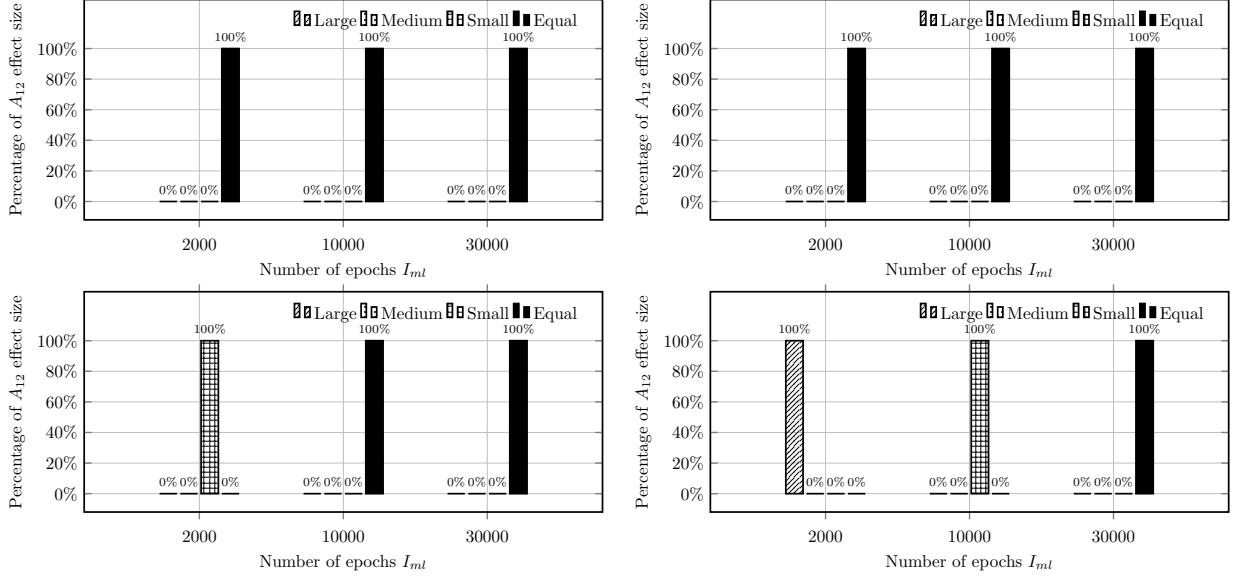


Figs. 6. Illustrative example of the  $AL_B$  and  $MP_B$  values during the meta-learning component when  $K = 1$ .

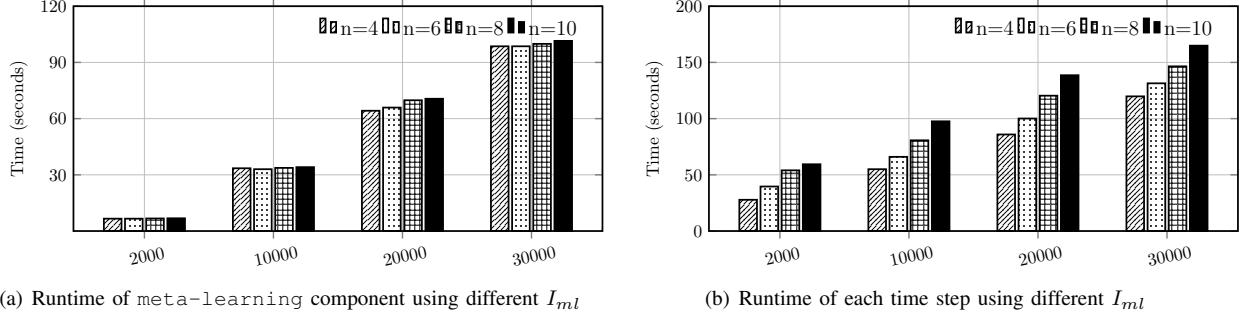
and Figs. 7, respectively. Similar to its performance in  $K$ , MLBO exhibits statistically equivalent performance across different  $I_{ml}$  in low-dimensional spaces. However, in relatively high-dimensional space, decreasing  $I_{ml}$  to 2000 results in an apparent degradation in the  $E_{BBC}$  values and a large classification in effect sizes. This might be because the model does not have enough training batches to learn the domain-specific features among tasks, thus leading to poor performance on new tasks. In addition, using more epochs will increase the training time. Figs. 8 presents a comparison of CPU time using different  $I_{ml}$ . From this figure, it is evident that a higher number of epochs leads to longer running time. Considering both the effectiveness and efficiency of the algorithm, we recommend setting  $I_{ml}$  as 20000.

3) *Sensitivity to the learning rate  $\alpha, \beta$ :* We present statistical comparison results of  $E_{BBC}$  values for MLBO with different inner-loop learning rate  $\alpha$  and outer-loop learning rate  $\beta$  in Table VI and VII, respectively. Furthermore, we evaluate the  $A_{12}$  effect size to compare MLBO with  $\alpha = 0.01$  and  $\beta = 0.01$  against other settings, as depicted in Figs. 9 and 10. As shown in Table VI and Figs. 9, the performance of MLBO under different inner-loop learning rate  $\alpha$  shows no significant differences, which illustrates MLBO is not very sensitive to inner-loop learning rate  $\alpha$ . By referring to other meta-learning studies [9], [10], we set  $\alpha$  as 0.01. Similarly, based on the statistical results provided in Table VII and Figs. 10, the proposed algorithm instance MLBO also shows little sensitivity to the outer-loop learning rate in the lower dimensionality, particularly when  $n \in \{4, 6\}$ . However, as dimensionality increases, we observe a noticeable performance degradation whether decreasing or increasing  $\beta$ . In particular, a too small outer-loop learning rate may result in very slow parameter updates, thereby reducing the convergence speed. As illustrated in Figs. 11 (a), when using  $\beta = 0.001$ , the model parameters in the GPR model (i.e., length-scale  $l$  and Gaussian noise  $\sigma_n^2$ ) exhibit slight increment during the meta-learning component. Conversely, increasing the outer-loop learning rate enhances the model's convergence speed, but it may also lead to overfitting on new tasks if the value becomes too large. As shown in Figs. 11 (c), the model parameters converge rapidly during the meta-learning component when  $\beta = 0.1$ . However, its performance on new tasks degrades compared to when  $\beta = 0.01$ , as demonstrated in Figs. 10. Therefore, it is recommended to set  $\beta$  as 0.01.

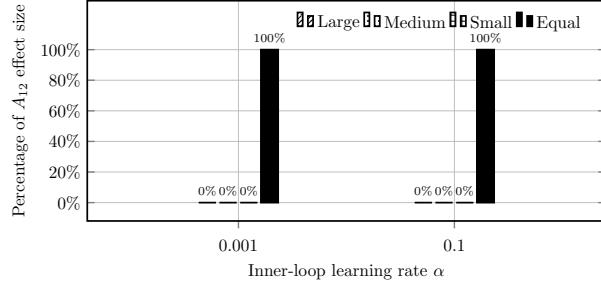
4) *Sensitivity to the batch size  $\xi$  for MLDDEO:* Table VIII and the  $A_{12}$  effect size shown in Figs. 12 demonstrate that MLSACMA-ES (NN) with  $\xi = 5$  exhibits superior performance compared to  $\xi = 1$ . Specifically, 25% of the comparisons



Figs. 7. Percentage of  $A_{12}$  effect size of  $EBBC$ , when comparing MLBO with the recommended settings (i.e.,  $I_{ml} = 20000$ ) against others (i.e.,  $I_{ml} = 2000, 10000, 30000$ ).

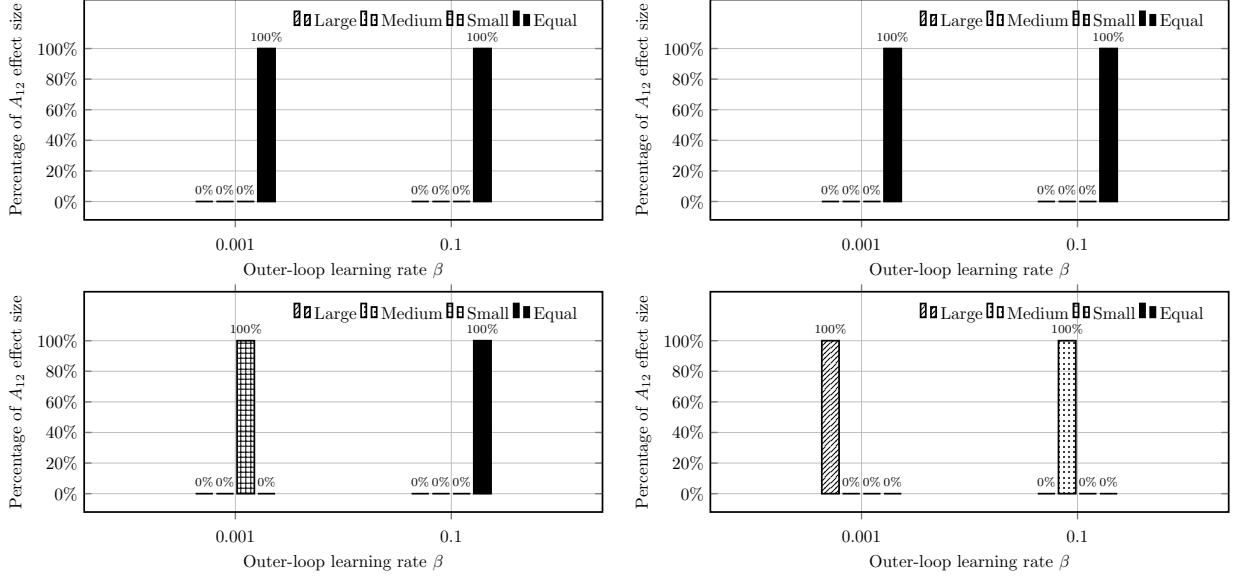


Figs. 8. Collected comparisons of CPU wall clock time on a computer with an Intel Core i9, 3.00-GHz CPU when using different  $I_{ml}$  settings.

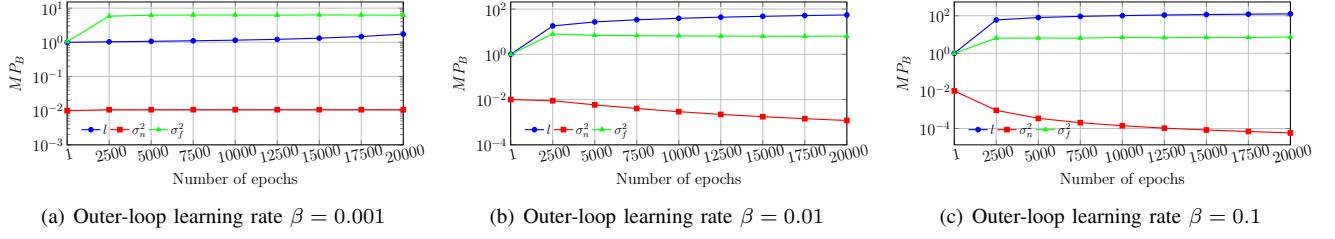


Figs. 9. Percentage of  $A_{12}$  effect size of  $EBBC$ , when comparing MLBO with the recommended settings (i.e.,  $\alpha = 0.01$ ) against others (i.e.,  $\alpha = 0.001, 0.1$ ).

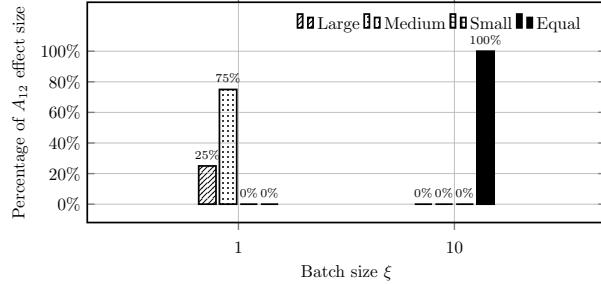
showed a large effect size, while 75% exhibited a medium effect size. When pick up multiple solutions per iteration, the NN model can more comprehensively explore the search space, thus increasing the possibility of discovering superior solutions. However, increasing  $\xi$  for selecting more solutions also diminishes the number of iterations available for updating the model. This is because the total number of FEs remains fixed, and sampling multiple solutions increases the FEs consumed per iteration. Therefore, beyond a certain threshold, a larger  $\xi$  does not necessarily improve algorithm performance. As shown in Figs. 12, the comparison results of  $A_{12}$  effect size demonstrate that MLSACMA-ES (NN) with  $\xi = 5$  is comparable to that of  $\xi = 10$ , with all differences classified as statistically equivalent. Based on these findings, we recommend setting  $\xi$  as 5.



Figs. 10. Percentage of  $A_{12}$  effect size of  $E_{BBC}$ , when comparing MLBO with the recommended settings (i.e.,  $\beta = 0.01$ ) against others (i.e.,  $\beta = 0.001, 0.1$ ).

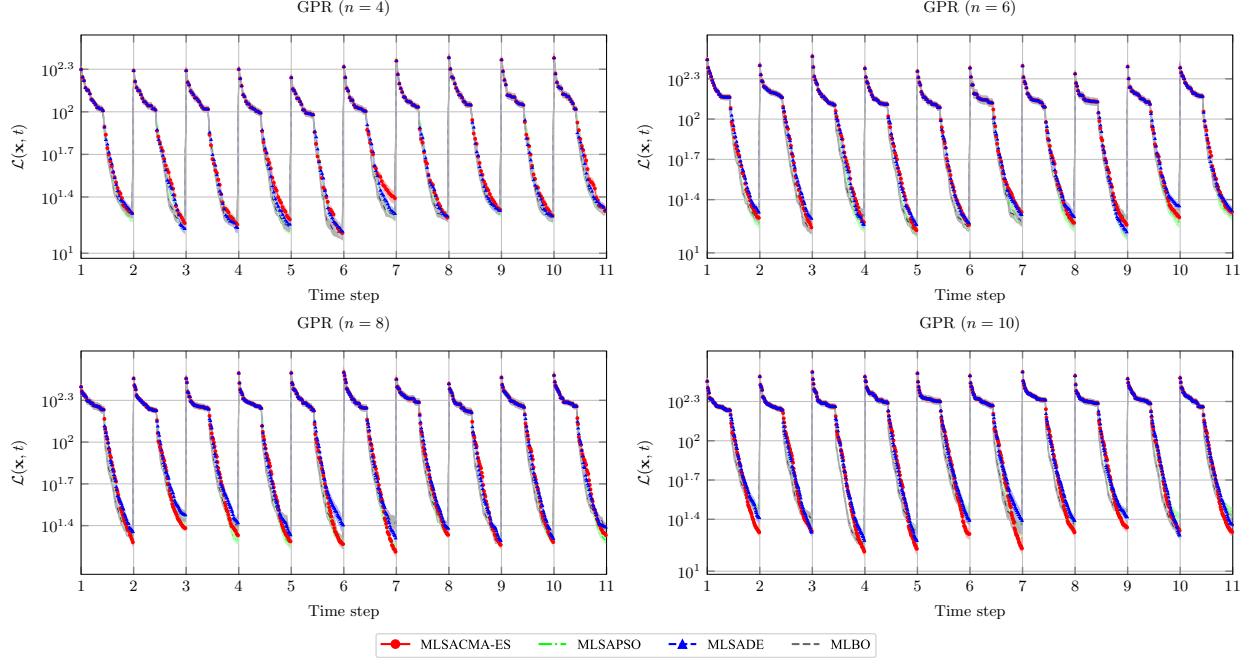


Figs. 11. Illustrative example of the  $MP_B$  values during the meta-learning component when  $\beta = 0.001, 0.01$ , and  $0.1$ .



Figs. 12. Percentage of  $A_{12}$  effect size of  $E_{BBC}$ , when comparing MLSACMA-ES (NN) with the recommended settings (i.e.,  $\xi = 5$ ) against others (i.e.,  $\xi = 1, 10$ ).

**Response to concern 5:** We have the following takeaways from the experiments. 1) In the lower-dimensional space, the proposed algorithm instance MLBO is not particularly sensitive to the parameters involved in meta-learning component, including few-shot samples size  $K$ , inner and outer learning rates  $\alpha, \beta$ , and the number of epochs  $I_{ml}$ . 2) However, in relatively high-dimensional space, an excessively large  $K$  or  $\beta$  introduces a higher risk of overfitting and can result in a performance degradation on new tasks. Conversely, using a too small  $K$  may compromise the opportunity to exploit previous information. The convergence speed of the algorithm instance becomes slower when using a small  $\beta$ . 3) If the number of epochs  $I_{ml}$  are too small, the model might not undergo enough training batches to learn the domain-specific features among tasks, thus leading to poor performance on new tasks. Furthermore, increasing  $I_{ml}$  will prolong the training time. 4) Using a small  $\xi$  may not fully explore the search space, whereas a too large  $\xi$  results in fewer model iterations.



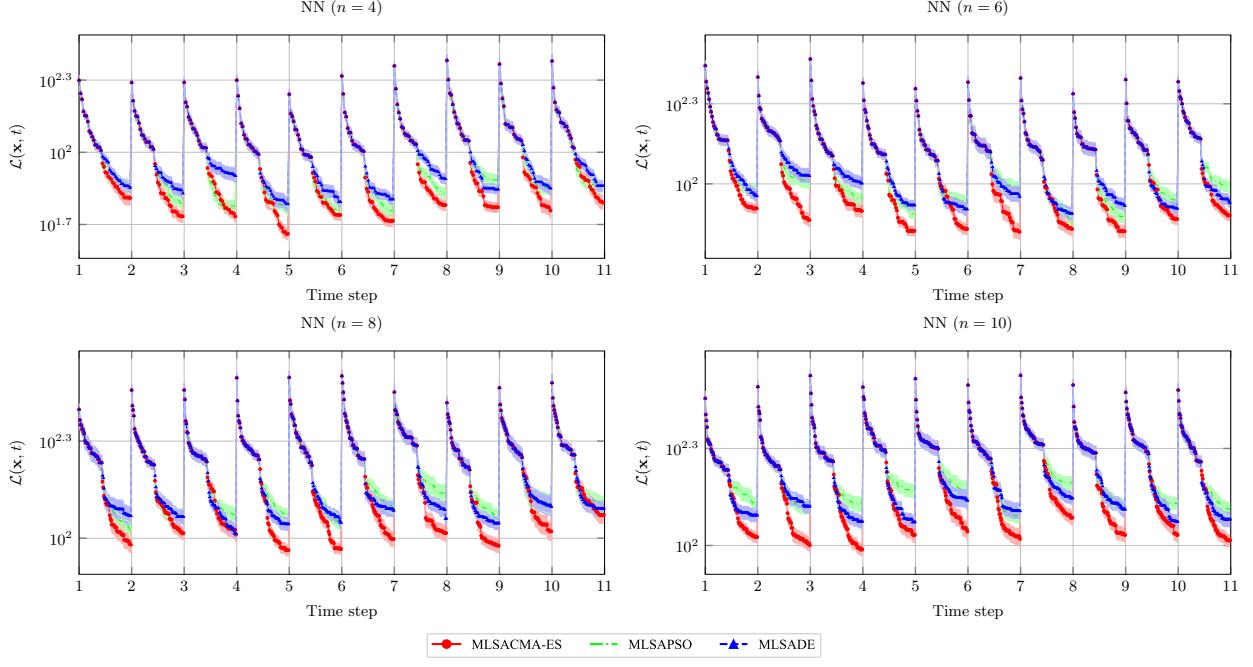
Figs. 13. Loss function of the mean errors between the true objective functions and the best objective values obtained by the proposed algorithm instances using GPR as the surrogate model along with a confidence level over time at different dimensions with  $h_{sev} = 7.0$  and  $x_{sev} = 5.0$ .

### C. Further studies of the proposed framework

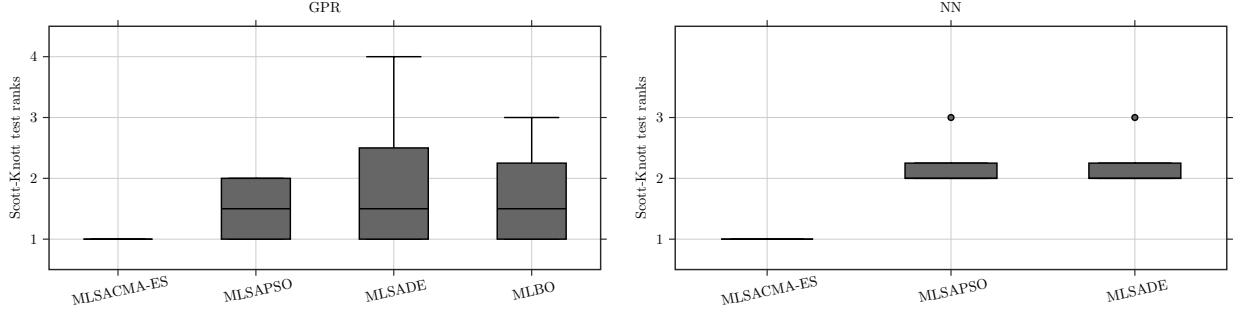
To investigate concern 6, we proceed to address the following two research questions. 1) Given a surrogate model, how does the performance differ in the proposed algorithm instances? 2) How is the performance using different surrogate models in the proposed method? Since we consider two different optimization mechanisms (i.e., MLDDEO and MLBO as introduced in Section III-A) and two surrogate models (i.e., GPR and NN) in the algorithm framework, this subsection aims to study the performance comparison of seven different algorithm instances under these two optimization mechanisms and two surrogate models separately. The statistical comparison results of  $E_{BBC}$  based on the Wilcoxon rank sum test are shown in Table II and III. In addition, the loss function curves during the evolutionary process among all algorithm instances can be found in Figs. 13 and Figs. 14. From these results, we can see that MLDDEO is more effective in handling higher dimensional problems compared to MLBO. In particular, the metric and loss values obtained by all algorithm instances are close in the lower dimensions (i.e.,  $n = 4, 6$ ). However, in higher dimensions, MLDDEO has shown better  $E_{BBC}$  values and smaller loss values than MLBO. One plausible explanation is that SAEAs utilize a population-based search strategy to explore the search space. On the one hand, this strategy maintains a diverse set of solutions. On the other hand, it guides the surrogate model to focus on the potential region during the evolutionary process where the parent population and offspring population reside. One advantage of finding diverse and better solutions is that the quality of the meta-training set for meta-learning component is improved, thus better facilitating to optimize the new environment. In contrast, BO relies on random sampling to evaluate a large number of points in the search space to find good solutions, which becomes infeasible as the dimensionality increases. It is interesting to note that MLSACMA-ES achieves better performance than MLSAPSO and MLSADE in 10-th dimension. One possible reason for this is that MLSACMA-ES uses a covariance matrix adaptation strategy to efficiently search for the optimal solution. This makes it less susceptible to getting stuck in local optima compared to MLSADE and MLSAPSO.

To facilitate an explicit analysis of ranking among these algorithm instances, the Scott-Knott test is used to classify them into different groups based on their performance on the MPB problems. All the Scott-Knott test results on different dimensions are pulled together, and the distribution and median are presented as box plots in Figs. 15. From this result, it is evident that MLSACMA-ES is the superior algorithm in our proposed framework, as it consistently ranks in the first place regardless of GPR or NN is used as the surrogate model.

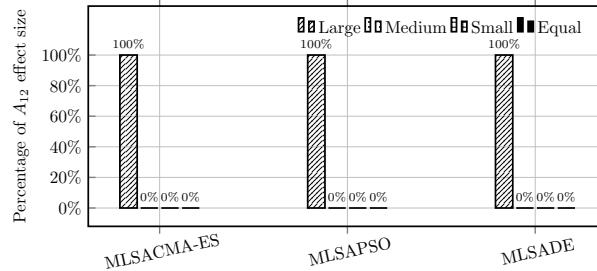
Furthermore, this subsection also investigates the performance using different surrogate models in the proposed method. Based on the results obtained in the previous subsection, we evaluate the  $A_{12}$  effect size of  $E_{BBC}$  between MLDDEO with regard to GPR and NN, respectively. We calculate the percentage of different effect sizes obtained by a pair of dueling algorithms. From the results depicted in Figs. 16, it is evident that using GPR as the surrogate model consistently outperforms that of NN. In particular, all comparison results for three SAEAs have a large effect size when employing GPR as the surrogate model in contrast to using NN. Overall, these comparison results suggest that GPR is more capable of modeling objective functions than NN. Nevertheless, as introduced in Section III-D, the computational cost for training a GPR model is higher



Figs. 14. Loss function of the mean errors between the true objective functions and the best objective values obtained by the proposed algorithm instances using NN as the surrogate model along with a confidence level over time at different dimensions with  $h_{sev} = 7.0$  and  $x_{sev} = 5.0$ .



Figs. 15. Box plots of Scott-Knott test ranks of  $E_{BBC}$  achieved by each algorithm instance of the proposed framework by using GPR and NN with  $h_{sev} = 7.0$  and  $x_{sev} = 5.0$ , respectively (the smaller rank is, the better performance achieved).



Figs. 16. Percentage of  $A_{12}$  effect size of  $E_{BBC}$  when comparing MLDDEO with GPR as the surrogate model against NN.

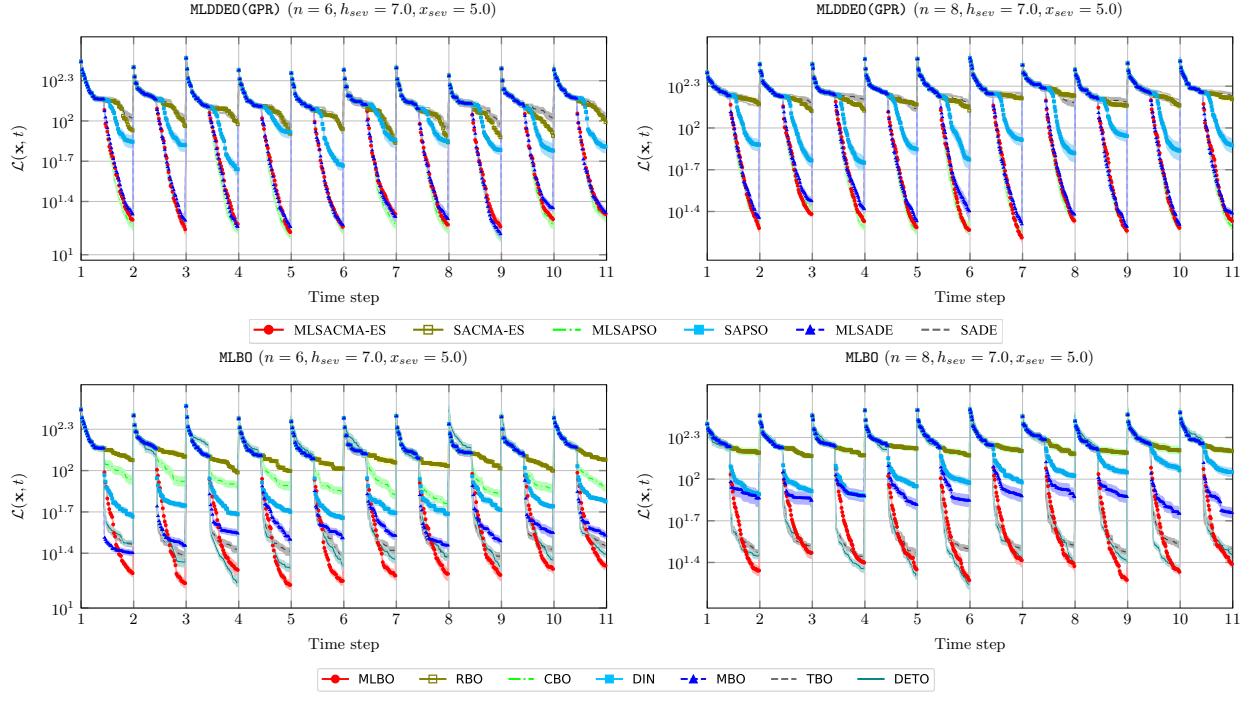
than that of NN.

Response to concern 6: We have the following takeaways from the empirical study. 1) All proposed algorithm instances show competitive results in both optimization mechanisms for solving relatively low-dimensional problems. When addressing higher-dimensional problems, MLDDEO outperforms MLBO, and MLSACMA-ES is the best algorithm instance in our proposed framework. 2) The population-based search strategy of SAEAs enables them to produce a higher quality meta-

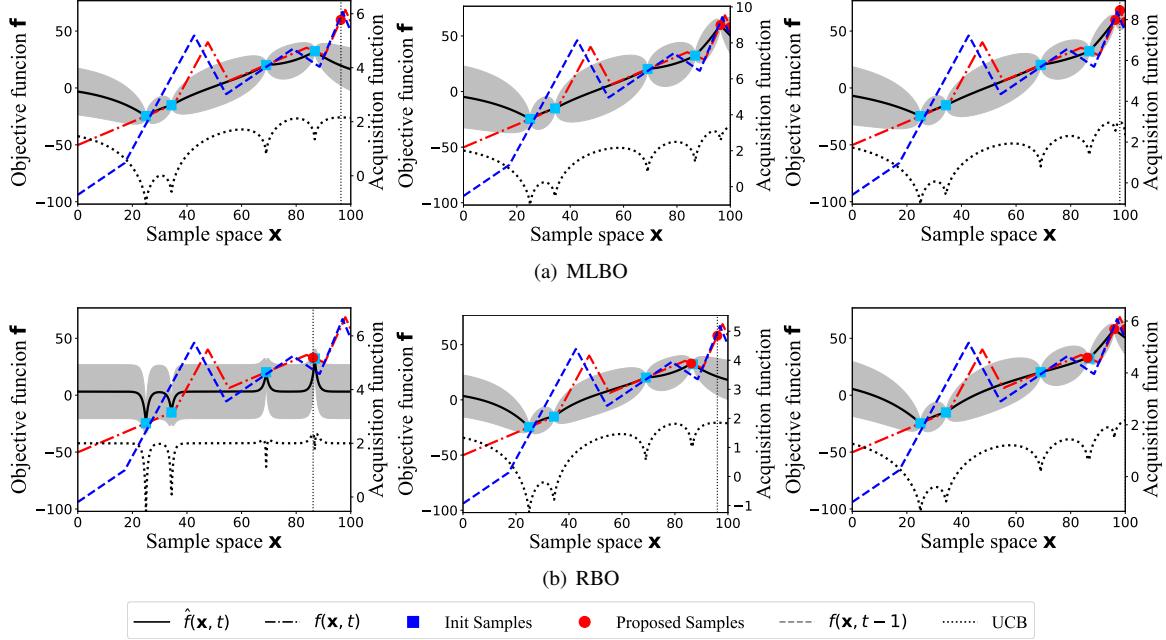
training set for the meta-learning component, which enhances the optimization of the new environment, particularly in high-dimensional ones. 3) MLSACMA-ES employs a covariance matrix adaptation strategy for effective optimal solution search, making it less prone to trapping in local optima compared to MLSADE and MLSAPSO. This observation is consistent when using both GPR and NN as the surrogate model. 4) Using GPR as the surrogate model is more capable than NN in our proposed MLDEO framework. The primary drawback of GPR is its cubic worst-case time complexity for model building.

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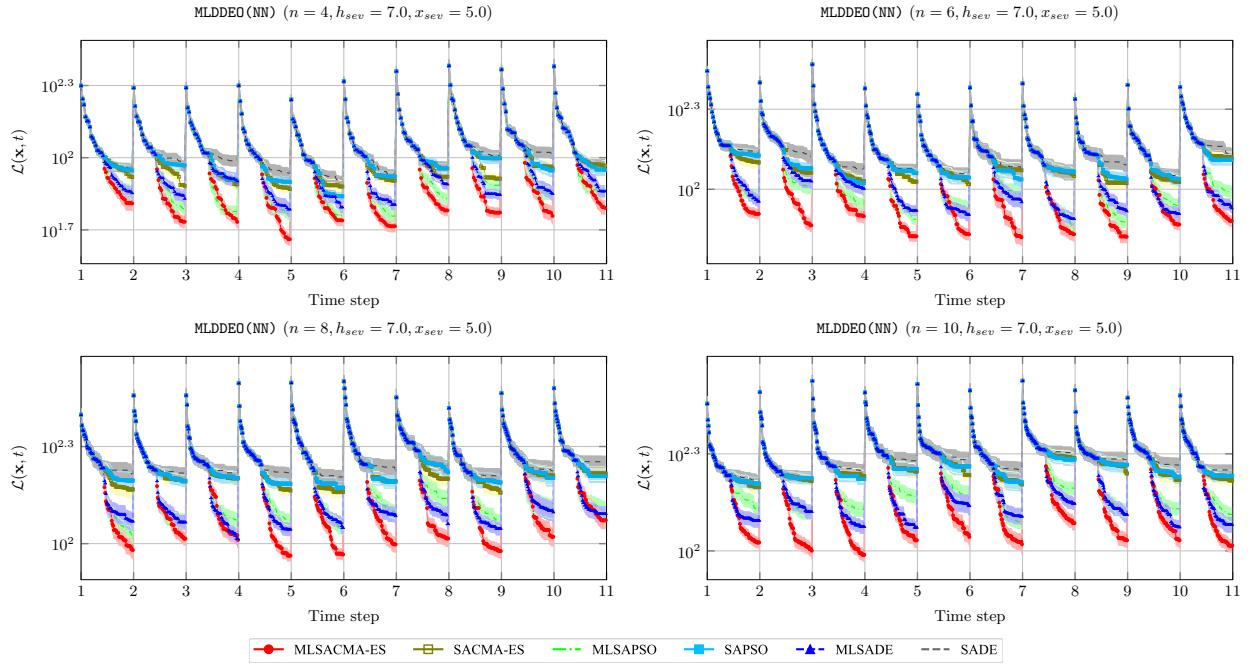
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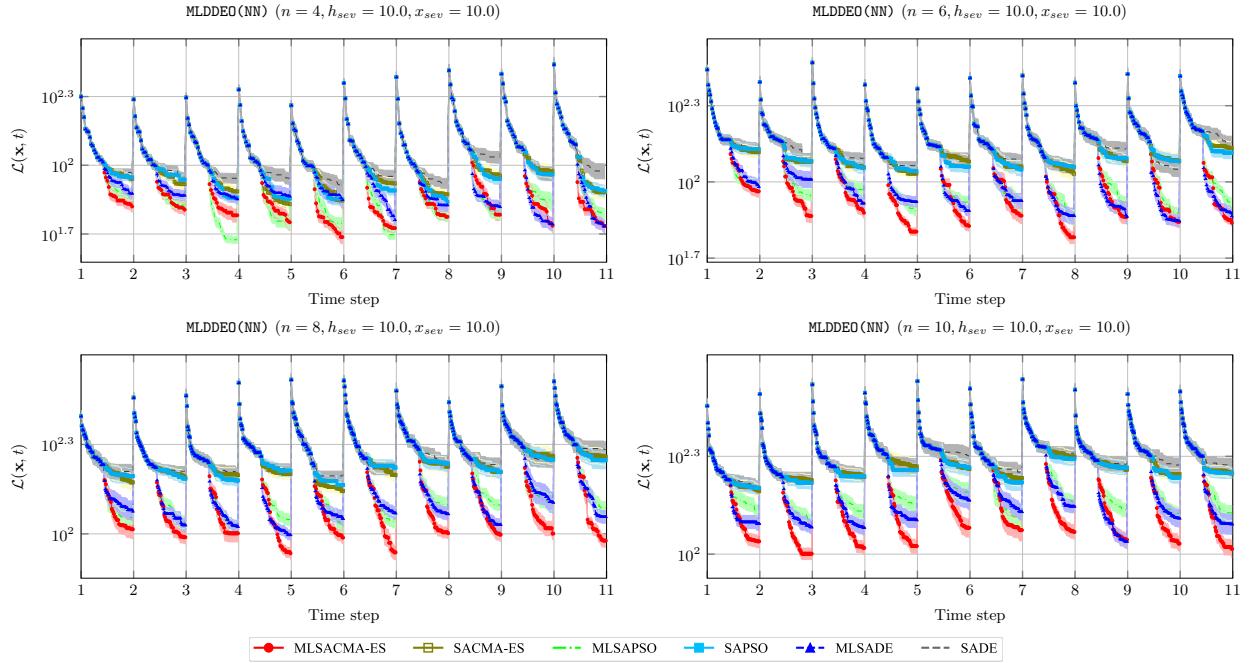
Figs. 17. Loss function of the mean errors between the true objective functions and the best objective values along with a confidence level over time at different dimensions with  $h_{sev} = 7.0$  and  $x_{sev} = 5.0$  when comparing MLDDEO by using GPR and MLBO with other peer algorithms, respectively.



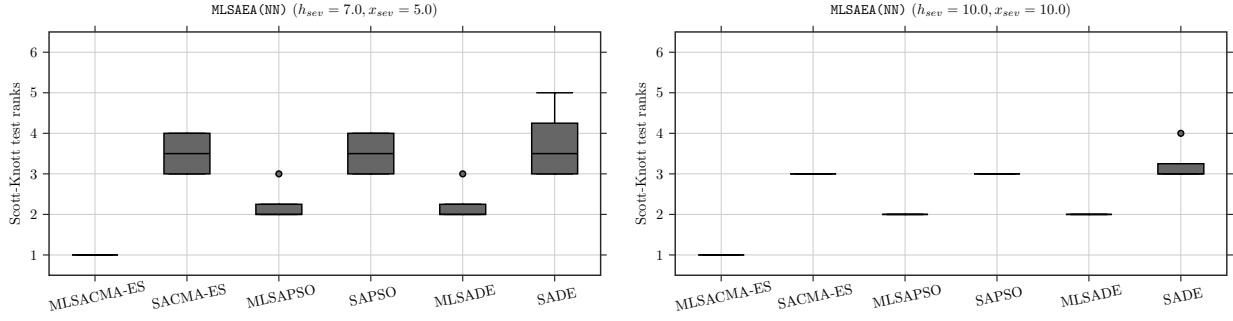
Figs. 18. Illustrative example of the search dynamics of MLBO and RBO across three new samples after environmental changes in the first scenario.



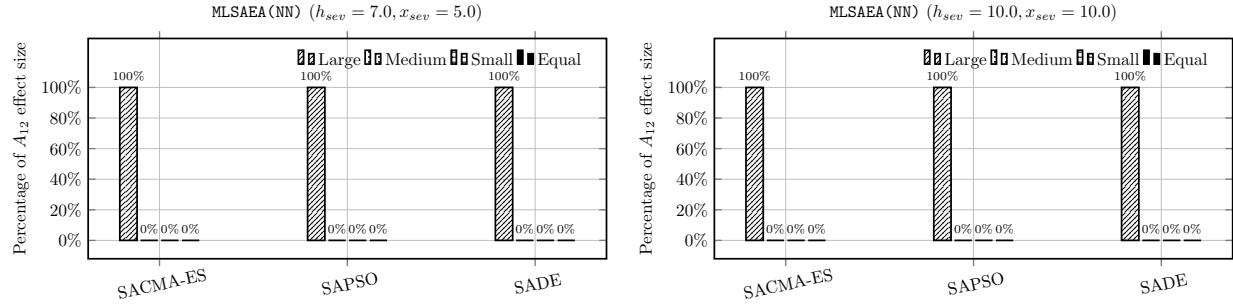
Figs. 19. Loss function of the mean errors between the true objective functions and the best objective values along with a confidence level over time at different dimensions with  $h_{sev} = 7.0$  and  $x_{sev} = 5.0$  when comparing MLDDEO by using NN with other peer algorithms.



Figs. 20. Loss function of the mean errors between the true objective functions and the best objective values along with a confidence level over time at different dimensions with  $h_{sev} = 10.0$  and  $x_{sev} = 10.0$  when comparing MLDDEO by using NN with other peer algorithms.



Figs. 21. Box plots of Scott-Knott test ranks of  $E_{BBC}$  achieved by MLDDEO using NN as the surrogate model compared against the corresponding SAEAs (the smaller rank is, the better performance achieved).



Figs. 22. Percentage of  $A_{12}$  effect size of  $E_{BBC}$  when comparing MLDDEO with corresponding SAEAs by using NN.

TABLE II  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY THE PROPOSED ALGORITHM INSTANCES WITH REGARD TO OTHER PEERS ON THE MPB PROBLEMS. IN PARTICULAR, GAUSSIAN PROCESS REGRESSION (GPR) IS USED AS THE SURROGATE MODEL.

$E_{BBC}$	n=4		n=6		n=8		n=10	
	(7, 5)	(10, 10)	(7, 5)	(10, 10)	(7, 5)	(10, 10)	(7, 5)	(10, 10)
MLSACMA-ES	1.84E+1(8.14E+0)†	1.73E+1(6.96E+0)†	1.77E+1(8.23E+0)†	1.83E+1(7.38E+0)†	<b>2.01E+1(6.43E+0)</b>	<b>2.04E+1(6.97E+0)</b>	<b>1.90E+1(5.99E+0)</b>	<b>2.08E+1(1.01E+1)</b>
SACMA-ES	2.77E+1(9.40E+0)‡	2.77E+1(1.11E+1)‡	7.94E+1(2.96E+1)‡	7.85E+1(3.11E+1)‡	1.46E+2(5.55E+1)‡	1.46E+2(4.91E+1)‡	1.67E+2(5.32E+1)‡	1.69E+2(5.31E+1)‡
MLSAPSO	<b>1.72E+1(7.71E+0)</b>	1.79E+1(7.40E+0)†	<b>1.64E+1(7.98E+0)</b>	2.60E+1(9.19E+0)‡	2.12E+1(7.11E+0)†	3.76E+1(1.26E+1)‡	2.51E+1(8.66E+0)‡	4.52E+1(1.47E+1)‡
SAPSO	3.70E+1(1.47E+1)‡	3.56E+1(1.52E+1)‡	6.24E+1(2.40E+1)‡	6.82E+1(2.53E+1)‡	7.01E+1(3.29E+1)‡	9.21E+1(3.97E+1)‡	7.79E+1(2.48E+1)‡	1.11E+2(3.41E+1)‡
MLSADE	1.76E+1(7.86E+0)†	1.71E+1(7.00E+0)†	1.86E+1(7.84E+0)†	1.98E+1(7.97E+0)†	2.48E+1(9.03E+0)†	2.41E+1(8.34E+0)†	2.38E+1(8.08E+0)‡	2.17E+1(7.71E+0)†
SADE	3.26E+1(1.50E+1)‡	3.26E+1(1.50E+1)‡	8.90E+1(3.80E+1)‡	8.90E+1(3.80E+1)‡	1.47E+2(5.28E+1)‡	1.47E+2(5.28E+1)‡	1.72E+2(5.54E+1)‡	1.72E+2(5.54E+1)‡
MLBO	1.76E+1(7.68E+0)†	<b>1.70E+1(7.03E+0)</b>	1.73E+1(8.68E+0)†	<b>1.77E+1(7.30E+0)</b>	2.35E+1(5.94E+0)‡	2.36E+1(6.83E+0)†	2.56E+1(7.11E+0)‡	3.36E+1(3.99E+1)‡
RBO	2.83E+1(1.19E+1)‡	2.63E+1(1.06E+1)‡	1.04E+2(4.06E+1)‡	1.06E+2(4.23E+1)‡	1.56E+2(5.34E+1)‡	1.60E+2(5.22E+1)‡	1.70E+2(5.72E+1)‡	1.75E+2(5.81E+1)‡
CBO	4.78E+1(1.41E+1)‡	5.60E+1(2.12E+1)‡	7.17E+1(3.39E+1)‡	8.34E+1(3.61E+1)‡	1.56E+2(5.35E+1)‡	1.60E+2(5.23E+1)‡	1.70E+2(5.72E+1)‡	1.75E+2(5.81E+1)‡
DIN	3.06E+1(1.12E+1)‡	3.44E+1(9.00E+0)‡	4.78E+1(1.57E+1)‡	5.00E+1(1.76E+1)‡	9.00E+1(3.93E+1)‡	8.93E+1(3.21E+1)‡	1.12E+2(3.46E+1)‡	1.18E+2(3.64E+1)‡
MBO	3.06E+1(9.71E+0)‡	4.45E+1(1.93E+1)‡	3.03E+1(1.16E+1)‡	4.70E+1(1.36E+1)‡	6.83E+1(6.31E+1)‡	7.87E+1(5.16E+1)‡	1.57E+2(5.64E+1)‡	1.59E+2(6.14E+1)‡
TBO	2.42E+1(1.01E+1)‡	2.42E+1(9.00E+0)‡	2.60E+1(1.03E+1)‡	2.76E+1(9.52E+0)‡	3.14E+1(9.13E+0)‡	3.22E+1(9.55E+0)‡	3.06E+1(9.02E+0)‡	3.20E+1(8.03E+0)‡
DETO	2.15E+1(8.92E+0)‡	2.19E+1(8.18E+0)‡	2.24E+1(9.13E+0)‡	2.26E+1(8.42E+0)‡	2.52E+1(8.20E+0)†	2.53E+1(9.53E+0)‡	2.71E+1(1.02E+1)‡	2.68E+1(8.31E+0)‡

‡ and † indicate the proposed algorithm instances performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE III  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY THE PROPOSED ALGORITHM INSTANCES WITH REGARD TO OTHER PEERS ON THE MPB PROBLEMS. IN PARTICULAR, A NEURAL NETWORK (NN) IS USED AS THE SURROGATE MODEL.

$E_{BBC}$	n=4		n=6		n=8		n=10	
	(7, 5)	(10, 10)	(7, 5)	(10, 10)	(7, 5)	(10, 10)	(7, 5)	(10, 10)
MLSACMA-ES	<b>5.74E+1(2.19E+1)</b>	<b>5.89E+1(2.42E+1)</b>	<b>7.52E+1(2.65E+1)</b>	<b>7.62E+1(2.89E+1)</b>	<b>1.05E+2(3.66E+1)</b>	<b>1.00E+2(3.11E+1)</b>	<b>1.10E+2(3.41E+1)</b>	<b>1.12E+2(3.69E+1)</b>
SACMA-ES	7.98E+1(2.73E+1)‡	7.94E+1(2.94E+1)‡	1.14E+2(4.42E+1)‡	1.18E+2(4.90E+1)‡	1.53E+2(5.44E+1)‡	1.60E+2(5.51E+1)‡	1.67E+2(5.00E+1)‡	1.74E+2(5.36E+1)‡
MLSAPSO	6.60E+1(2.49E+1)†	6.14E+1(2.31E+1)†	8.99E+1(3.27E+1)†	8.61E+1(3.16E+1)†	1.23E+2(4.35E+1)†	1.19E+2(3.67E+1)†	1.39E+2(4.24E+1)†	1.39E+2(4.43E+1)†
SAPSO	8.53E+1(2.91E+1)‡	7.91E+1(2.76E+1)‡	1.16E+2(4.50E+1)‡	1.19E+2(4.74E+1)‡	1.57E+2(5.27E+1)‡	1.62E+2(5.39E+1)‡	1.72E+2(5.34E+1)‡	1.74E+2(5.16E+1)‡
MLSADE	7.08E+1(2.40E+1)†	6.78E+1(2.55E+1)†	9.08E+1(3.60E+1)†	8.51E+1(3.43E+1)†	1.19E+2(3.93E+1)†	1.16E+2(3.97E+1)†	1.29E+2(3.74E+1)†	1.29E+2(4.27E+1)†
SADE	9.12E+1(3.08E+1)‡	8.94E+1(3.50E+1)‡	1.23E+2(4.97E+1)‡	1.24E+2(4.82E+1)‡	1.65E+2(5.83E+1)‡	1.67E+2(5.78E+1)‡	1.79E+2(5.60E+1)‡	1.81E+2(5.71E+1)‡

‡ and † indicate the proposed algorithm instances performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE IV  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY MLBO WITH DIFFERENT FEW-SHOT SIZE  $K$  AT  $h_{sev} = 7$  AND  $x_{sev} = 5$ .

$n$	$K = 5$	$K = 1$	$K = 15$	$K = 30$	$K = 50$
4	1.76E+1(7.68E+0)	<b>1.69E+1(7.58E+0)†</b>	1.76E+1(7.85E+0)‡	1.73E+1(7.97E+0)†	1.75E+1(7.86E+0)†
6	1.73E+1(8.68E+0)	2.13E+1(7.97E+0)†	1.71E+1(8.39E+0)‡	1.72E+1(8.33E+0)†	<b>1.69E+1(8.26E+0)†</b>
8	<b>2.35E+1(5.94E+0)</b>	1.39E+2(4.92E+1)‡	2.51E+1(7.61E+0)†	2.57E+1(7.90E+0)†	2.67E+1(9.29E+0)†
10	<b>2.56E+1(7.11E+0)</b>	1.57E+2(5.05E+1)‡	2.87E+1(9.48E+0)†	3.21E+1(1.02E+1)‡	3.49E+1(1.22E+1)‡

‡ and † indicate  $K = 5$  performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE V  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY MLBO WITH DIFFERENT NUMBER OF EPOCHS  $I_{ml}$  AT  $h_{sev} = 7$  AND  $x_{sev} = 5$ .

$n$	$I_{ml} = 20000$	$I_{ml} = 2000$	$I_{ml} = 10000$	$I_{ml} = 30000$
4	1.59E+1(7.00E+0)	<b>1.51E+1(6.90E+0)†</b>	1.54E+1(6.98E+0)†	1.60E+1(7.14E+0)†
6	1.58E+1(8.11E+0)	1.58E+1(7.52E+0)†	1.54E+1(7.93E+0)†	<b>1.51E+1(7.35E+0)†</b>
8	2.10E+1(5.40E+0)	<b>1.98E+1(6.21E+0)†</b>	2.05E+1(5.54E+0)†	2.13E+1(5.65E+0)†
10	<b>2.13E+1(6.08E+0)</b>	8.13E+1(7.97E+1)‡	2.86E+1(3.75E+1)†	2.39E+1(3.50E+1)†

‡ and † indicate  $I_{ml} = 20000$  performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE VI  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY MLBO WITH DIFFERENT INNER-LOOP LEARNING RATE  $\alpha$  AT  $h_{sev} = 7$  AND  $x_{sev} = 5$ .

$n$	$\alpha = 0.01$	$\alpha = 0.001$	$\alpha = 0.1$
4	<b>1.59E+1(7.00E+0)</b>	1.59E+1(7.03E+0)†	1.59E+1(7.03E+0)†
6	1.58E+1(8.11E+0)	1.59E+1(8.17E+0)†	<b>1.57E+1(8.01E+0)†</b>
8	<b>2.10E+1(5.40E+0)</b>	2.11E+1(5.69E+0)†	2.12E+1(5.70E+0)†
10	<b>2.13E+1(6.08E+0)</b>	2.93E+1(3.64E+1)‡	2.89E+1(3.64E+1)†

‡ and † indicate  $\alpha = 0.01$  performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE VII  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY MLBO WITH DIFFERENT OUTER-LOOP LEARNING RATE  $\beta$  AT  $h_{sev} = 7$  AND  $x_{sev} = 5$ .

$n$	$\beta = 0.01$	$\beta = 0.001$	$\beta = 0.1$
4	1.59E+1(7.00E+0)	<b>1.51E+1(6.81E+0)†</b>	1.58E+1(7.29E+0)†
6	1.58E+1(8.11E+0)	<b>1.55E+1(7.47E+0)†</b>	1.55E+1(7.72E+0)†
8	2.10E+1(5.40E+0)	<b>1.98E+1(5.60E+0)†</b>	2.39E+1(8.75E+0)†
10	<b>2.13E+1(6.08E+0)</b>	8.24E+1(7.94E+1)‡	3.51E+1(3.64E+1)‡

‡ and † indicate  $\beta = 0.01$  performs significantly better than and equivalently to the corresponding algorithm, respectively.

TABLE VIII  
PERFORMANCE COMPARISON RESULTS OF  $E_{BBC}$  OBTAINED BY MLSACMA-ES (NN) WITH DIFFERENT BATCH SIZE  $\xi$  AT  $h_{sev} = 7$  AND  $x_{sev} = 5$ .

$n$	$\xi = 5$	$\xi = 1$	$\xi = 10$
4	6.13E+1(2.22E+1)	7.30E+1(2.49E+1)†	<b>5.74E+1(2.19E+1)†</b>
6	7.65E+1(2.73E+1)	9.51E+1(3.99E+1)‡	<b>7.52E+1(2.65E+1)†</b>
8	<b>1.04E+2(3.39E+1)</b>	1.27E+2(4.67E+1)‡	1.05E+2(3.66E+1)†
10	1.16E+2(4.01E+1)	1.40E+2(4.43E+1)†	<b>1.10E+2(3.41E+1)†</b>

‡ and † indicate  $\xi = 5$  performs significantly better than and equivalently to the corresponding algorithm, respectively.