Supplementary material for MO-DEHB: Evolutionary-based Hyperband for Multi-Objective Optimization

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A More Details on Experiments

A.1 Baseline Methods

In our experiments, we use default settings to run the baselines methods as it is reported in their papers or implementations such as [Blank and Deb, 2020], [Balandat *et al.*, 2020].

Random Search (RS) In each generation, random architectures are sampled from the configuration space using a uniform distribution.

QNPAREGO We use the implementation from [Balandat *et al.*, 2020]. We use 20 initial samples and a batch size of 5

$SMAC_{RF}^{mean}$ We use the implementation from https://github.com/automl/SMAC3 we use HyperparameterOptimizationFacade with MeanAggregationStrategy as the multi-objective algorithm

NSGA-III We use the implementation for NSGA-III from pymoo repository[Blank and Deb, 2020]. we use 10 partitions to generate reference direction.

AGE-MOEA We used the implementation for AGE-MOEA from pymoo repository[Blank and Deb, 2020]. We use a population of size 100

MOEA/D We used the implementation for MOEA/D from pymoo repository[Blank and Deb, 2020]. we use 10 partitions to generate reference direction with the default setting of number of neighbors as 20. We use auto decomposition and a default setting for probability of neighbor mating as 0.9

A.2 Benchmarks

We collect benchmarks for multi-objective (MO) that optimize interesting objectives from three diverse domains: Neural Architecture Search (NAS), joint NAS and hyperparameter optimization (joint NAS & HPO), and algorithmic fairness. We build our collection of benchmarks on HPOBench library [Eggensperger *et al.*, 2021]. For NAS family, we conduct experiments on NAS-Bench-101 [Ying *et al.*, 2019b], NAS-Bench-1shot1 [Zela *et al.*, 2020b] and NAS-Bench-201 [Dong and Yang, 2020b], which are 9 tabular benchmarks. The joint NAS & HPO family involving tuning Convolutional Neural Networks (CNNs) the Oxford-Flowers dataset [Nilsback and Zisserman, 2008] and Fashion-MNIST [Xiao *et al.*, 2017], and also three surrogate benchmarks [Zela *et al.*, 2022] from the recently introduced JAHS-Bench-201 suite [Bansal *et al.*, 2022]. For algorithmic fairness, we have a fair model adopted from [Schmucker *et al.*, 2021a] on Adult dataset [Kohavi and others, 1996]. In Table 1, we provide a summary for all the benchmarks with details on search space and its type, optimized objectives and fidelity.

A.3 Results for Neural Architecture Search

In Figure 1, the performance of all baseline algorithms is evaluated on NAS-Bench-101. We observe that all baseline algorithms perform similarly except for MOEA/D. MO-DEHB$_{NSGA-II}$ slightly outperforms the rest on NAS-Bench-101-A and NAS-Bench-101-B, while QNPAREGO demonstrates the best overall performance on NAS-Bench-101-C. Figure 2 presents the results for NAS-Bench-1Shot1[1]. We observe that that all baseline algorithms, except MOEA/D, converge with a similar performance . Figure 3 presents the results on NAS-201. For Imagenet benchmark, we see that RS serves as a strong baseline. Also, however the MO-DEHB variants perform poorly initially for a short period of time, later they converge to a similar performance compared to other baselines. Furthermore, $SMAC_{RF}^{mean}$ demonstrates a strong performance on all benchmarks, although it is slightly outperformed by MO-DEHB on NAS-201-Cifar100.

A.4 Results for Joint NAS & HPO

Figure 4 presents the results for Fashion and Flower datasets. We observe that on Flower benchmark, MO-DEHB$_{EPSNET}$ performed well initially but it is outperformed by MO-DEHB$_{NSGA-II}$ later, with AGE-MOEA showing the final best performance. On the Fashion dataset, we see that while MO-DEHB$_{EPSNET}$ consistently outperforms all other baseline methods, it is outperformed by QNPAREGO in the end of optimization. In Figure 5 we show the results for JAHS-Bench-201 suite. We observe that MO-DEHB$_{NSGA-II}$ shows the final best performance on all three benchmarks while MO-DEHB$_{EPSNET}$ performs competitively. Additionally, we observe that $SMAC_{RF}^{mean}$ exhibits competitive performance on JAHS-Cifar10 and JAHS-Colorectal-Histology.

*Equal Contribution

[1] Due to minor integration issues, the observation for 1Shot_CS_3 is currently unavailable. However, it will be provided in the near future

Family	#benchs	#cont(log)	#int(log)	#cat	#ord	fidelity	type	objectives	opt. budget	#confs	Ref.
NAS101	3	0 0 21	0 0 1	26 14 5	0 0 0	epochs	Tabular	Accuracy Modelsize	10^7sec 428 TAE 435 TAE	423k	[Ying *et al.*, 2019a]
NAS201	3	0	0	6	0	epochs	Tabular	Accuracy Modelsize	10^7sec 216 TAE	15 625	[Dong and Yang, 2020a]
NAS1shot1	3	0	0	9 9 11	0	epochs	Tabular	Accuracy Model size	10^7sec 260 TAE 285 TAE	6 240 29 160 363 648	[Zela *et al.*, 2020a]
Joint Nas&HPO	2	1(1)	9(7)	3	0	epochs	raw	Accuracy Log Modelsize	86400 sec 309 TAE	-	[Izquierdo *et al.*, 2021]
JAHS-Bench-201	3	2(2)	0	9	3	epochs	surrogate	Accuracy Latency	10^7 sec 320 TAE	200k	[Bansal *et al.*, 2022]
Fairness$_{Adult}$	1	5(5)	5(4)	0	0	epochs	raw	Accuracy DSO	86400 sec 273 TAE	-	[Schmucker *et al.*, 2021b]

Table 1: Overview of used benchmark. We report the number of benchmarks per family (*#benchs*), the number of continuous (*#cont*), integer (*#int*), categorical (*#cat*), ordinal (*#ord*) hyperparameters and if they are on a log scale. We also report benchmark type, optimization objectives and budgets. We set a upper limit per benchmark of Target Algorithm Executions (TAE) depending on the search space ($20 + 80 * \sqrt{|\text{Search Space}|}$)

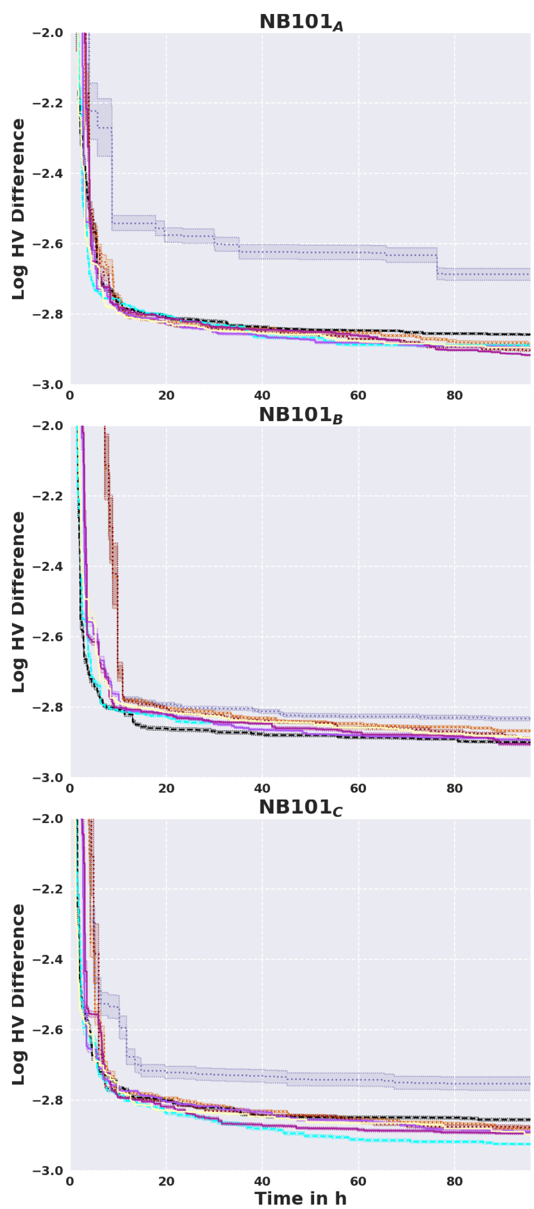

Figure 1: Log HV Differences between empirical best and trajectory on NAS-Bench 101.

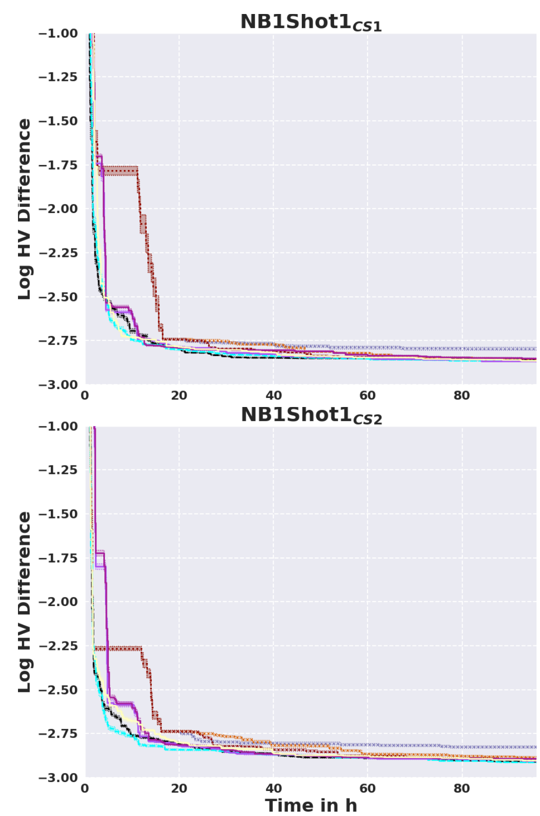

Figure 2: Log HV Differences between empirical best and trajectory on NAS-Bench 1shot1

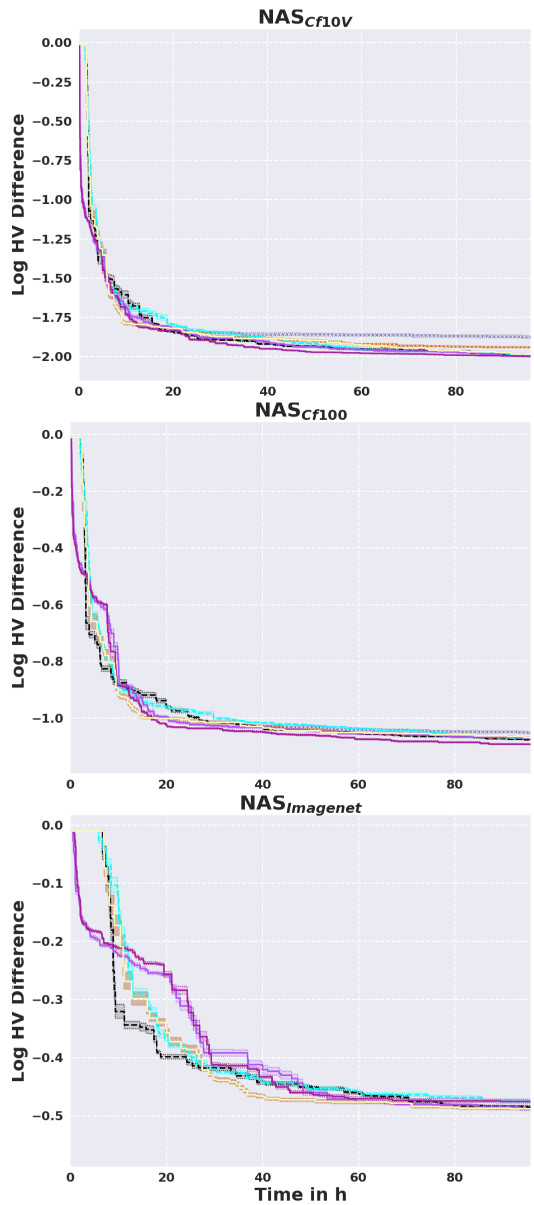

Figure 3: Log HV Differences between empirical best and trajectory on NAS-Bench 201

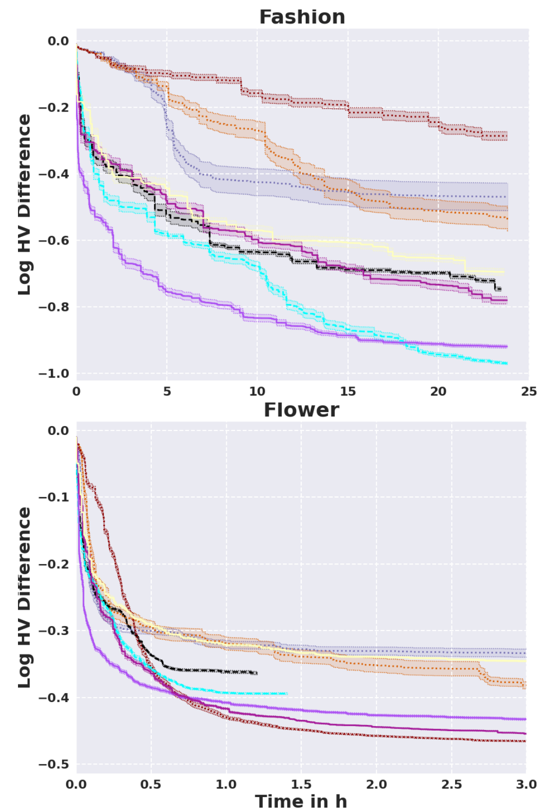

Figure 4: Log HV Differences between empirical best and trajectory on joint NAS & HPO for CNN Fashion and Flower datasets

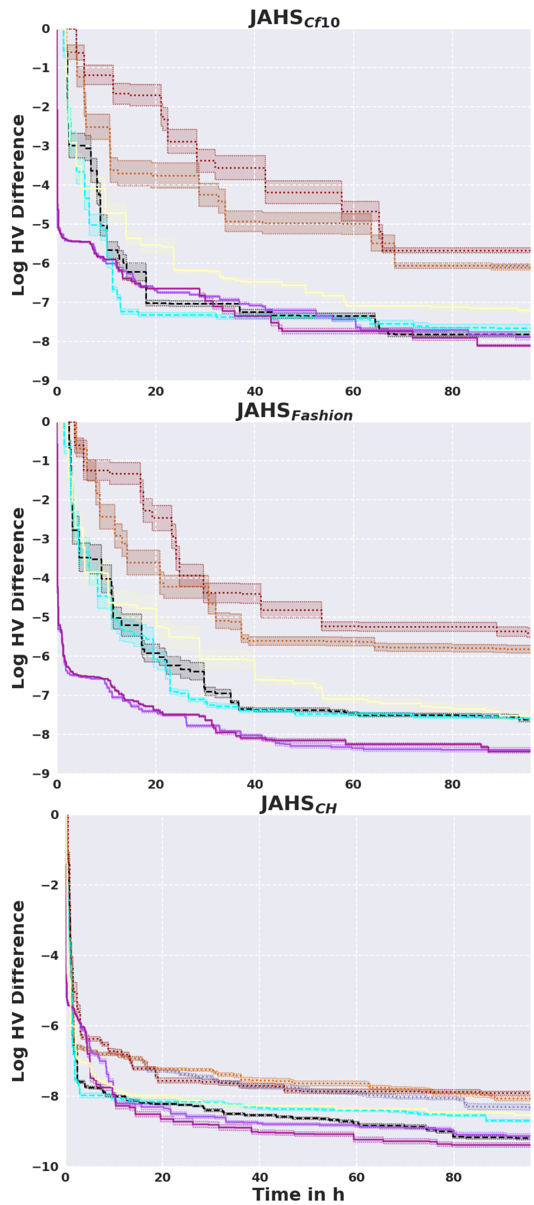

Figure 5: Log HV Differences between empirical best and trajectory on JAHS-Bench-201 Benchmark

A.5 Summary of Results

In Figure 6, we visualize the summary of attainment surfaces to evaluate the capacity of the baselines methods to approximate the entire Pareto front [Knowles, 2005]. To facilitate the visual inspection of the differences, we show the first, median and ninth attainment surfaces, rather than plotting all 10 attainment surfaces. In Figure 6, we observe that almost all baselines perform competitively on NAS-Bench-201 and NAS-Bench-1Shot1. For NAS-Bench-101, evolutionary algorithms (EAs) methods (i.e. AGE-MOEA, NSGA-III and our MO-DEHB variants) perform quite competitively. Moreover, we observe that while SMAC performs better than MO-DEHB variants on JAHS-Bench, MO-DEHB variants still exhibit consistent and good performance. For fashion dataset, we see QNPAREGO showing better performance than MO-DEHB while both variants of MO-DEHB shows better performance than other baselines. Additionally, we observe that MO-DEHB consistently shows superior performance on the Adult dataset. In conclusion, we observe that MO-DEHB consistently demonstrates strong performance on all benchmarks.

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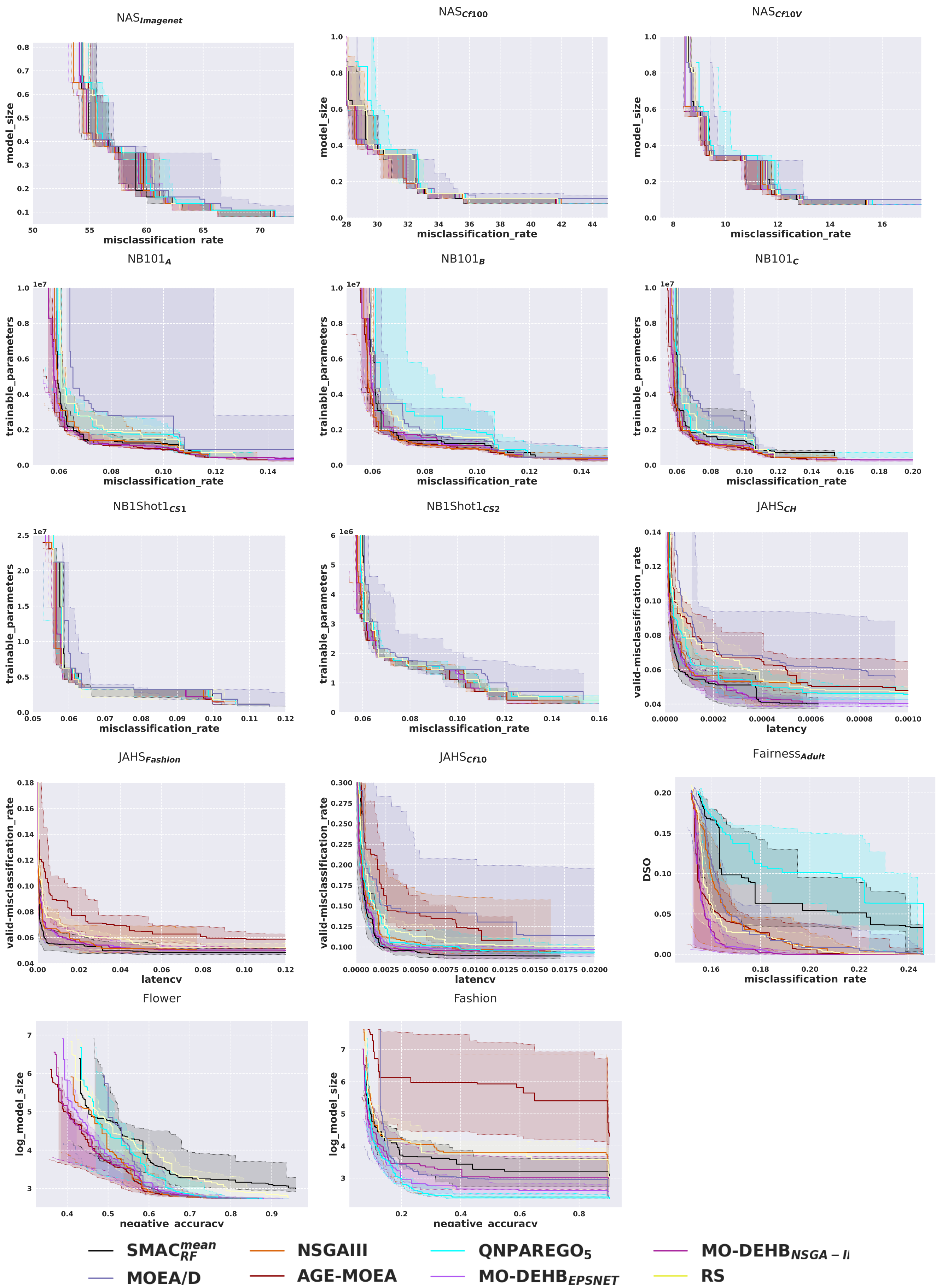

Figure 6: We report summary-attainment-surfaces for all benchmarks. Upper and lower bound correspond to the first and ninth summary-attainment-surface.