DEEP POWER LAWS FOR HYPERPARAMETER OPTIMIZATION

Anonymous authors
Paper under double-blind review

ABSTRACT

Hyperparameter optimization is an important subfield of machine learning that focuses on tuning the hyperparameters of a chosen algorithm to achieve peak performance. Recently, there has been a stream of methods that tackle the issue of hyperparameter optimization, however, most of the methods do not exploit the scaling law property of learning curves. In this work, we propose Deep Power Law (DPL), a neural network model conditioned to yield predictions that follow a power-law scaling pattern. Our model dynamically decides which configurations to pause and train incrementally by making use of multi-fidelity estimation. We compare our method against 7 state-of-the-art competitors on 3 benchmarks related to tabular, image, and NLP datasets covering 57 diverse search spaces. Our method achieves the best results across all benchmarks by obtaining the best any-time results compared to all competitors. We open-source our implementation and make our code publicly available at: `https://anonymous.4open.science/r/DeepRegret-0F61/`

1 INTRODUCTION

Hyperparameter Optimization (HPO) is a major challenge for the Machine Learning community. Unfortunately, HPO is not yet feasible for Deep Learning (DL) methods due to the high cost of evaluating multiple configurations. Recently, Gray-box HPO (a.k.a. multi-fidelity HPO) has emerged as a promising paradigm for HPO in DL, by discarding poorly-performing hyperparameter configurations after observing the validation error on the low-level fidelities of the optimization procedure (Li et al., 2017; Falkner et al., 2018; Awad et al., 2021; Li et al., 2020). The advantage of gray-box HPO compared to online HPO (Chen et al., 2017; Parker-Holder et al., 2020), or meta-gradient HPO (Maclaurin et al., 2015; Franceschi et al., 2017; Lorraine et al., 2020) is the ability to tune all types of hyperparameters.

In recent years, a stream of papers highlights the fact that the performance of DL methods is predictable (Hestness et al., 2017), concretely, that the validation error rate is a power law function of the model size, or dataset size (Rosenfeld et al., 2020; 2021). Such a power law relationship has been subsequently validated in the domain of NLP, too (Ghorbani et al., 2022). In this paper, we demonstrate that the power-law principle has the potential to be a game-changer in HPO, because we can evaluate hyperparameter configurations in low-budget regimes (e.g. after a few epochs), then estimate the performance on the full dataset using dataset-specific power law models.

We introduce Deep Power Law (DPL) ensembles, a probabilistic surrogate for Bayesian optimization (BO) that estimates the performance of a hyperparameter configuration at future budgets using ensembles of deep power law functions. Subsequently, a novel proposed flavor of BO dynamically decides which configurations to pause and train incrementally by relying on the performance estimations of the surrogate. We demonstrate that our method achieves the new state-of-the-art in HPO for DL by comparing against 8 strong HPO baselines, and 62 datasets of three diverse modalities (tabular, image, and natural language processing). As a result, we believe the proposed method has the potential to finally make HPO for DL a feasible reality. Overall, our contributions can be summarized as follows:

- We introduce a novel probabilistic surrogate for gray-box HPO based on ensembles of deep power law functions.

- We derive a simple mechanism to combine our surrogate with Bayesian optimization.
- Finally, we demonstrate the superiority of our method against the current state-of-the-art in HPO for Deep Learning, with a very large-scale HPO experimental protocol.

2 Related Work

Multi-fidelity HPO relaxes the black box assumption by assuming it has access to the learning curve of a hyperparameter configuration. Such a learning curve is the function that maps either training time or dataset size, to the validation performance. The early performance of configurations (i.e. first segment of the learning curve) can be used to discard unpromising configurations, before waiting for full convergence. Successive halving (Jamieson & Talwalkar, 2016) is a widely used multi-fidelity method that randomly samples hyperparameter configurations, starts evaluating them, and ends a fraction of them upon reaching a predefined budget. Afterward, the budget is multiplied by the fraction of discarded hyperparameter configurations and the process continues until the maximum budget is reached. Although the method relies only on the last observed value of the learning curve, it is very efficient. In recent years, various flavors of successive halving have been elaborated, including Hyperband (Li et al., 2017), which effectively runs successive halving in parallel with different settings. A major improvement to Hyperband is replacing random search with a more efficient sampling strategy (Awad et al., 2021; Falkner et al., 2018). However, the only assumption these methods make about the learning curve is that it will improve over time. In contrast, we fit surrogates that exploit a power law assumption on the curves.

Learning curve prediction is a related topic, where the performance of a configuration is predicted based on a partially observed learning curve. Typically, the assumptions about the learning curve are much stronger than those described above. The prediction is often based on the assumption that the performance increases at the beginning and then flattened towards the end. One way to model this behavior is to define a weighted set of parametric functions (Domhan et al., 2015; Klein et al., 2017). Then, the parameters of all functions are determined so that the resulting prediction best matches the observed learning curve. Another approach is to use learning curves from already evaluated configurations and to find an affine transformation that leads to a well-matched learning curve (Chandrashekaran & Lane, 2017). A more data-driven approach is to learn the typical learning curve behavior directly from learning curves across different datasets (Wistuba & Pedapati, 2020). Learning curve prediction algorithms can be combined with successive halving (Baker et al., 2018). In contrast to this line of research, we actually fit ensembles of power law surrogates for conducting multi-fidelity HPO with Bayesian optimization.

Scaling laws describe the relationship between the performance of deep learning models as a function of dataset size or model size. Concretely, Hestness et al. (2017) show empirically for different data modalities and neural architectures that a power law relationship holds when growing the dataset. Further work confirms this observation and extends it by demonstrating the power law relationship also with regard to the model size (Rosenfeld et al., 2020; 2021; Ghorbani et al., 2022). From a practical angle, Yang et al. (2022) propose to tune hyperparameters on a small-scale model and then transfer it to a large-scale version. In contrast to these papers, we directly use the power law assumption for training surrogates in Bayesian optimization for HPO.

3 Preliminaries

Hyperparameter Optimization (HPO) demands finding the configurations $\lambda \in \Lambda$ of a Machine Learning method that achieve the lowest validation loss $\mathcal{L}^{(\text{Val})}$ of a model (e.g. a neural network), which is parameterized with θ and learned to minimize the training loss $\mathcal{L}^{(\text{Train})}$ as:

$$\begin{aligned} \lambda^* &:= \underset{\lambda \in \Lambda}{\arg\min} \;\; \mathcal{L}^{(Val)}\left(\lambda, \theta^*\left(\lambda\right)\right), \\ \text{s.t.} \;\; \theta^*\left(\lambda\right) &:= \underset{\theta \in \Theta}{\arg\min} \;\; \mathcal{L}^{(Train)}\left(\lambda, \theta\right) \end{aligned} \tag{1}$$

For simplicity we denote the validation loss as our function of interest $f(\lambda) = \mathcal{L}^{(Val)}\left(\lambda, \theta^*\left(\lambda\right)\right)$. The optimal hyperparameter configurations λ^* of Equation 1 are found via **an HPO policy** $\mathcal{A}$ (also

called an HPO method) that given a history of N evaluated configurations $H := \{\lambda_i, f(\lambda_i)\}_{i=1}^{N}$ suggests the $(N+1)$-th configuration to evaluate as $\lambda_{N+1} := \mathcal{A}(H)$ where $A : [\Lambda \times \mathbb{R}_+]^N \rightarrow \Lambda$. The search for an optimal HPO policy is a bi-objective problem in itself, aiming at (i) finding a configuration out of N evaluations that achieves the smallest validation loss $f(\lambda)$, and (ii) ensuring that the costs of evaluating the N configurations do not exceed a total budget Ω, as shown in Equation 2.

$$\begin{aligned} \arg\min_{\mathcal{A}} \min_{i \in \{1,\dots,N\}} & f\left(\lambda_i = \mathcal{A}\left(H^{(i-1)}\right)\right), \\ \text{where:} \quad & H^{(i)} := \begin{cases} \{(\lambda_j, f(\lambda_j))\}_{j=1}^{i} & i > 0 \\ \emptyset & i = 0 \end{cases} \\ \text{subject to:} \quad & \Omega > \sum_{i=1}^{N} \text{cost}\left(f\left(\lambda_i\right)\right) \end{aligned} \tag{2}$$

Bayesian optimization (BO) is the most popular type of policy for HPO, due to its ability to balance the exploration and exploitation aspects of minimizing the loss f. Technically speaking, BO fits a surrogate $\hat{f}(\lambda; \theta)$ parametrized with θ to approximate the observed loss $f(\lambda)$ using the history H, as $\boldsymbol{\theta}^* := \arg\min_\theta \mathbb{E}_{(\lambda, f(\lambda)) \sim p_H}\, p(f(\lambda)|\lambda, \theta)$. Afterwards, BO uses an acquisition/utility function $a : \Lambda \rightarrow \mathbb{R}_+$ to recommend the next configuration as $\lambda_{N+1} := \mathcal{A}\left(H^{(N)}\right) = \arg\max_{\lambda \in \Lambda} a\left(\lambda; \boldsymbol{\theta}^*\right)$. A typical acquisition choice is the Expected Improvement (Mockus et al., 1978). For a more detailed introduction to BO and HPO we refer the interested reader to Hutter et al. (2019)

Gray-box (multi-fidelity) HPO refers to the case where an approximation of the validation loss can be measured at a lower budgets $b \in B$, where $B = (0, 1]$. For instance in Deep Learning we can measure the validation loss after few epochs ($0 < b < \epsilon$), rather than wait for a full convergence ($b = 1$). Throughout this paper the term budget refers to the number of optimization epochs. The evaluation of a configuration λ for a budget b is defined as $f(\lambda, b) := \mathcal{L}^{(Val)}\left(\lambda, \theta^*\left(\lambda, b\right)\right)$, where $f(\lambda, b) : \Lambda \times B \rightarrow \mathbb{R}_+$. The concept of budgets alters the HPO problem definition slightly. The history of N configurations evaluated at different budgets becomes a set of N triples (config, budget, eval) defined as $H := \{(\lambda_i, b_i, f(\lambda_i, b_i))\}_{i=1}^{N}$. A gray-box HPO policy is still optimized for Equation 2, however, the constraint is altered as $\Omega > \sum_{i=1}^{N} \text{cost}\left(f\left(\lambda_i, b_i\right)\right)$.

4 Power Law Surrogates for Bayesian Optimization

Prior work has demonstrated that the performance of Machine Learning methods as a function of budgets (i.e. dataset size, number of optimization epochs, model size, image resolution) follows a power law relationship (Rosenfeld et al., 2020; 2021). In this paper, we employ this power law dependence between the validation loss and the number of optimization epochs in Deep Learning. We propose a novel gray-box Hyperparameter Optimization method which is based on power law surrogates. We assume that every learning curve $f(\lambda, \cdot)$ can be described by a power law function defined by (α, β, γ). Concretely, we define a power law function modelling the validation loss for a configuration λ at budget b (a.k.a. number of epochs) as shown in Equation 3.

$$\hat{f}(\lambda, b) := \alpha_\lambda + \beta_\lambda\, b^{-\gamma_\lambda}, \quad \alpha, \beta, \gamma \in \mathbb{R} \tag{3}$$

We propose to use surrogate models employing the power law in Bayesian optimization (BO) to optimize hyperparameters. We suggest learning a **shared power law function** across all configurations by conditioning the power law coefficients α, β, γ on λ using a parametric neural network g that maps a configuration to the power law coefficients of its learning curve as $g : \Lambda \rightarrow \mathbb{R}^3$. The network g has three output nodes, corresponding to the power law coefficients, denoted as $g(\lambda)_\alpha, g(\lambda)_\beta, g(\lambda)_\gamma$. The configuration-conditioned power law surrogate becomes:

$$\hat{f}(\lambda, \mathbf{b}) := g(\lambda)_\alpha + g(\lambda)_\beta\, \mathbf{b}^{-g(\lambda)_\gamma}, \quad g : \Lambda \rightarrow \mathbb{R}^3 \tag{4}$$

Algorithm 1: Gray-box HPO with Deep Power Laws

Input : Search space Λ, initial design $H^{(0)}$, budget increment b^{step}
Output: Best hyperparameter configuration λ^*

Evaluate initial configurations and budgets $H := H^{(0)}$;
while *still budget* **do**
  Fit a DPL ensemble $\hat{f}^{(1)}(\lambda, b), \ldots, \hat{f}^{(K)}(\lambda, b)$ from history H using Equation 5;
  Define the posterior mean and variance $\mu_{\hat{f}}(\lambda, b), \sigma^2_{\hat{f}}(\lambda, b)$ using Equation 6;
  Recommend the next configuration λ^{next} using Equation 7;
  Compute the next budget b^{next} using Equation 8;
  Train λ^{next} until b^{next} and measure the validation loss $f\left(\lambda^{\text{next}}, b^{\text{next}}\right)$;
  Append to history $H \leftarrow H \cup \{(\lambda^{\text{next}}, b^{\text{next}}, f\left(\lambda^{\text{next}}, b^{\text{next}}\right))\}$;
end
return Best configuration λ^* with the smallest validation loss $\min_{(\lambda^*, b, f(\lambda^*, b)) \in H} f\left(\lambda^*, b\right)$;

Using a history of learning curve evaluations $H := \{(\lambda_i, b_i, f\left(\lambda_i, b_i\right))\}_{i=1}^{N}$ we can train the power law surrogate to minimize the following loss function using stochastic gradient descent:

$$\arg\min_{g} \; \mathbb{E}_{(\lambda, b, f(\lambda, \mathbf{b})) \sim p_H} \left(f\left(\lambda_i, \mathbf{b}_i\right) - \left[g(\lambda_i)_\alpha + g(\lambda_i)_\beta \; \mathbf{b}_i{}^{-g(\lambda_i)_\theta} \right] \right) \tag{5}$$

BO surrogates need to be probabilistic regression models because the acquisition functions require the posterior variance of the predictions. As a result, we train an ensemble of K diverse surrogates $\hat{f}^{(1)}(\lambda, b), \ldots, \hat{f}^{(K)}(\lambda, b)$ with the Deep Ensemble strategy (Lakshminarayanan et al., 2017), by initializing each surrogate with different weights and by training with a different sequence of mini-batches. The posterior mean μ and the posterior variance σ^2 of the power law ensemble are trivially computed as:

$$\begin{aligned} \mu_{\hat{f}}(\lambda, \mathbf{b}) &= \frac{1}{K} \sum_{k=1}^{K} \hat{f}^{(k)}(\lambda, \mathbf{b}), \\ \sigma^2_{\hat{f}}(\lambda, \mathbf{b}) &= \frac{1}{K} \sum_{k=1}^{K} \left(\hat{f}^{(k)}(\lambda, \mathbf{b}) - \mu_{\hat{f}}(\lambda, \mathbf{b}) \right)^2 \end{aligned} \tag{6}$$

The acquisition function of our approach relies on selecting the configuration λ with the lowest estimated loss at the full budget. In other words, we select the hyperparameter configurations that are expected to achieve the best performance at the end of the optimization procedure. Consequently, we use the Expected Improvement (EI) acquisition with the estimated full budget's ($b = 1$) posterior mean and variance. The best observed loss until a budget b is denoted as $f^{(best)}\left(b\right) := \min\left\{f\left(\lambda, b'\right) \mid \left(\lambda, b', f\left(\lambda, b\right)\right) \in H \wedge b' < b\right\}$. We briefly define the acquisition in Equation 7, and refer the reader to Mockus et al. (1978) for the details of the EI.

$$\lambda^{\text{next}} := \arg\max_{\lambda \in \Lambda} \; \text{EI}\left(\mu_{\hat{f}}(\lambda, \mathbf{b} = 1), \; \sigma^2_{\hat{f}}(\lambda, \mathbf{b} = 1); \; f^{(best)}\left(\mathbf{b} = 1\right) \right) \tag{7}$$

However, after selecting a configuration with our variant of the EI acquisition, we do not naively run it until convergence. Instead, we propose a novel multi-fidelity strategy that advances the selected λ^{next} of Equation 7 by a small budget of b^{step}, e.g. for few more mini-batches of training. Therefore, the selected λ^{next} will be evaluated at b^{next} as defined in Equation 8. Notice our proposed strategy also covers new configurations with no learning curve evaluations in H.

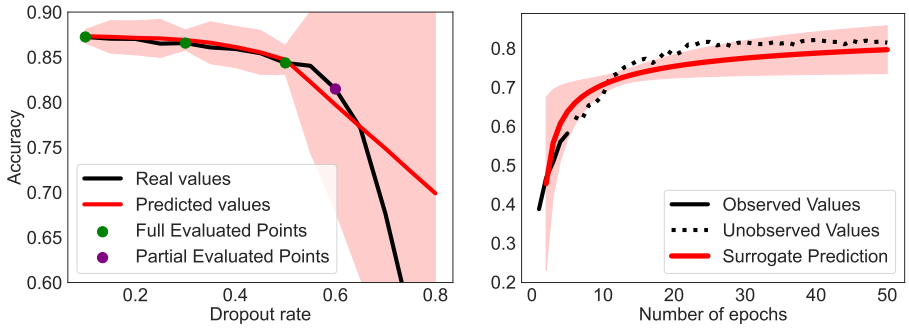


Figure 1: The power law predictions and uncertainty estimations on the CIFAR10 1-D search space. **Left:** The maximal budget across different hyperparameter configurations (dropout rates). **Right:** Across different budgets for the same hyperparameter configuration that was observed partially.

$$b^{\text{next}} := \begin{cases} b^{\text{step}}, & \nexists \lambda^{\text{next}} : (\lambda^{\text{next}}, \cdot, \cdot) \in H \\ b^{\text{step}} + \max\limits_{(\lambda^{\text{next}}, \mathbf{b}, \cdot) \in H} \mathbf{b}, & \text{otherwise} \end{cases} \tag{8}$$

The overall procedure for conducting HPO with our Deep Power Laws is shown in the pseudocode of Algorithm 1, illustrating how the aforementioned components fit a Bayesian optimization routine.

5 A Proof-of-concept Example

To visually demonstrate the power law surrogate, we created a 1-dimensional search space where we train a Preact ResNet (He et al., 2016) on the CIFAR-10 dataset (Krizhevsky et al., 2009). We train multiple versions of the model applying a different dropout hyperparameter $\lambda \in [0.1, 0.85]$ for 50 epochs, with a cosine annealed learning rate and an initial value of 10^{-2}. We train our power law surrogate on a subspace of the hyperparameter search space. We use the full validation curves for the aforementioned hyperparameter subspace, except for the hyperparameter configuration corresponding to 0.65, where, we use only a subset of the learning curve. Ideally, our power law surrogate should model a low uncertainty in the observed hyperparameter configurations and a higher uncertainty in the partial or unobserved regions.

As shown in Figure 1, our power law surrogate fits the training data well by generalizing correctly across different hyperparameter configurations. Furthermore, the power law surrogate models a low uncertainty in the region of observed hyperparameter configurations, and a higher uncertainty in the region of partially observed configurations that scales more the further we move from the region of observed points. Additionally, Figure 1 (right) conveys that when we evaluate the hyperparameter configuration that is only observed partially, the uncertainty scales with the budget. More concretely, the surrogate is more uncertain the higher the budget (epoch) for which we predict compared to the last observed value.

6 Experimental Protocol

In our experiments, we standardize the data by performing min-max scaling for our method and every baseline included. If a baseline has a specific preprocessing protocol, we do not apply min-max scaling but we apply the protocol as suggested by the authors. In the following experiments, we report the regret of configurations, which is defined as:

$$R(\lambda, b) = \max\left(0, f^{(best)}(b) - f(\lambda, b)\right) \tag{9}$$

In short, the regret is the distance from the best possible hyperparameter configuration on the dataset to the best-found hyperparameter configuration. On a dataset level, we report the average regret

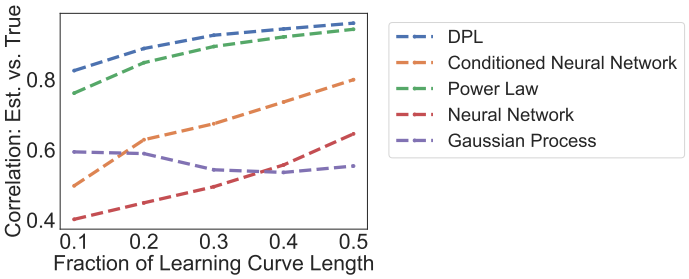


Figure 2: The correlations of individual models, and the DPL, for different fractions of observed learning curves across datasets.

across 10 repetitions with different seeds. When reporting results over all datasets, we report the averaged normalized regret. The normalized regret for each dataset is calculated by dividing the regret by the difference between the best value and the worst value. We normalize the regret since, over all datasets, there are regret distances of different scales, which in turn can lead to low regret values that can dominate the overall averaged results for all datasets.

6.1 BENCHMARKS

LCBench: A benchmark that features 2,000 hyperparameter configurations that parametrize the architecture of simple feedforward neural networks, as well as, the training pipeline (Zimmer et al., 2021). The benchmark features 7 numerical hyperparameters. The hyperparameter configurations were evaluated for 51 epochs on 35 different datasets from the AutoML benchmark (Gijsbers et al., 2019).

PD1: A deep learning benchmark (Wang et al., 2022) that consists of recent DL architectures run on large vision datasets such as CIFAR-10, CIFAR-100, ImageNet, as well as statistical modeling corpora and protein sequences datasets from the bioinformatics domain. Every search space features varying learning curve lengths, ranging from 5 to 1414, and a different number of evaluated hyperparameter configurations ranging from 807 to 2807.

TaskSet: A benchmark that features different optimization tasks evaluated in 5 different search spaces (Metz et al., 2020). For our work, we focus on the Adam8p search space, which is among the largest search spaces in the benchmark with 1000 hyperparameter configurations, every hyperparameter configuration featuring 8 continuous hyperparameters. The hyperparameters control the training pipeline and the optimizer. Every run consists of 50 steps, where, every step corresponds to 200 training iterations. For variety among our benchmarks, we focus on 12 NLP tasks.

6.2 BASELINES

Random Search: Randomly samples hyperparameter configurations for the largest possible budget.

Hyperband: Uses multiple brackets with different trade-offs of the initial budget and number of epochs to initially train (Li et al., 2017). It then further applies Successive Halving (SH) (Jamieson & Talwalkar, 2016) on every individual bracket to decide which configurations to further train and which configurations to stop training.

ASHA: An asynchronous version of SH (Li et al., 2018) that does not wait for all configurations to finish in a bracket before running for the next fidelity.

BOHB: An extension of Hyperband that replaces the random sampling of hyperparameter configurations in the initial brackets with model-based sampling (Falkner et al., 2018). BOHB uses TPE (Bergstra et al., 2011) as an inner model and has an individual model for every fidelity.

DEHB: An additional extension of Hyperband, which differs from BOHB by using evolutionary strategies to sample the initial hyperparameter configurations (Awad et al., 2021).

MF-DNN: A multi-fidelity method that makes use of deep neural networks (Li et al., 2020).

SMAC: A method that extends Hyperband but uses random forests to sample the initial hyperparameter configurations for a bracket (Lindauer et al., 2022).

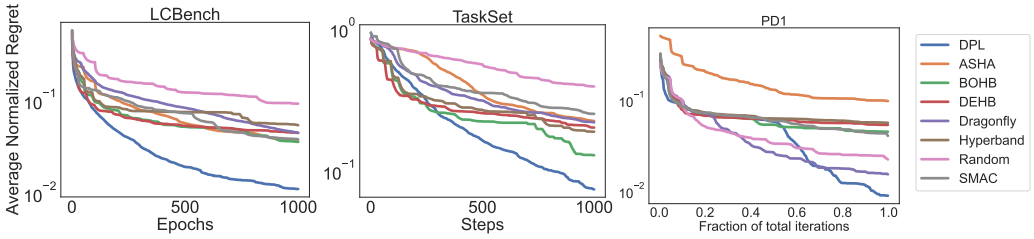


Figure 3: A comparison of all methods considered in the experiments over the number of epochs/steps for all the considered benchmarks. We report the average normalized regret for all methods. A step corresponds to 200 iterations in the case of TaskSet.

Dragonfly: We use the Dragonfly Library (Kandasamy et al., 2020) to compare against BOCA (Kandasamy et al., 2017), a multi-fidelity method that uses Gaussian processes to predict the next hyperparameter to evaluate and the fidelity for which it should be evaluated.

For all the baselines, we use their official public implementations. We provide additional details in Appendix C.

7 Research Hypotheses and Experimental Results

Hypothesis 1: *The power law assumption improves the quality of the learning curve predictions.*

We compare power laws against GPs and simple feedforward neural networks by fitting individual instances of every algorithm on a partially observed learning curve for every corresponding hyperparameter configuration. We repeat the procedure with different fractions of partially observed learning curves for every dataset in the LCBench benchmark. We check the accuracy of each model in predicting the final performance by calculating the correlation. Lastly, we investigate the performance of a simple feedforward neural network and Deep Power Law (DPL). In particular, we do not fit a model on the learning curve of every hyperparameter configuration, but, we fit a model for all learning curves of different hyperparameter configurations.

As can be seen in Figure 2, DPL manages to have the highest accuracy compared to all the considered model algorithms. Observing the results, fitting an individual power law to a learning curve achieves predictions of higher quality compared to fitting a simple feedforward neural network or Gaussian processes.

Furthermore, conditioning a neural network to output based on a power law formulation yields a DPL that can share information across hyperparameter configurations while improving accuracy compared to the individual power laws. As expected, the effect is more noticeable in the small data regime, where, we observe only a small subset of observed points from the learning curve. Lastly, a DPL is less expensive to fit on a benchmark compared to fitting an individual power law for every hyperparameter configuration, which does not scale. Based on the results, we consider Hypothesis 1 to be validated and that **DPLs yield qualitative predictions that surpass different models fitted on individual hyperparameter configurations**.

Hypothesis 2: *Our method DPL achieves state-of-the-art results in HPO.*

Initially, we compare the average normalized regret of our method against all competitors over the number of epochs for all the benchmarks. In Figure 3, we show the performance of all the methods considered in the experiments over the number of epochs, as observed, DPLs manage to outperform in all the considered baselines. In the case of LCBench, DPLs converge faster to a better solution compared to the competitor methods and continue to increase the gap in performance until the optimization process ends. Furthermore, we observe the same trend with TaskSet, only in 0.25% of the optimization process the DPLs converge to a better solution compared to all the considered baselines and increase the lead until the optimization process ends. Lastly, since PD1 features datasets with different learning curves, we consider a budget of 20 full function evaluations for every dataset (roughly the same number of full function evaluations as in the other two benchmarks). We normalize the budget by dividing the number of epochs by the total number of epochs per dataset.

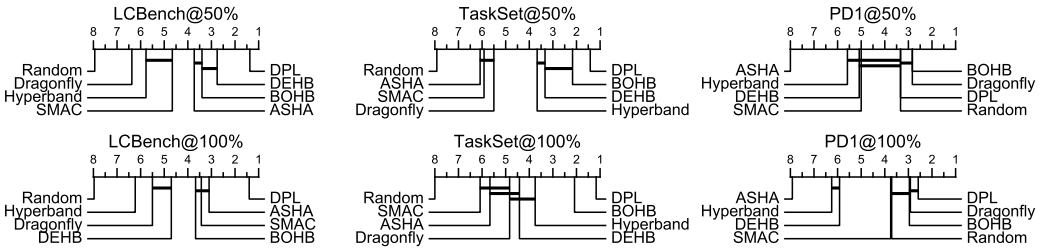
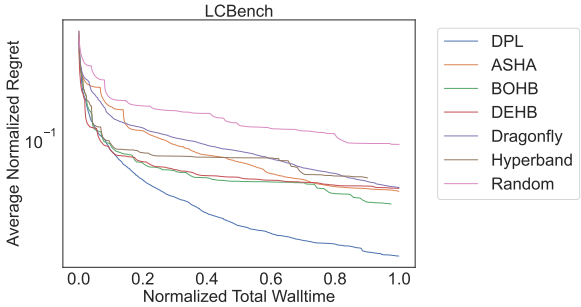


Figure 4: The critical difference diagrams for DPL and the other baselines in all the considered benchmarks. **Top**: The The numbers indicate the average ranks across all datasets (the lower the better). Connected lines correspond to methods whose result difference is not statistically significant.

Figure 5: The performance of rival methods over time in LCBench. We report the average normalized regret for all baselines.



As seen in Figure 3, our method converges slower compared to DragonFly, the closest baseline in the benchmark, however, when 75% of the optimization process is reached, our method matches the baseline in performance and continues to improve until the end of the optimization process, once again, performing best compared to all baselines.

In addition to the average normalized regret, Figure 4 shows the critical difference diagrams that show the ranks of all methods for the different benchmarks, where, DPL consistently achieves the best rank with a statistically significant difference in the majority of cases. In particular, we provide the critical difference diagrams during half the optimization procedure and at the end of the optimization procedure. As observed, for LCBench and TaskSet, DPL achieves the best performance with a statistically significant difference in results only halfway through the optimization procedure, retaining the statistical significance until the end of the HPO procedure. In the case of PD1, our method is among the best three methods during half of the optimization procedure, with a non-significant difference compared to the other two top-3 methods. Although at the end of the optimization procedure our method does not have a statistical difference in the results compared to the other methods, it still achieves the best rank over all datasets.

Lastly, we analyse the performance of DPL and all the other methods considered in the experiments in Figure 5, where, as it can be observed, DPL manages to outperform the competitors even when method's overhead time is included, showing that the time overhead of DPL is negligible in the results. In more detail, the time includes the time to evaluate a hyperparameter configuration and the time taken by each respective method in its inner process to suggest the next hyperparameter configurations to evaluate. TaskSet is not included in Figure 5 since it does not offer information regarding the time. Given the results, we conclude that Hypothesis 2 is validated and that **DPL manages to achieve state-of-the-art performance**.

Hypothesis 3: *DPL explores the search space more efficiently compared to the baselines.*

We conduct further analyses to understand the source of the efficiency of our method DPL versus the baselines. As a result, we analyze two important aspects, the quality of the evaluated configurations, as well as the exploration capability of our gray-box HPO. First of all, we measure what fraction of the top 1% configurations (ranked by accuracy) our method considers. Figure 6 (left) shows that until convergence our method can discover significantly more top configurations in the datasets of the LCBench benchmark, compared to baselines.

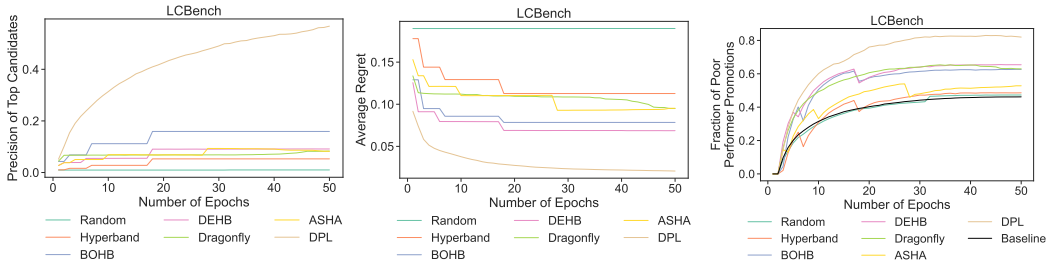


Figure 6: Study of DPL's efficiency over the course of HPO. **Left:** Share of the best candidates selected during training. **Middle:** Average regret of configurations chosen to be trained at each budget. **Right:** Share of top third configurations at a given budget which were bottom two third configurations at a previous budget.

The middle plot of Figure 6 shows the average regret for each configuration promoted to the respective budget. According to this plot, DPL is more efficient by assigning budget only to configurations with lower regret compared to the other methods. The precision and regret plots demonstrate that the quality of the evaluated configurations is largely better than all baselines, therefore, giving our method a significant lift in the performance rank. Last but not least, the right plot shows the percentage of configurations that were performing poor in an earlier epoch (i.e. accuracy-wise in the bottom $2/3$ of configurations up to the epoch indicated at the x-axis) but performed better at later epochs (i.e. at the top $1/3$ of configurations). Furthermore, we added a line labeled with "Baseline", which represents the fraction of previously poor-performing configurations of all configurations. Such behavior is observed often with learning curves, for instance, strongly regularized networks converge slowly. The results indicate that our method can better explore unpromising early configurations, by giving them a chance through the uncertainty estimation of our ensemble, and the respective Bayesian optimization mechanism.

8 LIMITATIONS

Our proposed ensemble of power law functions achieves an important gain in performance concerning the state-of-the-art in gray-box HPO and highlights the efficiency of modeling learning curves with the power law assumption. However, we believe that further research is needed to calibrate the power law model for the beginning and the end parts of the learning curves. Recent work highlighted that the error rate at very small fidelities (e.g. after a few mini-batches) is not a power law (Rosenfeld et al., 2021). Contrary to the common expectations, we experienced that the uncertainty estimation arising from the Deep Ensemble (Lakshminarayanan et al., 2017) is not very qualitative compared to standard BO surrogates such as Gaussian Processes. In addition, having to train an ensemble has additional computational costs, due to the necessity of training multiple power law models. In the future, we plan to re-conceptualize our surrogate, by combining power laws with Gaussian Processes.

9 CONCLUSIONS

In this work, we introduce Deep Power Law (DPL), a probabilistic surrogate based on an ensemble of power law functions. The proposed surrogate is used within a novel gray-box HPO method based on Bayesian optimization. In contrast to the prior work we exploit the recently-discovered scaling laws for estimating the performance of Deep Learning models. Through extensive experiments comprising 7 baselines, 57 datasets, and search spaces of diverse deep learning architectures, we showed that DPL outperforms strong HPO baselines for DL by a large margin. As an overarching contribution, we advanced the state-of-the-art in the important field of HPO for Deep Learning.

REFERENCES

Noor H. Awad, Neeratyoy Mallik, and Frank Hutter. DEHB: evolutionary hyberband for scalable, robust and efficient hyperparameter optimization. In *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence, IJCAI 2021, Virtual Event / Montreal, Canada, 19-27 August 2021*, pp. 2147–2153, 2021. doi: 10.24963/ijcai.2021/296. URL https://doi.org/10.24963/ijcai.2021/296.

Bowen Baker, Otkrist Gupta, Ramesh Raskar, and Nikhil Naik. Accelerating neural architecture search using performance prediction. In *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Workshop Track Proceedings*, 2018. URL https://openreview.net/forum?id=HJqk3N1vG.

James Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. *Advances in neural information processing systems*, 24, 2011.

Akshay Chandrashekaran and Ian R. Lane. Speeding up hyper-parameter optimization by extrapolation of learning curves using previous builds. In *Machine Learning and Knowledge Discovery in Databases - European Conference, ECML PKDD 2017, Skopje, Macedonia, September 18-22, 2017, Proceedings, Part I*, volume 10534 of *Lecture Notes in Computer Science*, pp. 477–492. Springer, 2017.

Yutian Chen, Matthew W. Hoffman, Sergio Gomez Colmenarejo, Misha Denil, Timothy P. Lillicrap, Matthew Botvinick, and Nando de Freitas. Learning to learn without gradient descent by gradient descent. In *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, pp. 748–756, 2017. URL http://proceedings.mlr.press/v70/chen17e.html.

Tobias Domhan, Jost Tobias Springenberg, and Frank Hutter. Speeding up automatic hyperparameter optimization of deep neural networks by extrapolation of learning curves. In *Proceedings of the Twenty-Fourth International Joint Conference on Artificial Intelligence, IJCAI 2015, Buenos Aires, Argentina, July 25-31, 2015*, pp. 3460–3468. AAAI Press, 2015.

Stefan Falkner, Aaron Klein, and Frank Hutter. BOHB: robust and efficient hyperparameter optimization at scale. In *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*, pp. 1436–1445, 2018. URL http://proceedings.mlr.press/v80/falkner18a.html.

Luca Franceschi, Michele Donini, Paolo Frasconi, and Massimiliano Pontil. Forward and reverse gradient-based hyperparameter optimization. In *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, pp. 1165–1173, 2017. URL http://proceedings.mlr.press/v70/franceschi17a.html.

Behrooz Ghorbani, Orhan Firat, Markus Freitag, Ankur Bapna, Maxim Krikun, Xavier Garcia, Ciprian Chelba, and Colin Cherry. Scaling laws for neural machine translation. In *The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022*. OpenReview.net, 2022. URL https://openreview.net/forum?id=hR_SMu8cxCV.

Pieter Gijsbers, Erin LeDell, Janek Thomas, Sébastien Poirier, Bernd Bischl, and Joaquin Vanschoren. An open source automl benchmark. *arXiv preprint arXiv:1907.00909*, 2019.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Identity mappings in deep residual networks. In *European conference on computer vision*, pp. 630–645. Springer, 2016.

Joel Hestness, Sharan Narang, Newsha Ardalani, Gregory F. Diamos, Heewoo Jun, Hassan Kianinejad, Md. Mostofa Ali Patwary, Yang Yang, and Yanqi Zhou. Deep learning scaling is predictable, empirically. *CoRR*, abs/1712.00409, 2017. URL http://arxiv.org/abs/1712.00409.

Frank Hutter, Lars Kotthoff, and Joaquin Vanschoren (eds.). *Automated Machine Learning - Methods, Systems, Challenges*. Springer, 2019.

Kevin G. Jamieson and Ameet Talwalkar. Non-stochastic best arm identification and hyperparameter optimization. In *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics, AISTATS 2016, Cadiz, Spain, May 9-11, 2016*, pp. 240–248, 2016. URL http://proceedings.mlr.press/v51/jamieson16.html.

Kirthevasan Kandasamy, Gautam Dasarathy, Jeff G. Schneider, and Barnabás Póczos. Multi-fidelity bayesian optimisation with continuous approximations. In *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, pp. 1799–1808, 2017. URL http://proceedings.mlr.press/v70/kandasamy17a.html.

Kirthevasan Kandasamy, Karun Raju Vysyaraju, Willie Neiswanger, Biswajit Paria, Christopher R. Collins, Jeff Schneider, Barnabás Póczos, and Eric P. Xing. Tuning hyperparameters without grad students: Scalable and robust bayesian optimisation with dragonfly. *J. Mach. Learn. Res.*, 21:81:1–81:27, 2020. URL http://jmlr.org/papers/v21/18-223.html.

Aaron Klein, Stefan Falkner, Jost Tobias Springenberg, and Frank Hutter. Learning curve prediction with bayesian neural networks. In *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*, 2017. URL https://openreview.net/forum?id=S11KBYclx.

Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009.

Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and scalable predictive uncertainty estimation using deep ensembles. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper/2017/file/9ef2ed4b7fd2c810847ffa5fa85bce38-Paper.pdf.

Liam Li, Kevin Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Moritz Hardt, Benjamin Recht, and Ameet Talwalkar. Massively parallel hyperparameter tuning. *arXiv preprint arXiv:1810.05934*, 5, 2018.

Lisha Li, Kevin G. Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. Hyperband: A novel bandit-based approach to hyperparameter optimization. *J. Mach. Learn. Res.*, 18: 185:1–185:52, 2017. URL http://jmlr.org/papers/v18/16-558.html.

Shibo Li, Wei Xing, Robert M. Kirby, and Shandian Zhe. Multi-fidelity bayesian optimization via deep neural networks. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/60e1deb043af37db5ea4ce9ae8d2c9ea-Abstract.html.

Marius Lindauer, Katharina Eggensperger, Matthias Feurer, André Biedenkapp, Difan Deng, Carolin Benjamins, Tim Ruhkopf, René Sass, and Frank Hutter. Smac3: A versatile bayesian optimization package for hyperparameter optimization. *Journal of Machine Learning Research (JMLR) – MLOSS*, 23(54):1–9, 2022.

Jonathan Lorraine, Paul Vicol, and David Duvenaud. Optimizing millions of hyperparameters by implicit differentiation. In *The 23rd International Conference on Artificial Intelligence and Statistics, AISTATS 2020, 26-28 August 2020, Online [Palermo, Sicily, Italy]*, pp. 1540–1552, 2020. URL http://proceedings.mlr.press/v108/lorraine20a.html.

Dougal Maclaurin, David Duvenaud, and Ryan P. Adams. Gradient-based hyperparameter optimization through reversible learning. In *Proceedings of the 32nd International Conference on Machine Learning, ICML 2015, Lille, France, 6-11 July 2015*, pp. 2113–2122, 2015. URL http://proceedings.mlr.press/v37/maclaurin15.html.

Luke Metz, Niru Maheswaranathan, Ruoxi Sun, C. Daniel Freeman, Ben Poole, and Jascha Sohl-Dickstein. Using a thousand optimization tasks to learn hyperparameter search strategies. *CoRR*, abs/2002.11887, 2020. URL https://arxiv.org/abs/2002.11887.

Jonas Mockus, Vytautas Tiesis, and Antanas Zilinskas. The application of Bayesian methods for seeking the extremum. *Towards Global Optimization*, 2(117-129):2, 1978.

Jack Parker-Holder, Vu Nguyen, and Stephen J. Roberts. Provably efficient online hyperparameter optimization with population-based bandits. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/c7af0926b294e47e52e46cfebe173f20-Abstract.html.

Jonathan S. Rosenfeld, Amir Rosenfeld, Yonatan Belinkov, and Nir Shavit. A constructive prediction of the generalization error across scales. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net, 2020. URL https://openreview.net/forum?id=ryenvpEKDr.

Jonathan S. Rosenfeld, Jonathan Frankle, Michael Carbin, and Nir Shavit. On the predictability of pruning across scales. In Marina Meila and Tong Zhang (eds.), *Proceedings of the 38th International Conference on Machine Learning, ICML 2021, 18-24 July 2021, Virtual Event*, volume 139 of *Proceedings of Machine Learning Research*, pp. 9075–9083. PMLR, 2021. URL http://proceedings.mlr.press/v139/rosenfeld21a.html.

David Salinas, Matthias Seeger, Aaron Klein, Valerio Perrone, Martin Wistuba, and Cedric Archambeau. Syne tune: A library for large scale hyperparameter tuning and reproducible research. In *First Conference on Automated Machine Learning (Main Track)*, 2022.

Zi Wang, George E Dahl, Kevin Swersky, Chansoo Lee, Zelda Mariet, Zachary Nado, Justin Gilmer, Jasper Snoek, and Zoubin Ghahramani. Pre-training helps bayesian optimization too. *arXiv preprint arXiv:2207.03084*, 2022.

Martin Wistuba and Tejaswini Pedapati. Learning to rank learning curves. In *Proceedings of the 37th International Conference on Machine Learning, ICML 2020, 13-18 July 2020, Virtual Event*, pp. 10303–10312, 2020. URL http://proceedings.mlr.press/v119/wistuba20a.html.

Greg Yang, Edward J. Hu, Igor Babuschkin, Szymon Sidor, Xiaodong Liu, David Farhi, Nick Ryder, Jakub Pachocki, Weizhu Chen, and Jianfeng Gao. Tensor programs V: tuning large neural networks via zero-shot hyperparameter transfer. *CoRR*, abs/2203.03466, 2022. doi: 10.48550/arXiv.2203.03466. URL https://doi.org/10.48550/arXiv.2203.03466.

Lucas Zimmer, Marius Lindauer, and Frank Hutter. Auto-pytorch tabular: Multi-fidelity metalearning for efficient and robust autodl. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 43(9):3079 – 3090, 2021.

A Implementation Details

For our method, we use a 2-layer feedforward neural network with 128 units per layer. Additionally, we use batch normalization after every linear layer. We use Leaky ReLU as our non-linearity. Our network has 3 output units, which, are then combined to yield the power law output. We apply the Sigmoid non-linearity activation only on the β and γ output units. For the experiments in the pd1 benchmark, we apply a Leaky ReLU non-linearity to improve convergence, since, the benchmark features low error rate values. We use PyTorch version 1.12 as the main library on top of which we build our method.

We use the L1 loss to train our network, coupled with Adam featuring an initial learning rate of 10^{-2}. We train every network of our ensemble for 250 epochs only in the beginning of the hpo optimization process and we continuously refine the model for 10 epochs every hpo iteration. Lastly, we use 5 models to build our ensemble of DPLs.

B Benchmarks

LCBench We use the official implementation as the interface for the LCBench benchmark [1].

[1] https://github.com/automl/LCBench

TaskSet: The TaskSet benchmark features 1000 diverse tasks. We decide to focus on only 12 NLP tasks from the TaskSet benchmark to add variety to our entire collection of datasets. Our limitation on the number of tasks included is related to the limited compute power, we are unable to run for the entire suite of datasets offered in TaskSet.

PD1: We use the synetune library (Salinas et al., 2022) for our interface to the PD1 benchmark. From the Benchmark, we only include datasets that have a learning curve of length greater than 10. We furthermore only include datasets that have a learning curve lower or equal to 50 to have a fair comparison between all benchmarks, to have approximately 20 full function evaluations.

C BASELINES

Random Search: We implemented random search by randomly sampling hyperparameter configurations from the benchmarks with the maximal budget.

Hyperband, BOHB, LCNet: We use version 0.7.4 of the HpBandSter library as a common codebase for all 3 baselines [2]. For the last approach mentioned, despite heavy hyperparameter tuning of the method, we could not get stable results across all the benchmarks and hence dropped partial results from all our analyses.

ASHA: For the implementation of ASHA we use the public implementation from the optuna library , version 2.10.0.

DEHB: We use the public implementation offered by the authors [3].

MF-DNN: In our experiments we used the official implementation from the authors [4].

SMAC: For our experiment with SMAC we used the official code base from the authors [5].

Dragonfly: We use version 0.1.6 of the publicly available Dragonfly library.

For all the multi-fidelity methods considered in the experiments, we use the same minimal and maximal fidelities. In more detail, for the LCBench and TaskSet benchmarks we use a minimal fidelity lower bound of 1 and a maximal fidelity lower bound equal to the max budget. In the case of PD1, where, the learning curves have different lengths, we use a minimal bound that allows for a maximal amount of 4 brackets, if no more than 4 brackets can be achieved we use a minimal budget of 1.

[2] https://github.com/automl/HpBandSter
[3] https://github.com/automl/DEHB/
[4] https://github.com/shib0li/DNN-MFBO
[5] https://github.com/automl/SMAC3