Speedup Techniques for Hyperparameter Optimization

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Outline

1. Overview
2. Meta-Learning
3. Overview of Multi-Fidelity Optimization
4. Hyperband
5. BOHB
6. Multi-fidelity Bayesian optimization
7. Predicting Learning Curves
8. Success Stories and Practical Recommendations

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Overview

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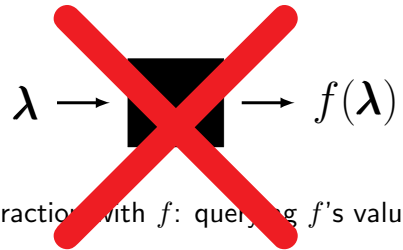
Beyond Black-box Optimization

Recall general blackbox optimization:

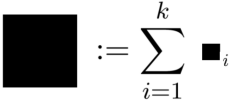


Only mode of interaction with f: querying f's value at a given $\boldsymbol{\lambda}$

Too slow for tuning expensive models

Methods for Going Beyond Blackbox Bayesian Optimization

- Sum of little black boxes
  - Each little black box is fast but only yields a noisy estimate
  - SMAC [Hutter et al. 2011] directly solves $\arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \sum_{i=1}^{N} c(\boldsymbol{\lambda}, i)$
  - Auto-WEKA [Thornton et al. 2013] used this to optimize 10-fold cross-validation performance



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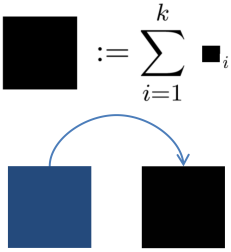
- Meta-learning across problems / datasets



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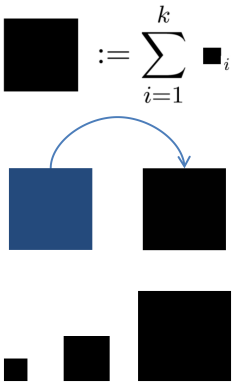
- Multi-fidelity optimization



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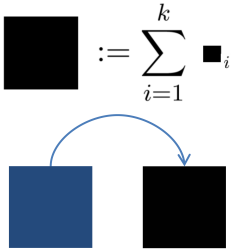

- Meta-learning across problems / datasets

- Multi-fidelity optimization

- Graybox optimization / learning curve prediction

Learning Goals of this Lecture

After this lecture, students can ...

- Describe many different ways of using meta-learning to speed up HPO
- Explain the concept of multi-fidelity optimization to speed up HPO
- Explain the Successive Halving and Hyperband algorithms
- Explain how to combine Bayesian optimization and Hyperband in BOHB
- Describe how to exploit multiple fidelities in Bayesian optimization
- Discuss several ways of predicting learning curves
- Discuss success stories of speeding up Bayesian optimization

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Meta-Learning

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Introduction

- Learning essentially never stops:
  - Many models are periodically re-fit to track changes in the data
  - Many models are re-fit to perform well on new tasks
- The best hyperparameter configuration tends to remain quite stable across tasks

For a good introduction to meta-learning in general, see [AutoML Book: Chapter 2]

Problem Statement

Given:

- a set of prior tasks: $t_j \in \mathcal{T}_{\text{meta}} \subset \mathcal{T}$,
- a set of new tasks: $t_{\text{new}} \in \mathcal{T}$,
- a set of learning algorithms, fully defined by $\theta_i \in \Theta$
- a set of prior evaluations $\mathcal{D}_{\text{meta}}$ on $t_j \in \mathcal{T}_{\text{meta}}$
- a set of evaluations $\mathcal{D}_{\text{new}}$ on new task t_{new}

Goal of meta-learning:

- use meta-data $\mathcal{D}_{\text{meta}}$ to choose $\theta_i \in \Theta$ for t_{new} better than only based on $\mathcal{D}_{\text{new}}$.

[adapted from AutoML Book: Chapter 2]

The Role of Meta-Features

- We can often extract additional characteristics for each task, called meta-features
- Each task t_j can be described by a vector of K meta-features:

$$m(t_j) = (m_{j,1}, \ldots, m_{j,K})$$

- This vector can be used to define a similarity measure between two tasks
  - e.g., calculating the Euclidean distance between $m(t_i)$ and $m(t_j)$
  - Based on similarity, we can transfer information from the most similar tasks to new task t_{new}

Overview of Meta-Features in Machine Learning

- Simple - easily extracted from the data, describe the basic dataset structure
  - e.g., number of features, data points or classes
- Statistical - characterize the data via descriptive statistics:
  - e.g., average or standard deviation of features, or their correlation with the labels
- Information-theoretic - measure the class entropy in the data
  - capture the amount of information in the data
- Model-based - extracted from a model induced using the training data
  - these are often based on properties of decision tree models
  - e.g., number of leaves, number of nodes, shape of the tree
- Landmarking - computed by running several fast ML algorithms on the dataset
  - e.g., is fast algorithm A better than fast algorithm B on this dataset?
  - this can capture different properties of the dataset, e.g., linear separability
- Others - not included in the previous groups
  - e.g., time related measures, clustering and distance-based measures

Meta-Learning for HPO Approach 1: Warmstarting

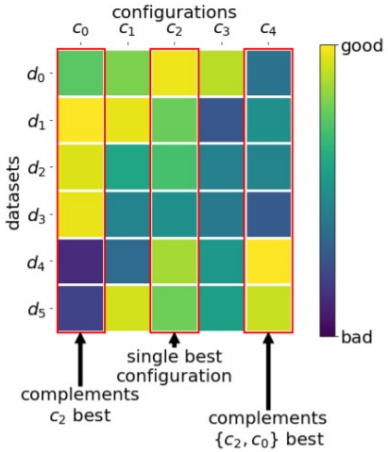
- Experts often start HPO from a strong default (rather than random configurations)
- Can we learn from meta-data $\mathcal{D}_{\text{meta}}$ how to initialize HPO?
- Note: just a single default configuration often does not perform great on a new dataset
  - Otherwise there would be no point in HPO

Meta-Learning for HPO Approach 2: Model-Warmstarting

- Many HPO methods use a predictive model (e.g., Bayesian optimization)
- By running HPO on different datasets, we learn something about the search landscape
  - E.g., what are bad regions of the configuration space in general
- Given: n predictive models $\hat{c}_{\mathcal{D}_i} : \mathbf{\Lambda} \rightarrow \mathbb{R}$ from HPO on $\mathcal{T}_{\text{meta}}$
- How can we use these $\hat{c}_{\mathcal{D}_i}$ to speed up HPO?

Meta-Learning for HPO Approach 3: Task-independent Recommendations

- *Idea:* learn a sorted list of defaults
- *Method:* mostly greedy on $\mathcal{T}_{\text{meta}}$
- *Results:* surprisingly strong, better than Bayesian Optimization



[Wistuba et al. 2017; Feurer et al. 2018; Pfisterer et al. 2018]

Meta-Learning for HPO Approach 3: Task-independent Recommendations

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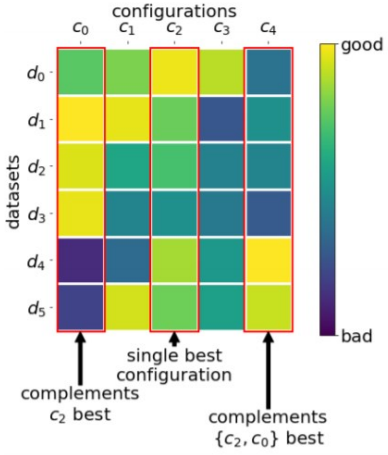
Advantages

- Easy to share and use
- Strong anytime performance
- Embarrassingly parallel

Disadvantages

- Not adaptive



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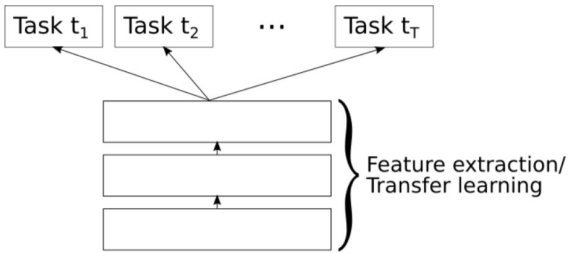
Meta-Learning for HPO Approach 4: Joint model for Bayesian optimization

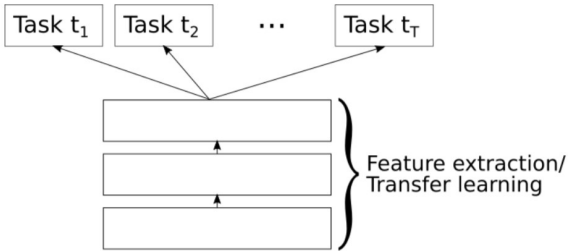
- Jointly train a "deep" neural network on all tasks



[Perrone et al. 2018]

Meta-Learning for HPO Approach 4: Joint model for Bayesian optimization

- Jointly train a "deep" neural network on all tasks
  - Have a separate output layer (head) for each task
  - Each head is a Bayesian linear regression (recall DNGO)



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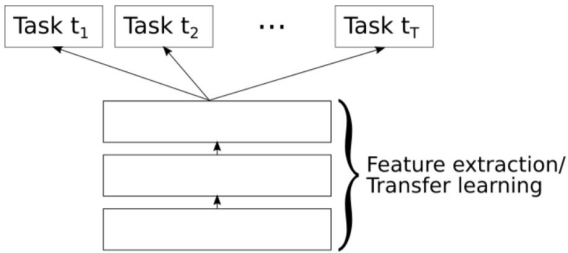
Meta-Learning for HPO Approach 4: Joint model for Bayesian optimization

- Jointly train a "deep" neural network on all tasks
  - Have a separate output layer (head) for each task
  - Each head is a Bayesian linear regression (recall DNGO)
- This uses meta-learning for feature extraction on the hyperparameter configurations



[Perrone et al. 2018]

Meta-Learning for HPO Approach 5: Learning a Black-box Optimization Algorithm from Data

- Learning a blackbox optimization algorithm
  - Use $\mathcal{D}_{\text{meta}}$ to learn a mapping from $\mathcal{D}_{\text{new}}$ to the next configuration $\boldsymbol{\lambda}$ to evaluate
  - This mapping can be a (recurrent) neural net $\text{NN}_\phi : \mathcal{D}_{\text{new}} \mapsto \boldsymbol{\lambda}$ parameterized by weights ϕ
  - This mapping NN_ϕ constitutes a blackbox optimization algorithm

- Existing approaches for learning a blackbox optimizer
  - Gradient descent on ϕ [Chen et al. 2016]
    - ⋆ Simplest technique, but requires backpropagation through the optimization trace
    - ⋆ This also requires the blackbox functions f used for training to be differentiable
  - Reinforcement learning [Li and Malik. 2016]
    - ⋆ Can be harder to get to work, but does not require differentiable f

Meta-Learning for HPO Approach 6: Learning Algorithm Parts

- Learning a complete optimization algorithm requires a lot of data
- It would be more sample-efficient to only replace hand-designed parts of an algorithm

- In Bayesian optimization, a critical hand-designed heuristic is the acquisition function
  - Trade-off between exploitation and exploration, e.g., via PI, EI, UCB, ES, KG, ...
  - Depending on the problem at hand, you might need a different acquisition function

- Idea: Learn a neural acquisition function from data, but still make use of the sample efficiency of Gaussian processes [Volpp et al. 2019]

- Two options:
  - Only depend on predicted mean and variance: $u_\phi(\boldsymbol{\lambda}) = u_\phi(\mu_t(\boldsymbol{\lambda}), \sigma_t(\boldsymbol{\lambda}))$
    - ⋆ This allows to learn a general acquisition function
  - Also depend on the $\boldsymbol{\lambda}$ value: $u_\phi(\boldsymbol{\lambda}) = u_\phi(\mu_t(\boldsymbol{\lambda}), \sigma_t(\boldsymbol{\lambda}), \boldsymbol{\lambda})$
    - ⋆ This allows to fine-tune to the characteristics of $\mathcal{D}_{\text{meta}}$ (e.g., avoid poor parts of the space)

Questions to Answer for Yourself / Discuss with Friends

- Repetition. What are the different kinds of meta-features which can be used to describe machine learning datasets?
- Repetition. List all the different ways of using the meta data for HPO you recall
- Discussion. In the various meta-learning approaches, what will happen if all prior tasks are dissimilar to the target task?

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Overview of Multi-Fidelity Optimization

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Motivating Example

- One possible cheap approximation of an expensive function: use a data subset
  - Many cheap evaluations on small subsets
  - Few expensive evaluations on the full data

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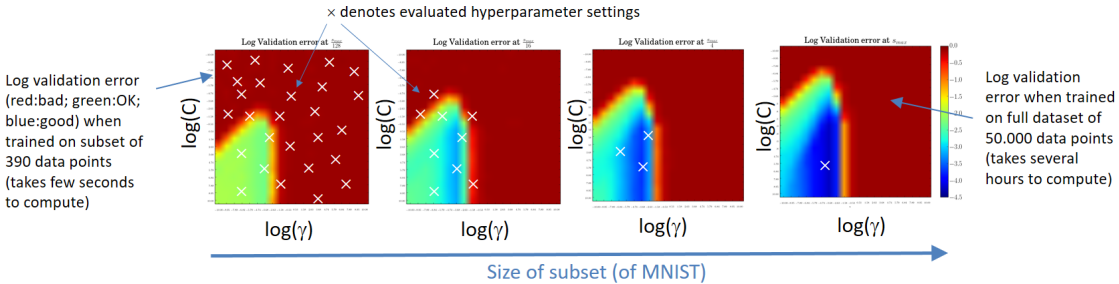
- E.g.: Support Vector Machines (SVM) on MNIST dataset (hyperparameters: C, γ)



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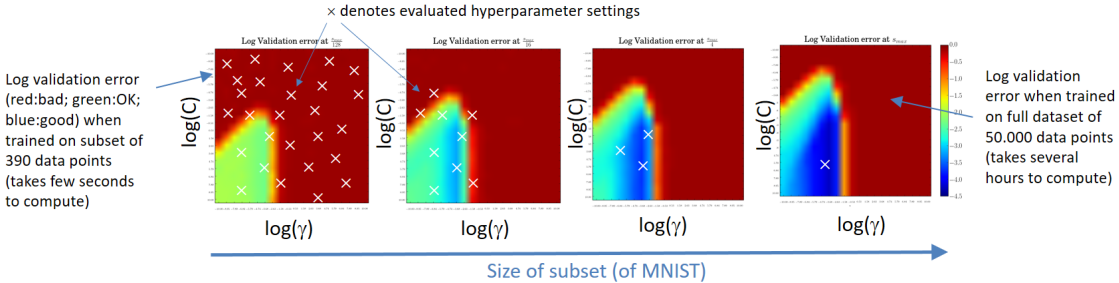
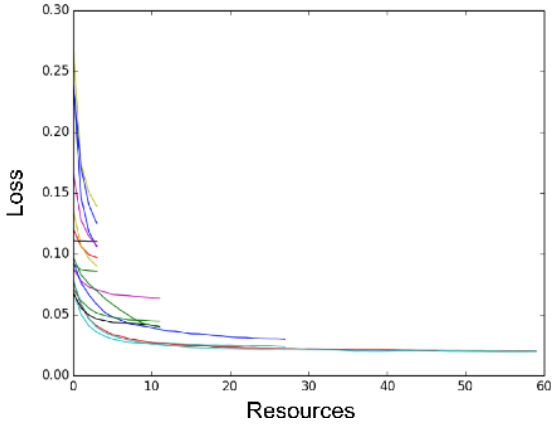


→ up to 1000x speedups over blackbox optimization on full data [Klein et al. 2017]

Motivating Example 2: Shorter Runs of Anytime Algorithms

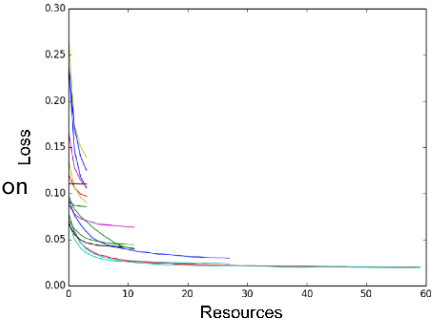
- Performance with shorter runs of an anytime algorithm (such as SGD):



Multi-Fidelity Optimization In General

Exploit cheap approximations of an expensive blackbox function $\rightarrow$ afford more configurations

- Idea: eliminate poor configurations early, allocate more resources to promising ones.
- Possible Resources:
  - Data subset size
  - Runtime / # epochs / # iterations
  - Downsampled size of images in object recognition
  - Depth / width of neural networks
  - Number of trees
  - Number of features
  - Number of cross validation folds
  - General concept, applicable even in fields outside ML, e.g., fluid simulation:
    - ★ Number of particles
    - ★ Time scale of simulation



General Remarks on Multi-Fidelity Optimization

- Often, we have a choice which resources we use as budget
- For multi-fidelity optimization to be helpful, performance with low budgets should be informative about performance with high budgets
- In the simplest case: good with low resources $\leftrightarrow$ good with high resources.
  - In practice, this is of course not always true

How Useful is the Cheap Approximation? The Rank Correlation

Given:

- A set of configurations $\mathbf{\Lambda} = \{\boldsymbol{\lambda}_1, ..., \boldsymbol{\lambda}_n\}$
- The performances $f(\boldsymbol{\lambda}_1), ..., f(\boldsymbol{\lambda}_n)$ on the expensive black box
- The performances $g(\boldsymbol{\lambda}_1), ..., g(\boldsymbol{\lambda}_n)$ on a cheap approximation of the black box

We compute the Spearman rank correlation between $[f(\boldsymbol{\lambda}_1), ..., f(\boldsymbol{\lambda}_n)]$ and $[g(\boldsymbol{\lambda}_1), ..., g(\boldsymbol{\lambda}_n)]$

- If this is high (in the extreme: 1), the relative ranking of the configurations is the same on f and g
  - In that case, we can optimize cheaply on g and also obtain an optimum for f
- If it is low (≈ 0), optimizing g does not tell us anything about f

Goal: find approximations g that are very cheap but have high rank correlations with f

Questions to Answer for Yourself / Discuss with Friends

- Repetition. Which cheap approximation is better in this hypothetical case?
  - Downscaling images (5x cheaper, rank correlation of 0.8)
  - Less epoch of SGD (4x cheaper, rank correlation of 0.75)
- Discussion. Can you think of an application of your interest where you would likely have a good multi-fidelity approximation?

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Hyperband

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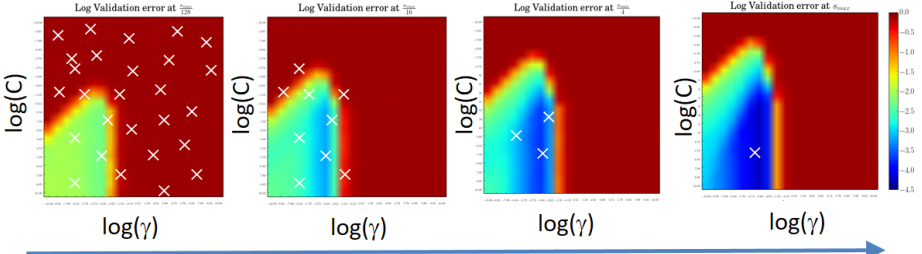
A Simple Multi-Fidelity Algorithms: Successive Halving (SH)

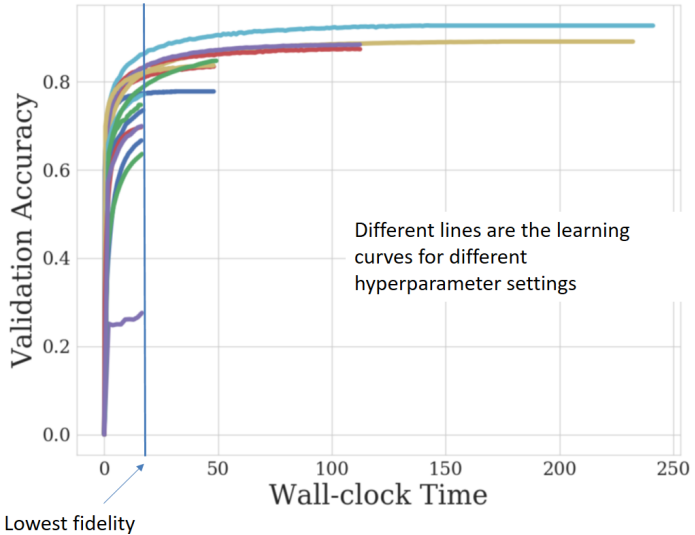
[Jamieson and Talwalkar. 2016]

- A very simple algorithm:
  - Sample N configurations uniformly at random & evaluate them on the cheapest fidelity
  - Keep the best half (or third), move them to the next fidelity
  - Iterate until the most expensive fidelity (= original expensive black box)



The Same SH Algorithm When the Fidelity is Runtime

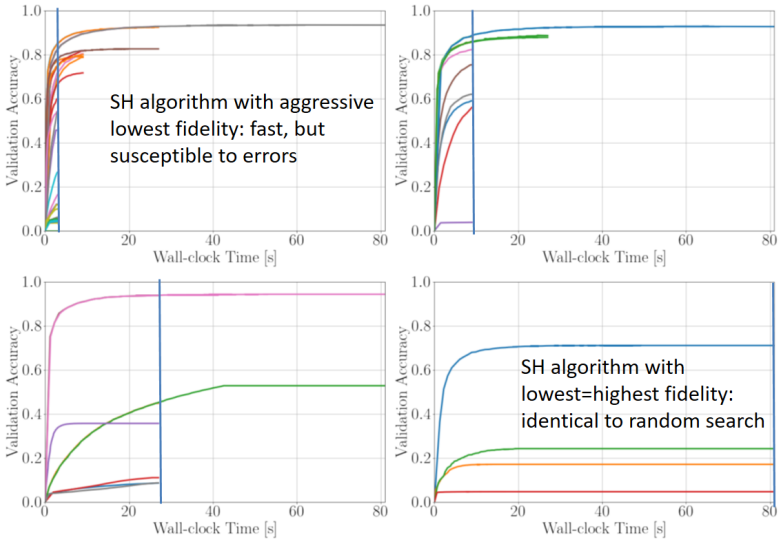
[Jamieson and Talwalkar. 2016]



An Extension of SH with Theoretical Guarantees: Hyperband

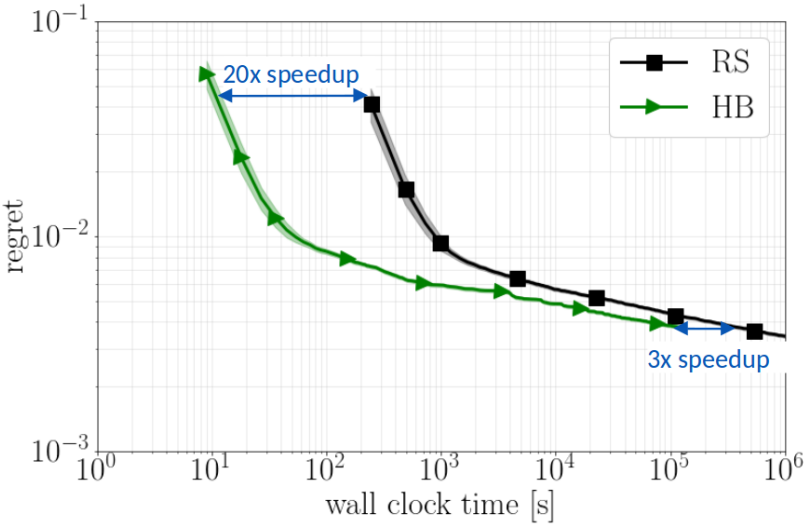
- Main Idea: hedge against errors in cheap approximations
- Algorithm: run multiple copies of SH in parallel, starting at different cheapest fidelities

[Li et al. 2018]



Empirical Evaluation: Hyperband vs. Random Search

[Falkner et al. 2018]



Questions to Answer for Yourself / Discuss with Friends

- Discussion. How do you think Hyperband would compare to successive halving using the most aggressive fidelity?
- Discussion. How slow is Hyperband in the worst case?

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BOHB

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Robust and Efficient Hyperparameter Optimization at Scale

Desiderata for a practical solution to the hyperparamenter optimization problem:

- Strong Anytime Performance
- Strong Final Performance
- Scalability
- Robustness & Flexibility
- Computational Efficiency
- Effective Use of Parallel Resources
- Conceptual / Algorithmic Simplicity

To fulfill all of these desiderata, BOHB combines Bayesian Optimization with Hyperband [Falkner et al. 2018]

BOHB

- BOHB combines the advantages of Bayesian Optimization and Hyperband
  - Bayesian Optimization for choosing configurations to achieve strong final performance
  - Hyperband to choose the budgets for good anytime performance
- BOHB replaces the random selection of configurations at the beginning of each HB iteration by a model-based search
- Details of the model
  - Variant of the Tree Parzen Estimator, with a product kernel
  - Models are fitted independently to the data for one budget at a time
    - Specifically, always the highest budget that has enough data points

BOHB: Algorithm

Pseudocode for sampling in BOHB

Input : observations D, fraction of random runs ρ, percentile γ, number of samples N_s, minimum number of points N_{min} to build a model, and bandwidth factor b_w

Output: next configuration to evaluate

if $rand() < \rho$ **then return** *random configuration*
$b = \arg\max\{D_b : |D_b| \geq N_{min} + 2\}$
if $b = \varnothing$ **then return** *random configuration*
Fit KDEs according to Equation 1
Draw N_s samples acoording to $l'(\boldsymbol{\lambda})$
return *sample with highest ratio* $l(\boldsymbol{\lambda})/g(\boldsymbol{\lambda})$

$$l(\boldsymbol{\lambda}) = p(c(\boldsymbol{\lambda}) \leq \gamma | D_b) \qquad g(\boldsymbol{\lambda}) = p(c(\boldsymbol{\lambda}) > \gamma | D_b) \tag{1}$$

- Note: $l'(\boldsymbol{\lambda})$ is similar to $l(\boldsymbol{\lambda},)$ but has larger bandwidths

BOHB: Empirical Evaluation

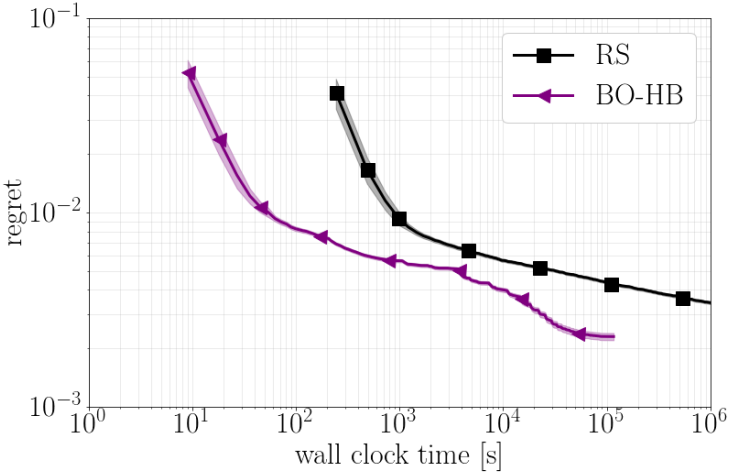
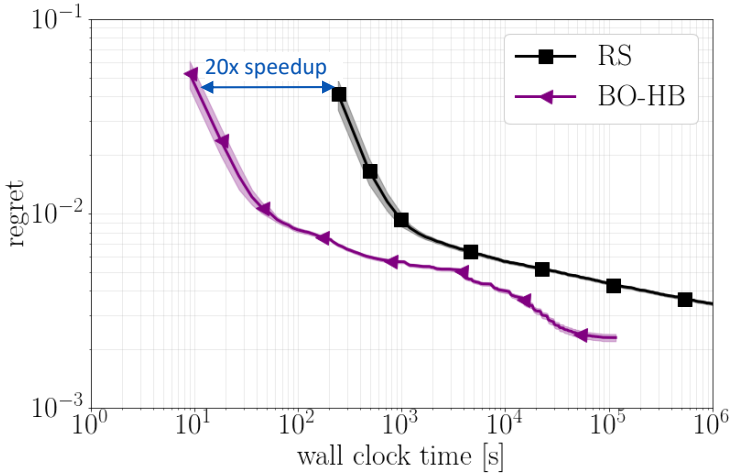


Figure: Performance of RS and BOHB on Auto-Net on dataset Adult

BOHB: Empirical Evaluation



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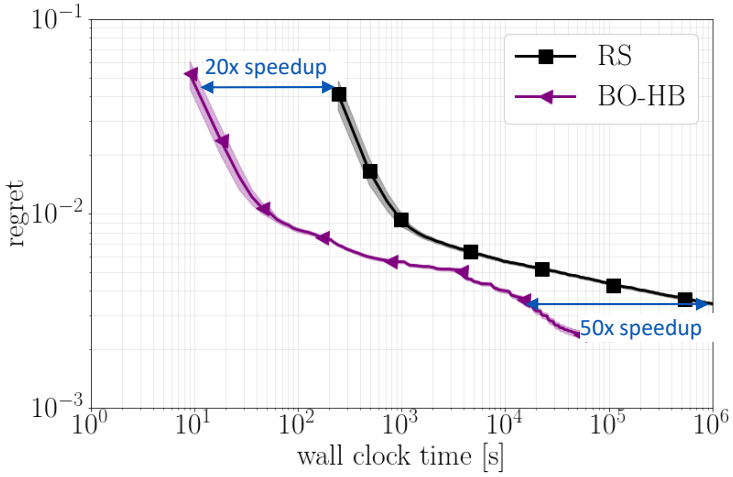

Figure: Performance of RS and BOHB on Auto-Net on dataset Adult

BOHB: Empirical Evaluation

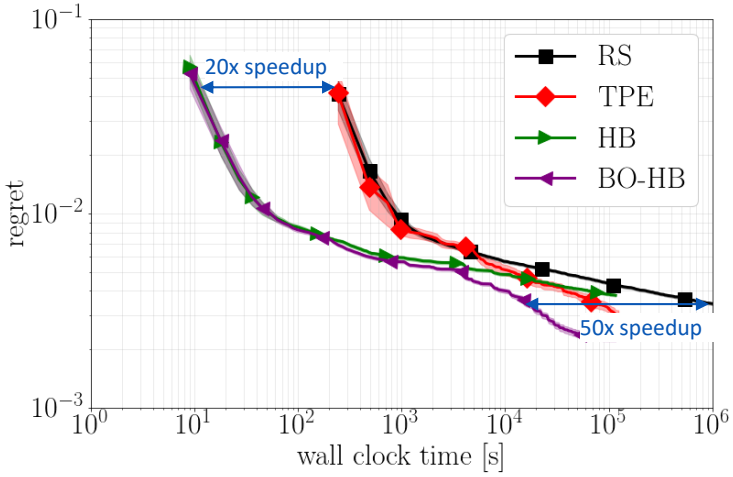

Figure: Performance of RS, TPE, HB and BOHB on Auto-Net on dataset Adult

BOHB: Different number of parallel workers

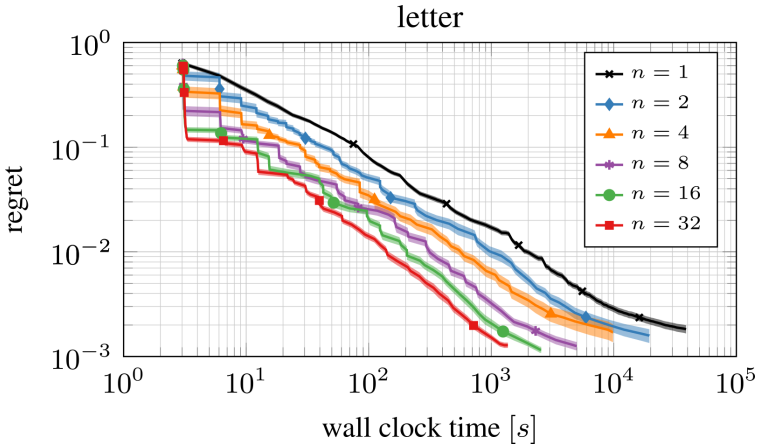

Figure: Performance of BOHB with different number of parallel workers on the letter surrogate benchmark for 128 iterations

BOHB: Optimization of a Bayesian Neural Network

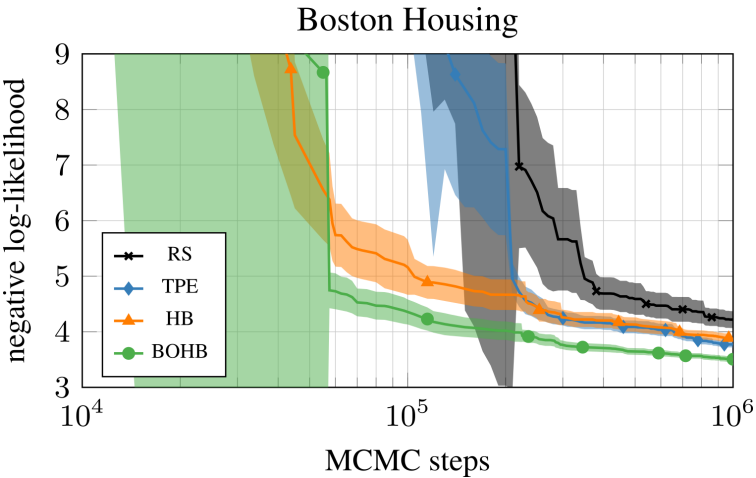

Figure: Optimization of 5 hyperparameters of a Bayesian neural network trained with SGHMC.

BOHB: Optimization of a Reinforcement Learning Agent

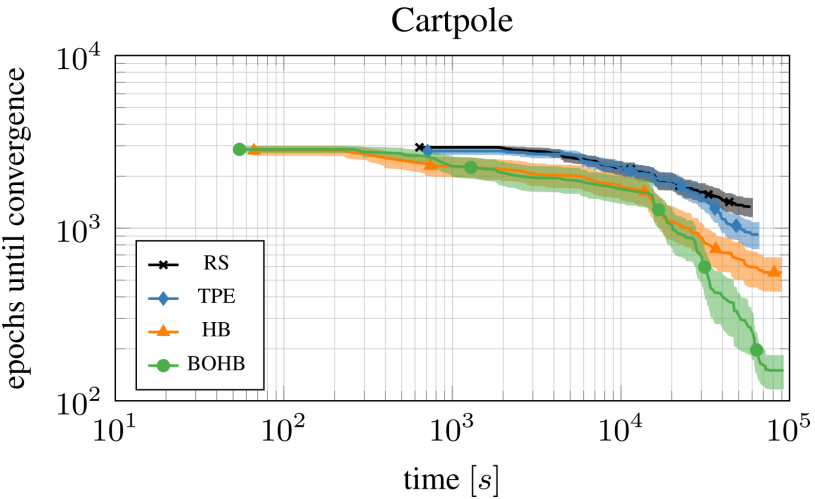

Figure: Hyperparameter optimization of 8 hyperparameters of PPO on the cartpole task.

BOHB: Optimization of an SVM

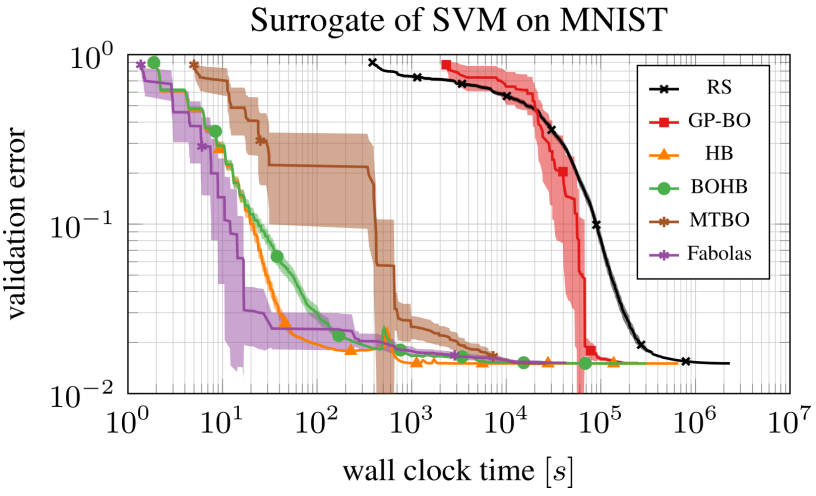

Figure: Comparison on the SVM on MNIST surrogate benchmark

BOHB: Counting Ones

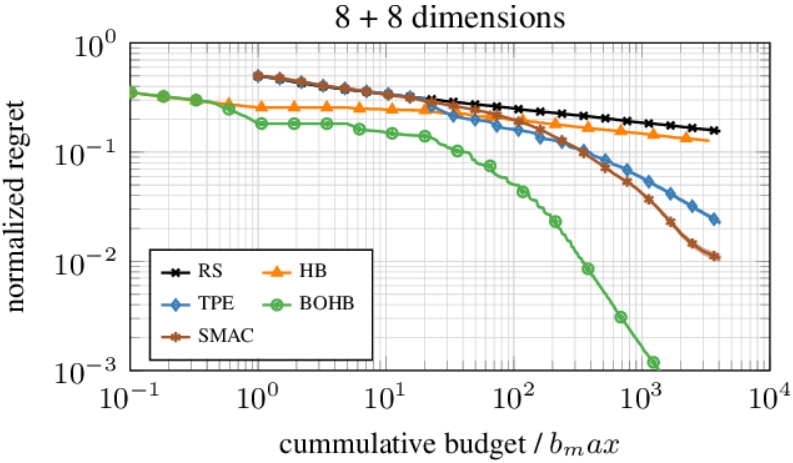

Figure: Results for the counting ones problem in 16 dimensional space with 8 categorical and 8 continuous hyperparameters.

BOHB: Optimization of a Feedforward Network

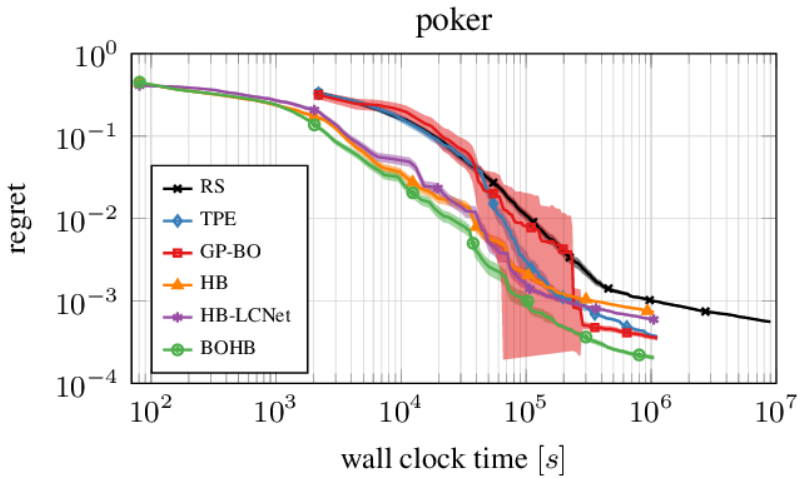

Figure: Optimizing six hyperparameters of a feed-forward neural network on featurized datasets; results are based on surrogate benchmarks.

Questions to Answer for Yourself / Discuss with Friends

- Repetition. Why does BOHB interleave randomly sampled configurations in the optimization process?
- Discussion. What are the advantages of the Parzen estimator model over more advanced models such as random forests or Gaussian processes?

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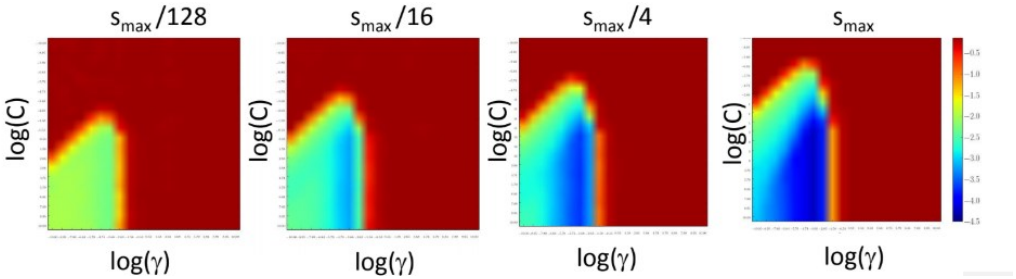
Speedup Techniques for Hyperparameter Optimization

Multi-fidelity Bayesian optimization

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Motivating example

- Performance of an SVM on MNIST and subsets of it:



  - Computational cost grows quadratically in dataset size z
  - Error shrinks smoothly with z
- Evaluations on the smallest subset (about 400 data points) cost $10\,000\times$ less than on the full data set

Idea of Multi-fidelity Bayesian optimization [Kandasamy et al. 2017; Klein et al. 2016]

- Recall: standard Bayesian optimization uses a model $\hat{c}(\boldsymbol{\lambda}) \approx y$ to select the next $\boldsymbol{\lambda}$
- Multi-fidelity Bayesian optimization uses a model $\hat{c}(\boldsymbol{\lambda}, z) \approx y$ to select the next $(\boldsymbol{\lambda}, z)$
  - Here, $z \in \mathcal{Z}$ is the fidelity; $\mathcal{Z}$ is the fidelity space, e.g., $\mathcal{Z} = [1, N_\bullet] \times [1, T_\bullet]$
- Denoting $z_\bullet$ as the maximum fidelity (e.g., $z_\bullet = [N_\bullet, T_\bullet]$), our goal is to find:

$$\boldsymbol{\lambda}^* = \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} f(\boldsymbol{\lambda}) = \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \hat{c}(\boldsymbol{\lambda}, z_\bullet)$$

- Implications for Bayesian optimization
  - Model $\hat{c}$ needs to be good at extrapolating from small to large z
  - Acquisition function now also needs to select z (i.e., take into account cost of evaluations)

Entropy Search: Reminder

- Define the p_{min} distribution given data $\mathcal{D}$:

$$p_{\text{min}}(\boldsymbol{\lambda}^* \mid \mathcal{D}) := p(\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} f(\boldsymbol{\lambda}) \mid \mathcal{D})$$

- Entropy search aims to minimize the entropy $\mathcal{H}[p_{\text{min}}]$ [Hennig and Schuler. 2012]
  - It aims to be maximally certain about the location of $\boldsymbol{\lambda}^*$

- In a nutshell: select $\boldsymbol{\lambda}$ that maximizes the following acquisition function:

$$u_{ES}(\boldsymbol{\lambda}) := \mathcal{H}[p_{\text{min}}(\cdot \mid \mathcal{D})] - \mathbb{E}_{p(\tilde{c}|\boldsymbol{\lambda},\mathcal{D})}\left[\mathcal{H}[p_{\text{min}}(\cdot \mid \mathcal{D} \cup \langle \boldsymbol{\lambda}, \tilde{c} \rangle)]\right]$$

Entropy Search for Multi-Fidelity Optimization [Klein et al. 2017]

- We now care about the p_{min} distribution for the maximal budget $z_\bullet$:

$$p_{\text{min}}(\boldsymbol{\lambda}^* \mid \mathcal{D}) := p(\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} f(\boldsymbol{\lambda}, z_\bullet) \mid \mathcal{D})$$

- We still want to minimize the entropy $\mathcal{H}[p_{\text{min}}]$
- Now we aim for the biggest reduction in entropy per time spent
  - Now we don't model only f, but also the cost $c(\boldsymbol{\lambda}, z)$
  - We choose the next $(\boldsymbol{\lambda}, z)$ by maximizing:

$$u_{ES}(\boldsymbol{\lambda}, z \mid \mathcal{D}) := \mathbb{E}_{p(\tilde{c} \mid (\boldsymbol{\lambda}, z), \mathcal{D})} \left[\frac{\mathcal{H}[p_{\text{min}}(\cdot \mid \mathcal{D})] - \mathcal{H}[p_{\text{min}}(\cdot \mid \mathcal{D} \cup \langle (\boldsymbol{\lambda}, z), \tilde{c} \rangle]}{c(\boldsymbol{\lambda}, z)} \right]$$

Entropy Search for Multi-Fidelity Optimization [Klein et al. 2017]

- The entire algorithm iterates the following 2 steps until time is up:
  1. Select $(\boldsymbol{\lambda}, z)$ by maximizing:

$$u_{ES}(\boldsymbol{\lambda}, z \mid \mathcal{D}) := \mathbb{E}_{p(\tilde{c}|(\boldsymbol{\lambda},z),\mathcal{D})}\left[\frac{\mathcal{H}[p_{\min}(\cdot \mid \mathcal{D})] - \mathcal{H}[p_{\min}(\cdot \mid \mathcal{D} \cup \langle(\boldsymbol{\lambda}, z), \tilde{c}\rangle}{c(\boldsymbol{\lambda}, z)}\right]$$

  2. Observe performance $f(\boldsymbol{\lambda}, z)$ and cost $c(\boldsymbol{\lambda}, z)$ and update models for f and c
- The algorithm originally focussed on data subsets and is therefore dubbed Fabolas: "Fast Bayesian Optimization on Large Datasets"

Advantages

- Conceptually beautiful
- 1 000-fold speedups for optimizing SVMs on MNIST

Disadvantages

- Scalability of GPs is a big problem (limits size of initial design)
- Limited applicability of Gaussian processes

Questions to Answer for Yourself / Discuss with Friends

- Discussion. What kind of cost model would you use in Fabolas?
- Discussion. Could one use an acquisition function other than entropy search for Fabolas?

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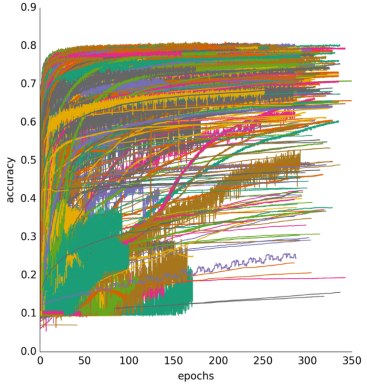
Speedup Techniques for Hyperparameter Optimization

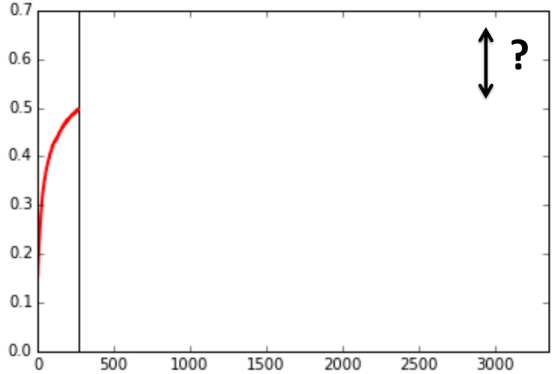
Predicting Learning Curves

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Learning Curves

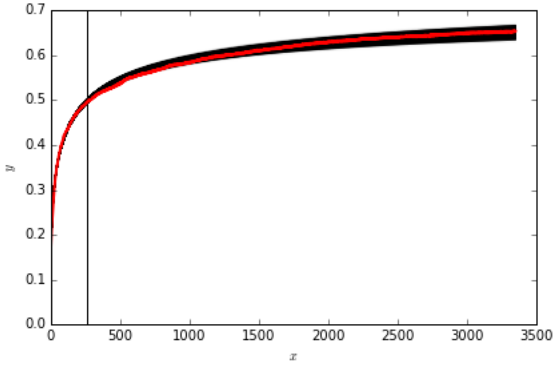


Learning Curve Predictions



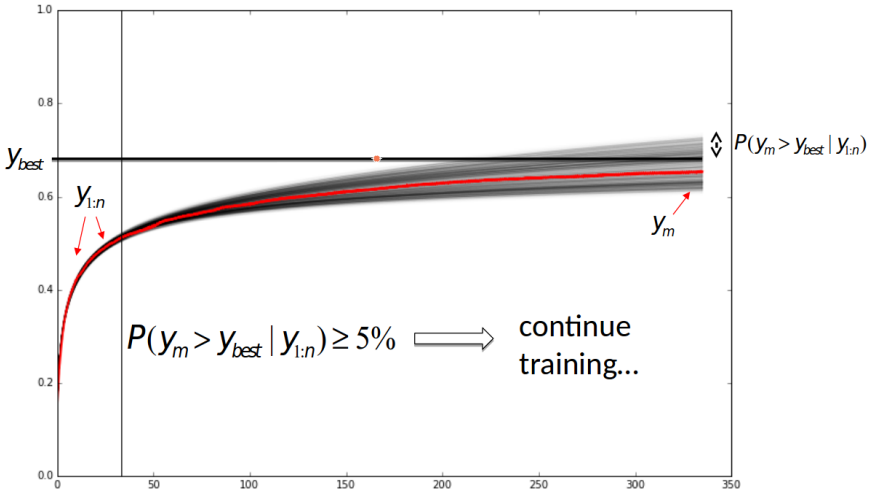
1. Observe learning curve for the first n steps (here $n = 250$)
2. Extrapolation: fit parametric model on partial learning curve to predict remaining learning curve
   - Various models can be used (see following slides)

Learning Curve Predictions



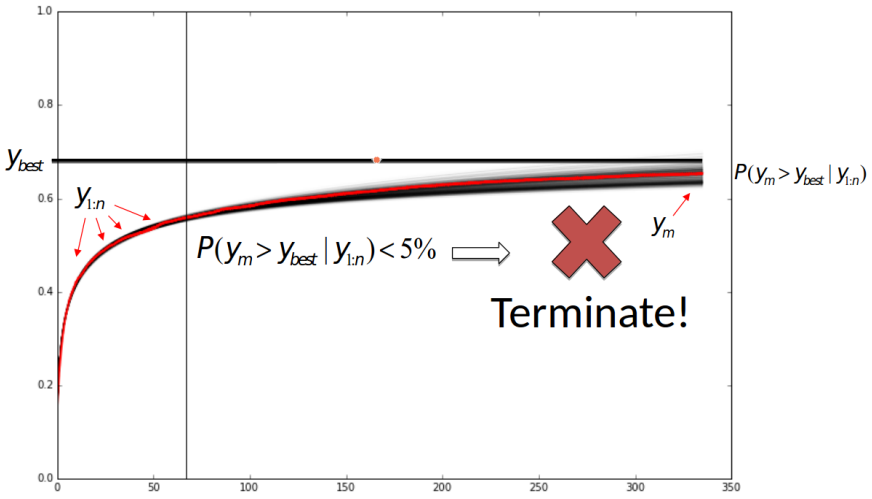
1. Observe learning curve for the first n steps (here $n = 250$)
2. Extrapolation: fit parametric model on partial learning curve to predict remaining learning curve
   - Various models can be used (see following slides)

Learning Curves: Early Termination



$\rightarrow$ need for probabilistic predictions / quantification of uncertainty

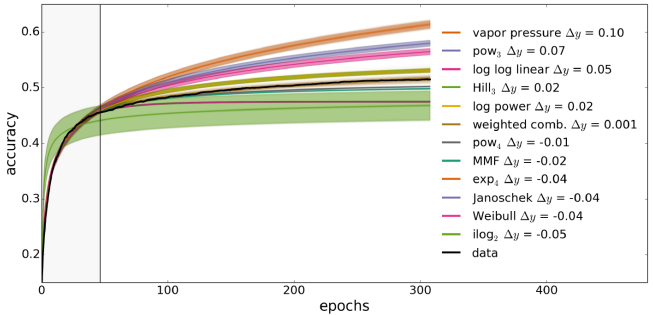
Learning Curves: Early Termination



$\rightarrow$ need for probabilistic predictions / quantification of uncertainty

Parametric Learning Curves [Domhan et al. 2015]

- Use a parametric model f_k with parameters $\boldsymbol{\theta}$ to model performance at step t as: $y_t = f_k(t|\boldsymbol{\theta}) + \epsilon$, with $\epsilon \sim \mathcal{N}(0, \sigma^2)$.
- Linear combination of $K = 11$ parametric types of models: $f_{comb}(t|\boldsymbol{\xi}) = \sum_{k=1}^{K} w_k f_k(t|\boldsymbol{\theta}_k)$, where $\boldsymbol{\xi} = (w_1, \ldots, w_K, \boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K, \sigma^2)$

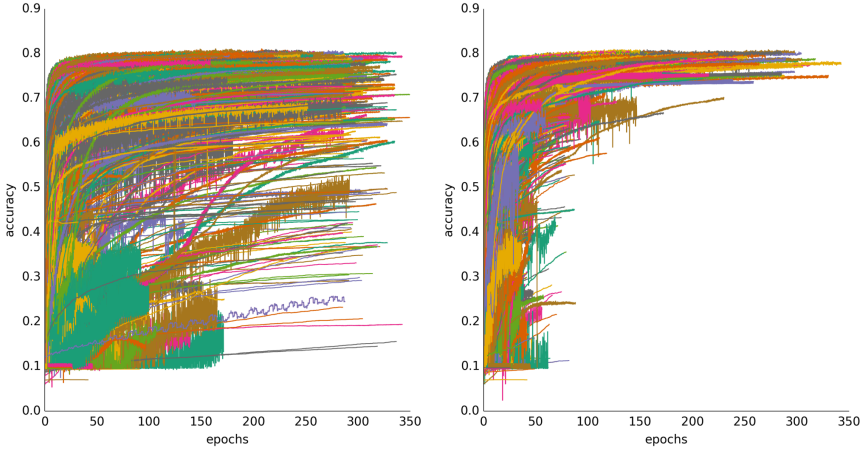


Reference name	Formula
vapor pressure	$\exp(a + \frac{b}{x} + c\log(x))$
pow_3	$c - ax^{-\alpha}$
log log linear	$\log(a\log(x) + b)$
Hill_3	$\frac{y_{\max} x^\eta}{\kappa^\eta + x^\eta}$
log power	$\frac{a}{1+\left(\frac{x}{e^b}\right)^c}$
pow_4	$c - (ax + b)^{-\alpha}$
MMF	$\alpha - \frac{\alpha - \beta}{1 + (\kappa x)^\delta}$
exp_4	$c - e^{-ax^\alpha + b}$
Janoschek	$\alpha - (\alpha - \beta)e^{-\kappa x^\delta}$
Weibull	$\alpha - (\alpha - \beta)e^{-(\kappa x)^\delta}$
ilog_2	$c - \frac{a}{\log x}$

$K = 11$ parametric families for modelling learning curves

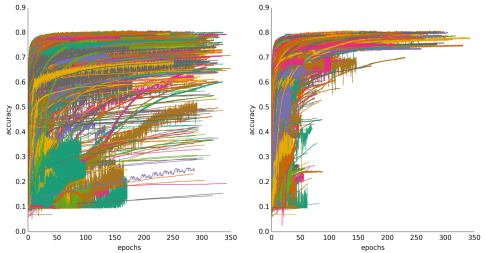
- Use Markov Chain Monte Carlo sampling of $\boldsymbol{\xi}$ to obtain uncertainties

Predictive Termination



All learning curves vs. learning curves with early termination

Predictive Termination



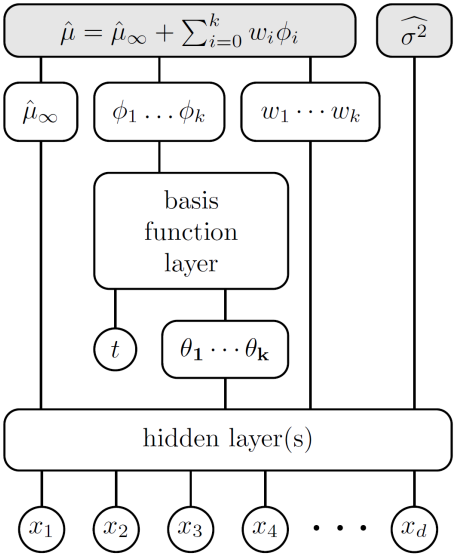
All learning curves vs. learning curves with early termination

- Disadvantages of this model?
  - Relies on manually-selected parametric families of curves
  - Does not take into account hyperparameters used

    → can't learn across hyperparameters

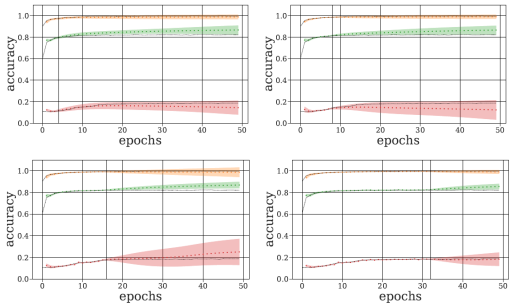
LC-Net [Klein et al. 2017]

- Make a layer out of the parametric learning curves by Domhan et al.
- Also support hyperparameters as inputs (in the figure denoted by $x_1, \ldots, x_d$)
- Disadvantages of this model?
  - Relies on manually-selected parametric families of curves
  - Cannot quickly integrate new information from extending the current curve (or from new runs)
  - Also, the model is very hard to train



Sequence Models (e.g., Bayesian RNN) [Gargiani et al. 2019]

- Learning curves are sequences
  - Previous models don't treat them like this
  - We can use an RNN (in particular, an LSTM) to predict the next value from a given sequence
  - We can use variational dropout to obtain uncertainty estimates:



Note: we can also use a simpler model

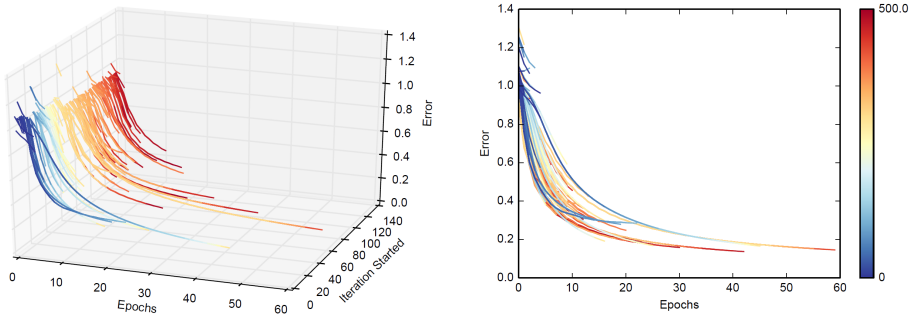
- E.g., a random forest to map from a fixed-size window to the next value

Compare: Baker et al, 2017 [Baker et al. 2018]

- Idea: map from configurations (including architectural hyperparameters) and partial learning curves to the final performance
- Advantages
  - Much simpler idea than all the approaches just discussed: no need to model the entire learning curve
  - Much easier to implement
- Disadvantage? $\rightarrow$ requires many (e.g., 100) fully-evaluated learning curves as training data
  - After 100 full function evaluations we want to be pretty much converged in practice
  - But definitely helpful for speeding up RL

Freeze-Thaw Bayesian Optimization [Swersky et al. 2014]

- Use a Gaussian process with inputs $\boldsymbol{\lambda}$ and t; special kernel for t
- For N configurations and T epochs each: $O(N^3t^3) \rightarrow$ approximation
- Iteratively: either extend existing configuration or try new one
- Result for probabilistic matrix factorization:



- Unfortunately, no results for DNNs; no code available

Questions to Answer for Yourself / Discuss with Friends

- Repetition. List all learning curve prediction methods you recall, along with their pros and cons.
- Discussion. Could predictive termination cut off evaluations early that would turn out to be the best?
- Discussion. How would you determine a learning curve prediction method's own hyperparameters (such as the 5% for early learning curve termination), in practice?
- Discussion. How could we exploit additional side information we gain about the learning curve, such as, e.g., statistics for the size of the gradients and activations over time?

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Success Stories and Practical Recommendations

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Large-scale Meta-Learning for HPO in Industry (Facebook)

- Facebook has an internal self-service machine learning (ML) system
  - Non-ML departments can integrate highly optimized ML models into their workflow
  - Hyperparameters of the ML models are optimized with Bayesian optimization
- Training data for the models changes over time
  - Hyperparameters are constantly re-optimized
  - For efficiency: meta-learning Bayesian optimization, as described in [Feurer et al. 2018]

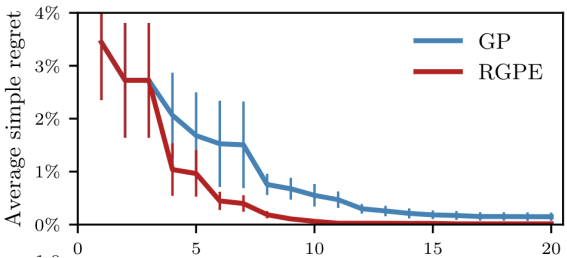
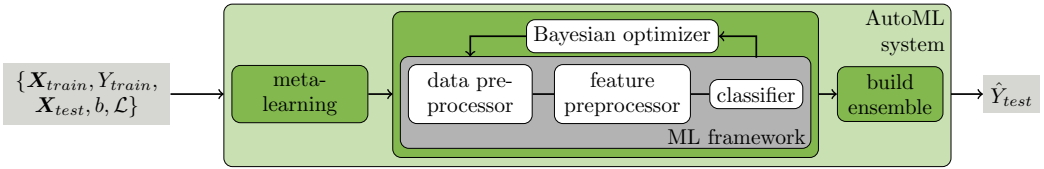


Figure: Bayesian optimization with meta-learning (RGPE) vs. vanilla Bayesian optimization (GP)

Auto-sklearn [Feurer et al. 2015]

Extension of Auto-WEKA with focus on speed improvements and robustness:



- Uses meta-learning to warmstart Bayesian optimization
- Won the 1st AutoML challenge
- Open source (BSD) and trivial to use

Used by 82 | Watch 211 | Star 4.5k | Fork 866

```
>>> import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

Available at `https://automl.github.io/auto-sklearn`; frequently used in industry

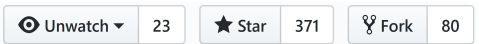
BOHB [Falkner et al. 2018]

- Robust and efficient
- Only published in 2018, adopted by the community very quickly

Scholar articles

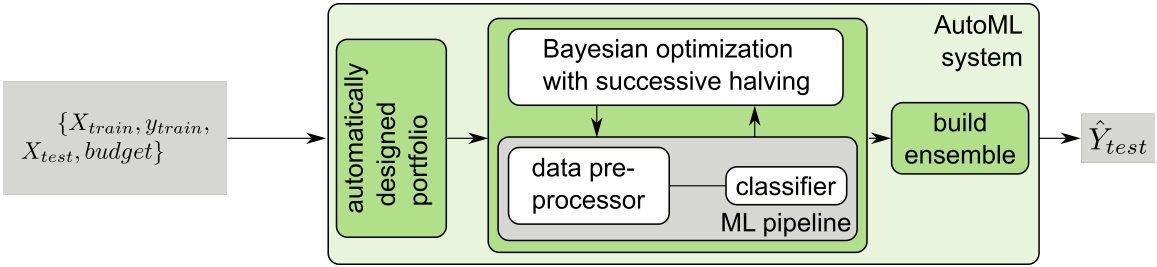
BOHB: Robust and efficient hyperparameter optimization at scale
S Falkner, A Klein, F Hutter - arXiv preprint arXiv:1807.01774, 2018
Cited by 129 Related articles All 8 versions

- Available at `https://github.com/automl/HpBandSter`



PoSH-Auto-sklearn [Feurer et al. 2018]

Idea: integrate warmstarting and a BOHB-like approach for Auto-sklearn



- Uses task-independent meta-learning to warmstart Bayesian optimization
  - Therefore, no need for (potentially unreliable) meta-features
- Uses successive halving to quickly go through proposed configurations
  - Therefore, scales better to larger datasets
- Followed by BOHB-like approach (uses successive halving instead of Hyperband)
- Won the 2nd AutoML challenge

Auto-sklearn 2.0

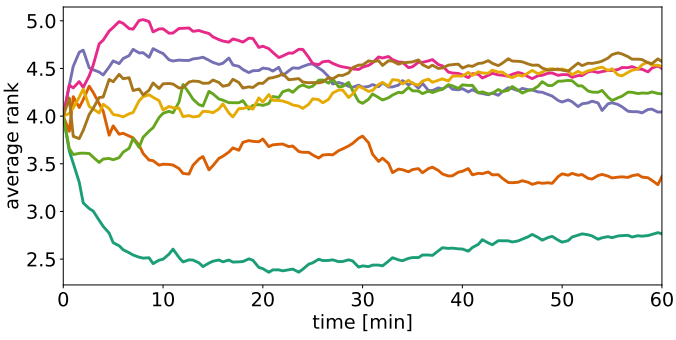
- Idea: automatically choose on a per-dataset basis
  - holdout or cross-validation
  - optimization on the full budget or optimization with successive halving

Auto-sklearn 2.0

- Idea: automatically choose on a per-dataset basis
  - holdout or cross-validation
  - optimization on the full budget or optimization with successive halving
- Can be done based on algorithm selection

Auto-sklearn 2.0

- Idea: automatically choose on a per-dataset basis
  - holdout or cross-validation
  - optimization on the full budget or optimization with successive halving
- Can be done based on algorithm selection
- Substantial improvements over Auto-sklearn 1.0
  - $5\times$ reduction of average error
  - $6\times$ speedup (same performance in 10 minutes as Auto-sklearn 1.0 in 1 hour)



Practical Recommendations Which HPO Method to Use [Feurer and Hutter. 2019]

- If multiple fidelities available: BOHB [Falkner et al. 2018]
- Otherwise
  - Low-dimensional continuous parameter space:
    - ⋆ GP-based BO, e.g., Spearmint [Snoek et al. 2012]
  - High-dimensional discrete parameter space:
    - ⋆ RF-based BO, e.g., SMAC [Hutter et al. 2011]
  - Purely continuous, cheap function evaluations:
    - ⋆ CMA-ES [Hansen et al. 2001]; evaluated for HPO by [Loshchilov and Hutter. 2016]
- Just submitted: DEHB combines differential evolution and Hyperband and largely dominates BOHB. Especially good for high dimensions.

Questions to Answer for Yourself / Discuss with Friends

- Repetition. Discuss several success stories of speeding up Bayesian optimization.
- Repetition. What differs between Auto-sklearn 1.0 and Auto-sklearn 2.0?

Further Reading

Survey on hyperparameter optimization: [Feurer and Hutter. 2019]