

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

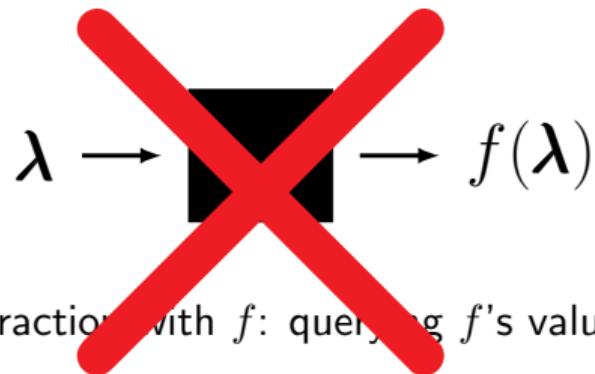
Speedup Techniques for Hyperparameter Optimization

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 λ

Too slow for tuning expensive models

Methods for Going Beyond Blackbox Bayesian Optimization

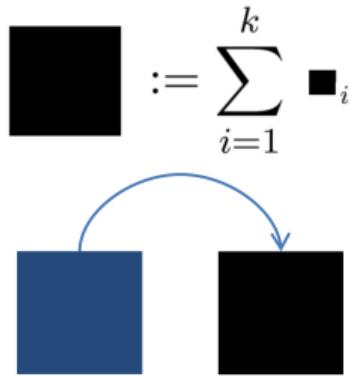
- Sum of little black boxes

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

$$\blacksquare := \sum_{i=1}^k \blacksquare_i$$

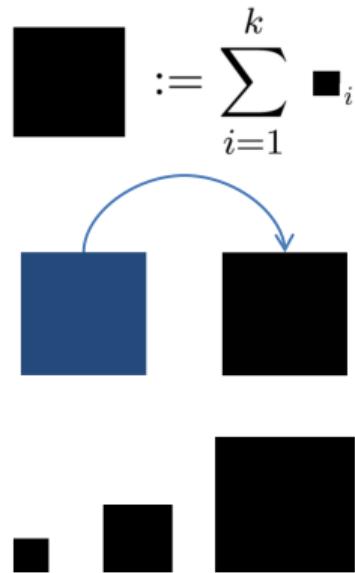
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- Meta-learning across problems / datasets



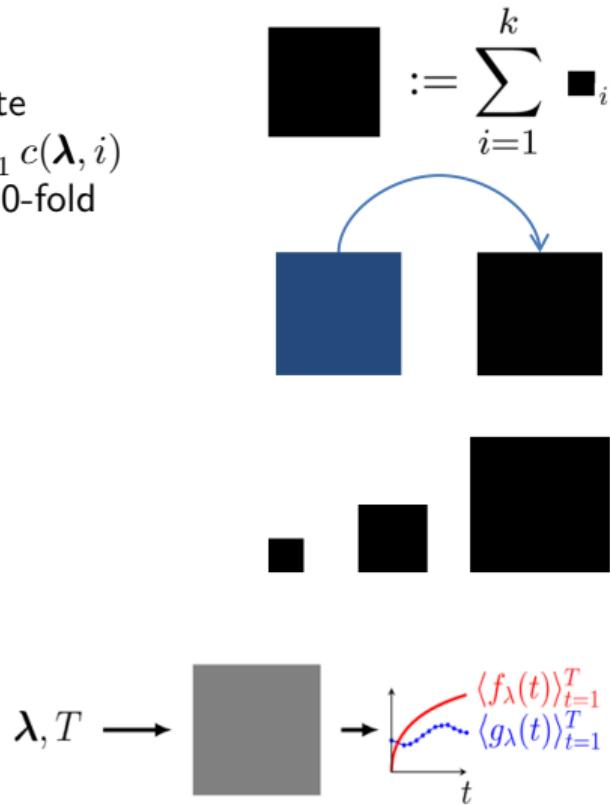
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- Meta-learning across problems / datasets
- Multi-fidelity optimization



Methods for Going Beyond Blackbox Bayesian 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

Outline

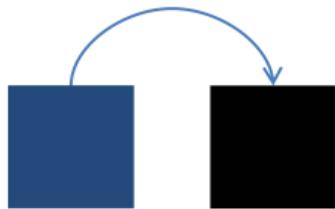
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Speedup Techniques for Hyperparameter Optimization

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}_{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}_{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:

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

- 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

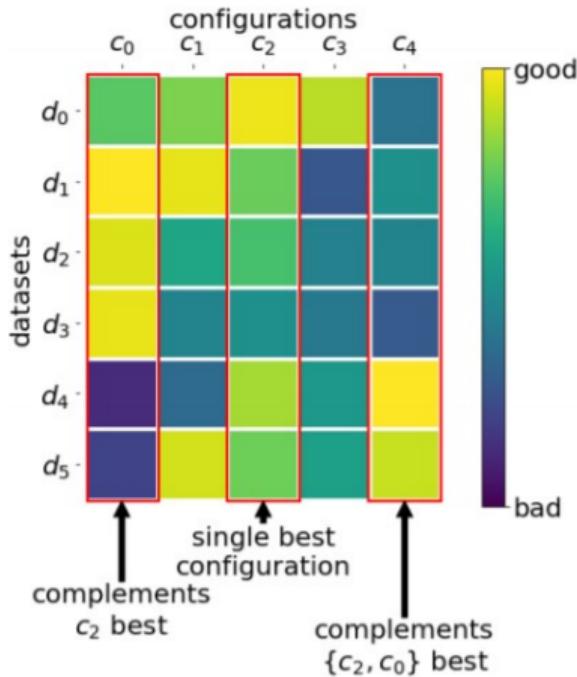
- Experts often start HPO from a strong default (rather than random configurations)
- Can we learn from meta-data $\mathcal{D}_{\text{meta}}$ how to [initialize](#) HPO?
- Note: just a single default configuration often does not perform great on a new dataset
 - ▶ Otherwise there would be no point in 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 $\hat{c}_{\mathcal{D}_i} : \Lambda \rightarrow \mathbb{R}$ 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. 2015a], [Feurer et al. 2018], [Pfisterer et al. 2018]

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

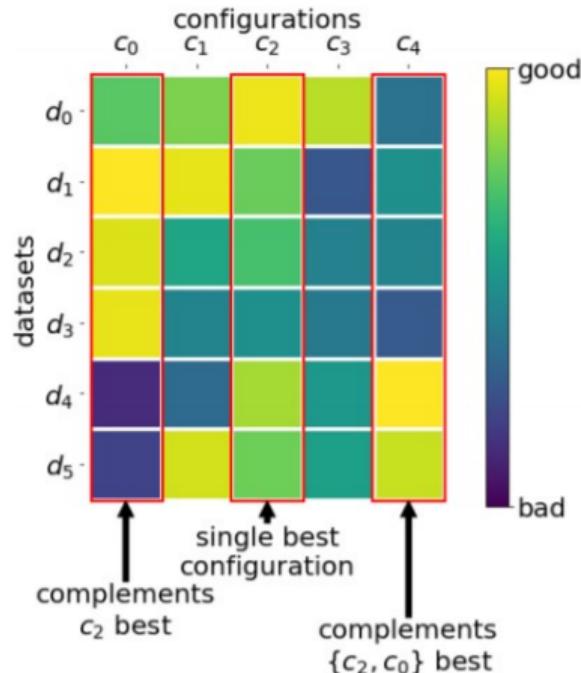
- Idea: learn a sorted list of defaults
- Method: mostly greedy on $\mathcal{T}_{\text{meta}}$
- Results: surprisingly strong,
better than Bayesian Optimization

Advantages

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

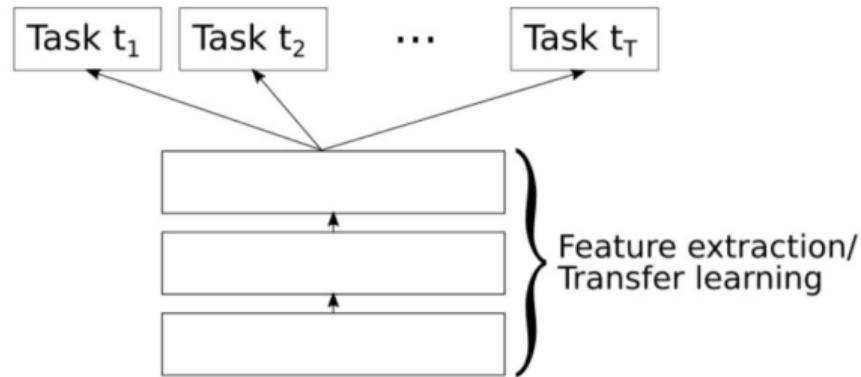
Disadvantages

- Not adaptive



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

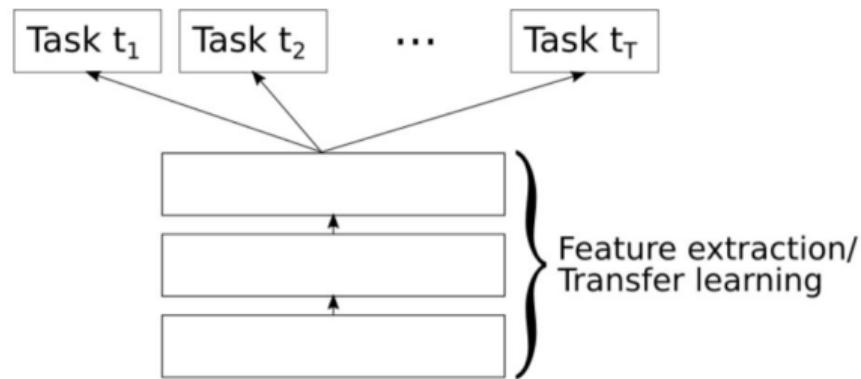
- Jointly train a “deep” neural network **on all tasks**



[Perrone et al. 2018]

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

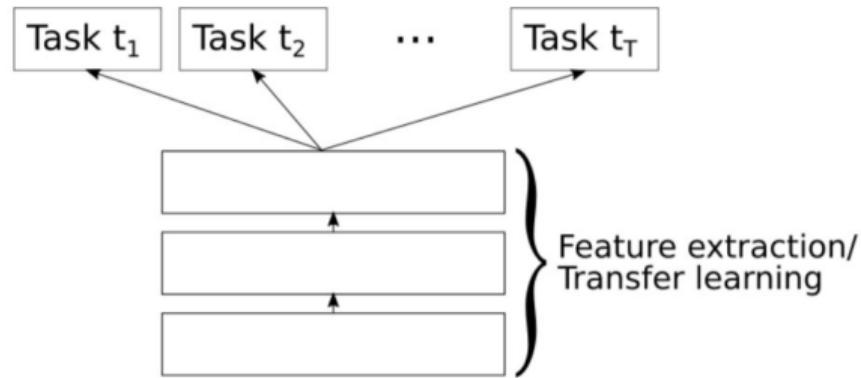
- **Jointly train a “deep” neural network **on all tasks****
 - ▶ Have a separate output layer (head) for each task
 - ▶ Each head is a Bayesian linear regression (recall DNGO)



[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)
- 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}_{new} to the next configuration λ to evaluate
 - ▶ This mapping can be a (recurrent) neural net $\text{NN}_\phi : \mathcal{D}_{\text{new}} \mapsto \lambda$ 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. 2017]
 - ★ 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 & 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. 2020]
- Two options:
 - ▶ Only depend on predicted mean and variance: $u_\phi(\lambda) = u_\phi(\mu_t(\lambda), \sigma_t(\lambda))$
 - ★ This allows to learn a general acquisition function
 - ▶ Also depend on the λ value: $u_\phi(\lambda) = u_\phi(\mu_t(\lambda), \sigma_t(\lambda), \lambda)$
 - ★ 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



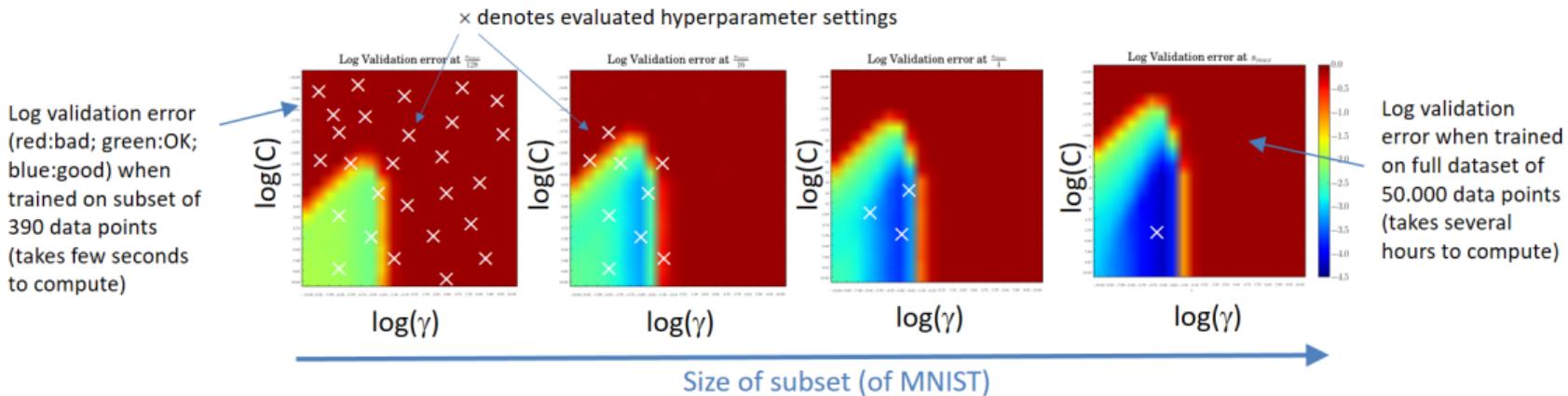
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- E.g.: Support Vector Machines (SVM) on MNIST dataset (hyperparameters: C , γ)



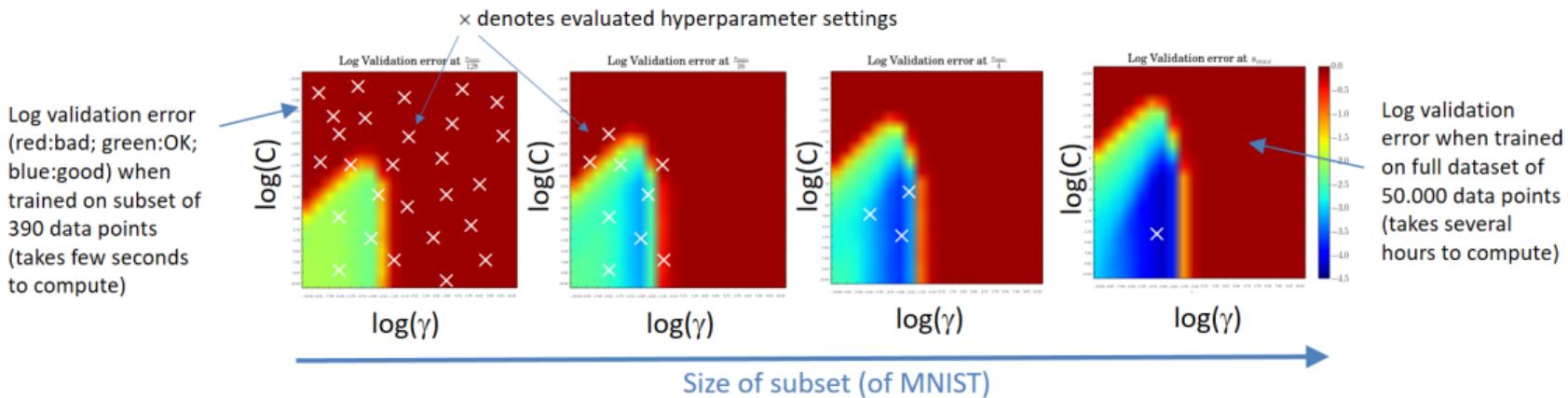
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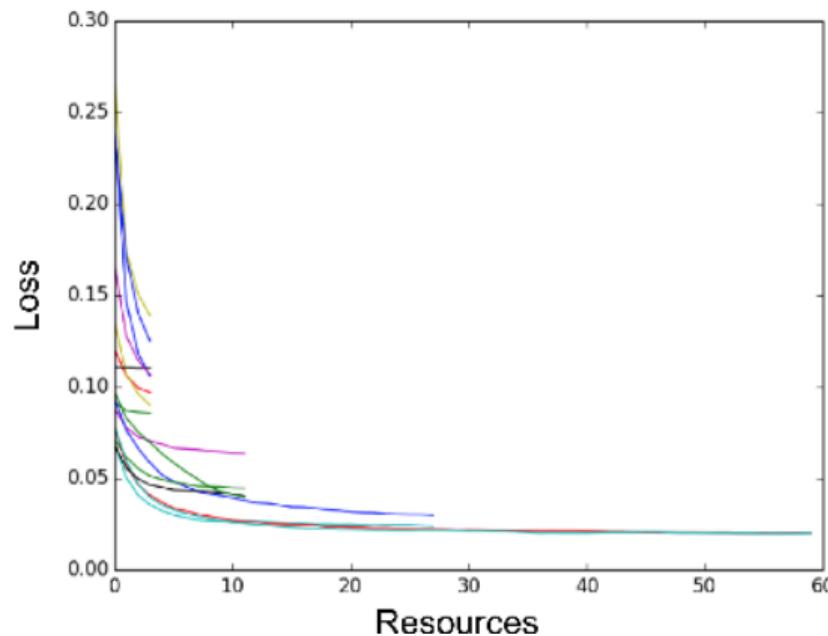
- E.g.: Support Vector Machines (SVM) on MNIST dataset (hyperparameters: C , γ)



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

Motivating Example 2: Shorter Runs of Anytime Algorithms

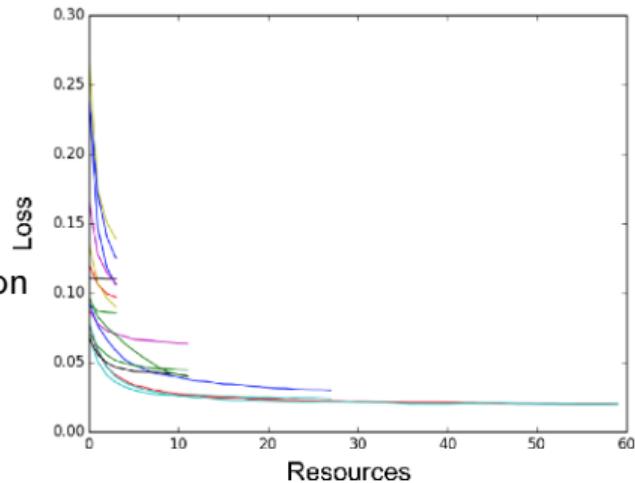
- Performance with shorter runs of an anytime algorithm (such as SGD):



Multi-Fidelity Optimization In General

Exploit cheap approximations of an expensive blackbox function → 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 $\Lambda = \{\lambda_1, \dots, \lambda_n\}$
- The performances $f(\lambda_1), \dots, f(\lambda_n)$ on the expensive black box
- The performances $g(\lambda_1), \dots, g(\lambda_n)$ on a cheap approximation of the black box

We compute the **Spearman rank correlation** between $[f(\lambda_1), \dots, f(\lambda_n)]$ and $[g(\lambda_1), \dots, g(\lambda_n)]$

- 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

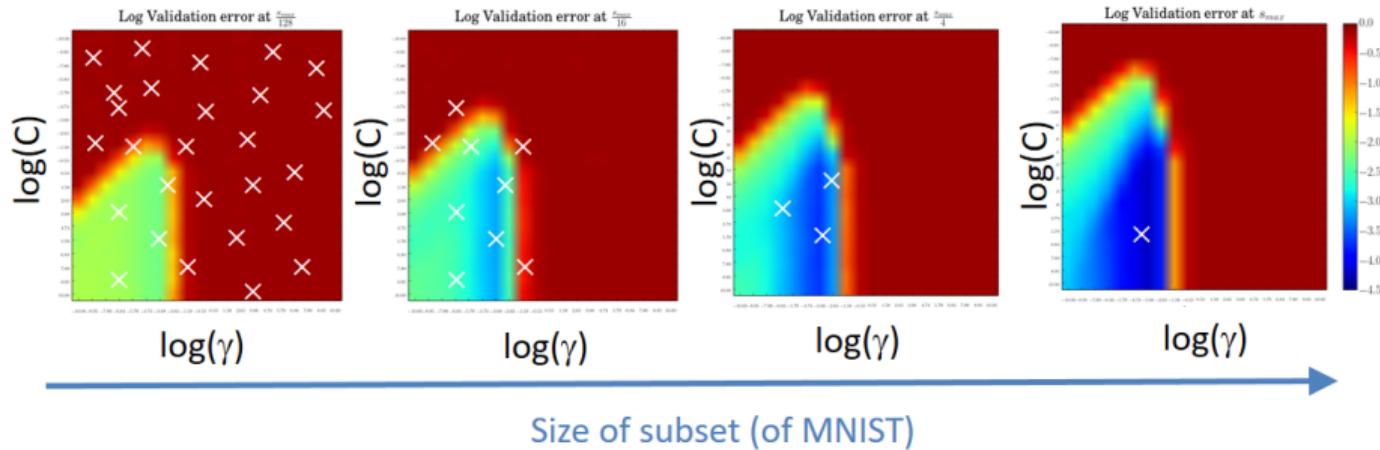
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A Simple Multi-Fidelity Algorithms: Successive Halving (SH)

[Jamieson and Talwalkar, AISTATS 2016]

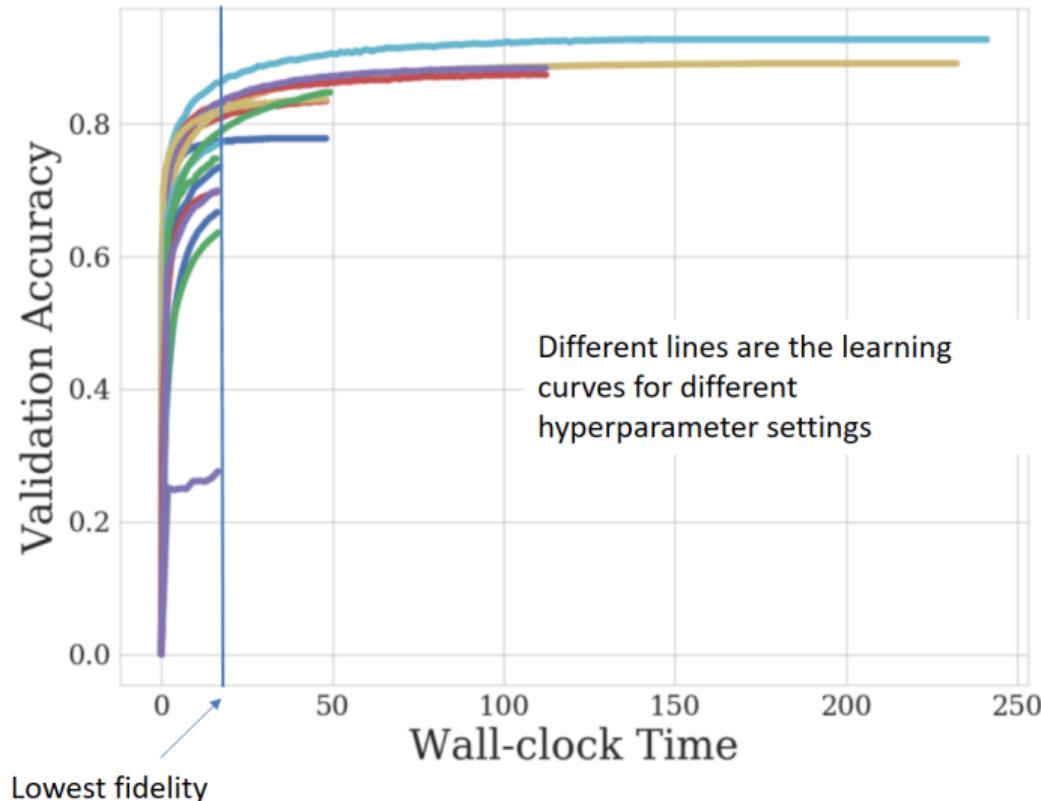
- A very simple algorithm:

- ▶ 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

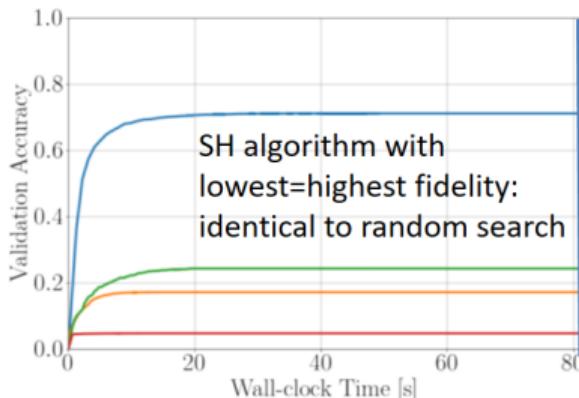
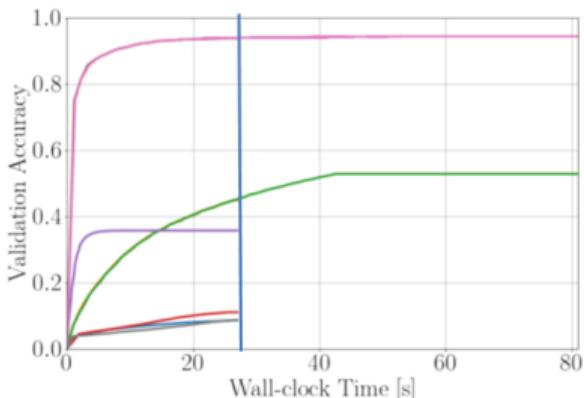
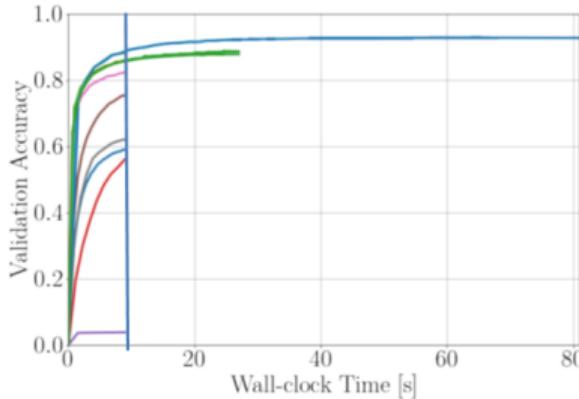
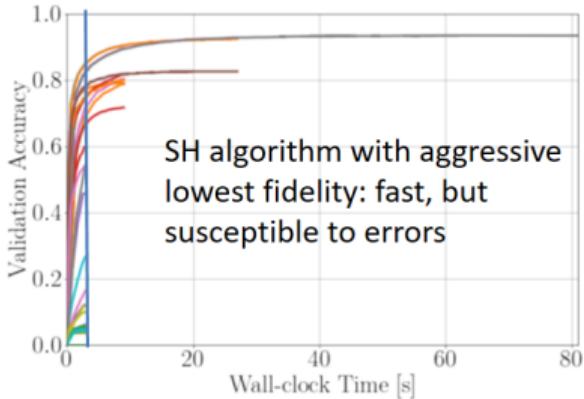
[Jamieson and Talwalkar, AISTATS 2016]



An Extension of SH with Theoretical Guarantees: Hyperband

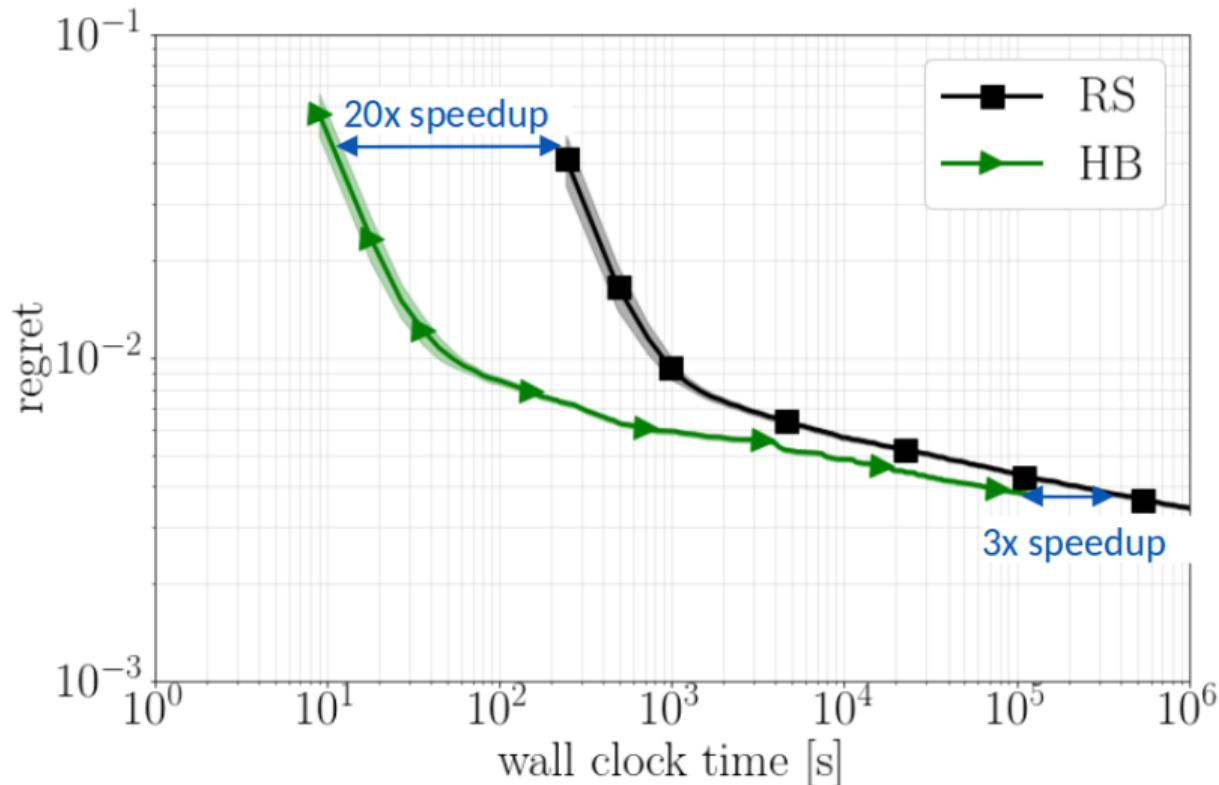
[Li et al., JMLR 2018]

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



Empirical Evaluation: Hyperband vs. Random Search

[Falkner, Klein & Hutter, ICML 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 hyperparameter 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 [Falkner, Klein and Hutter, ICML 2018] combines Bayesian Optimization with Hyperband

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

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

$$l(\lambda) = p(c(\lambda) \leq \gamma | D_b) \quad g(\lambda) = p(c(\lambda) > \gamma | D_b) \quad (1)$$

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

BOHB: Empirical Evaluation

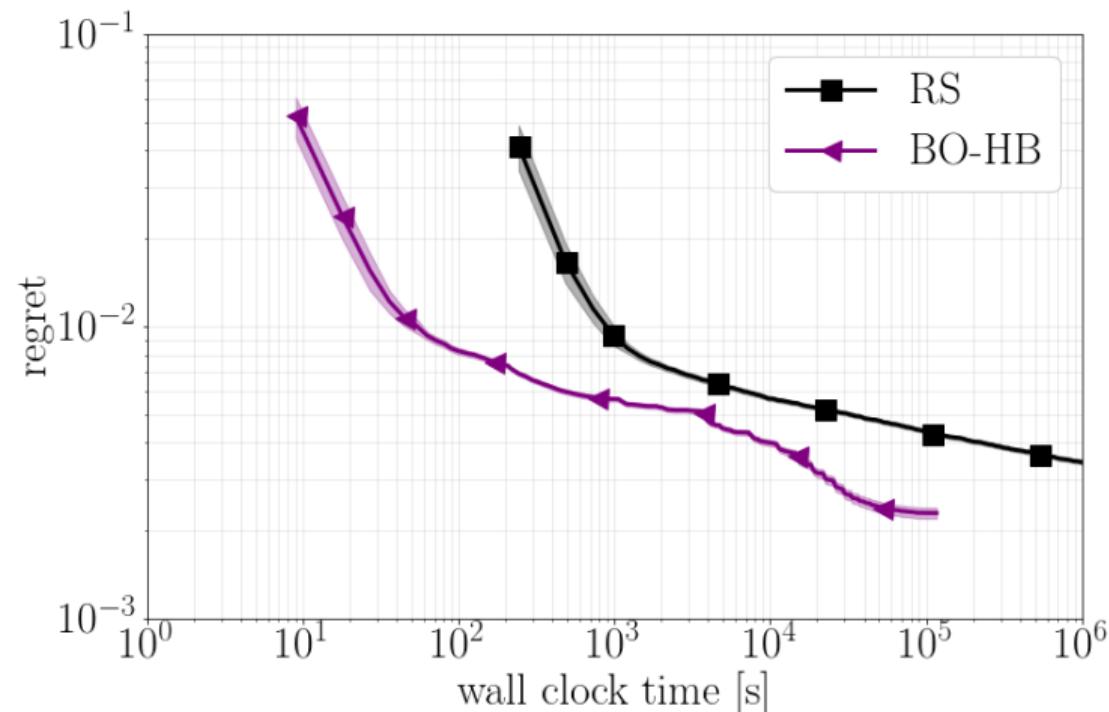


Figure: Performance of RS and BOHB on Auto-Net on dataset Adult

BOHB: Empirical Evaluation

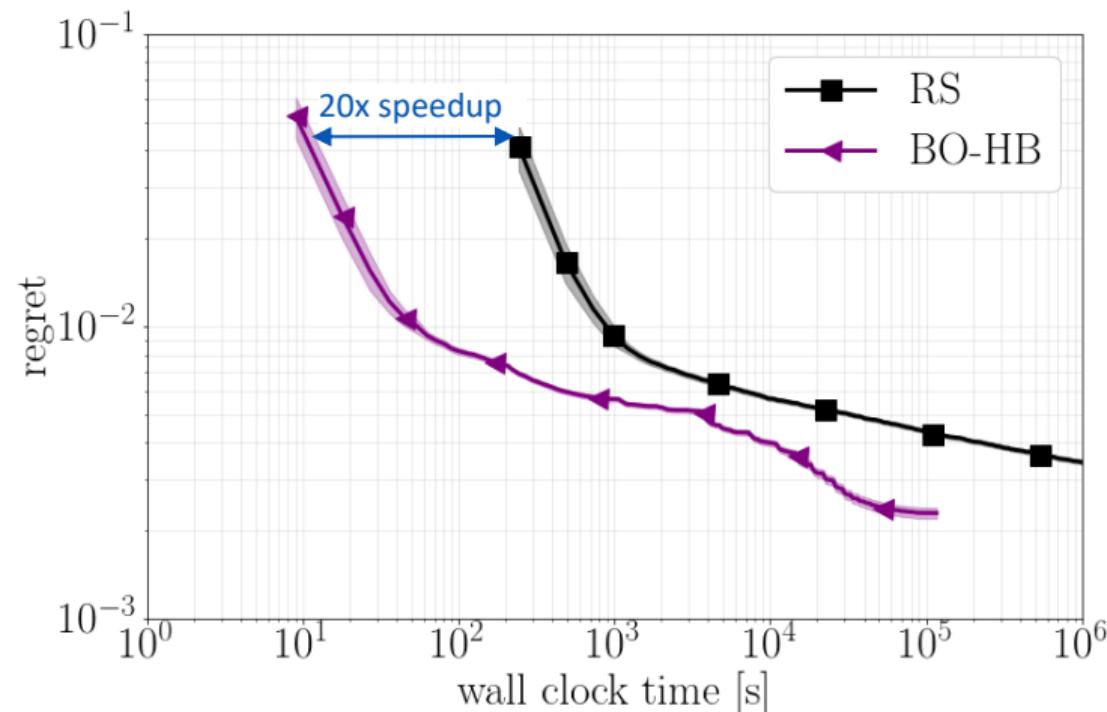


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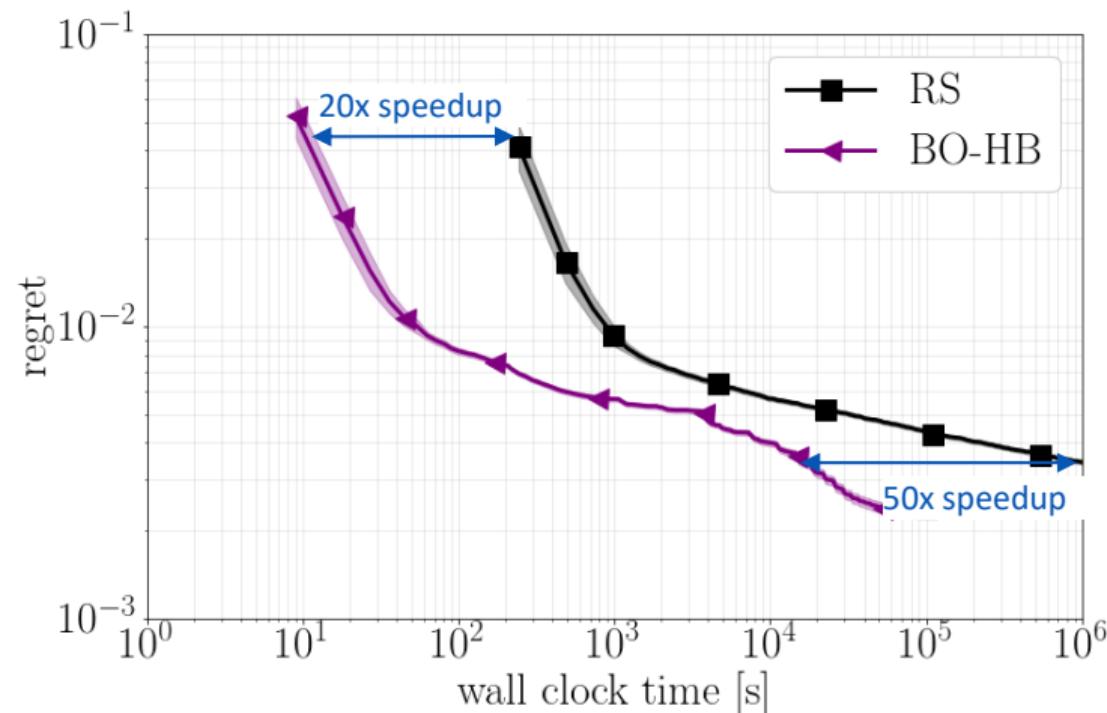


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BOHB: Empirical Evaluation

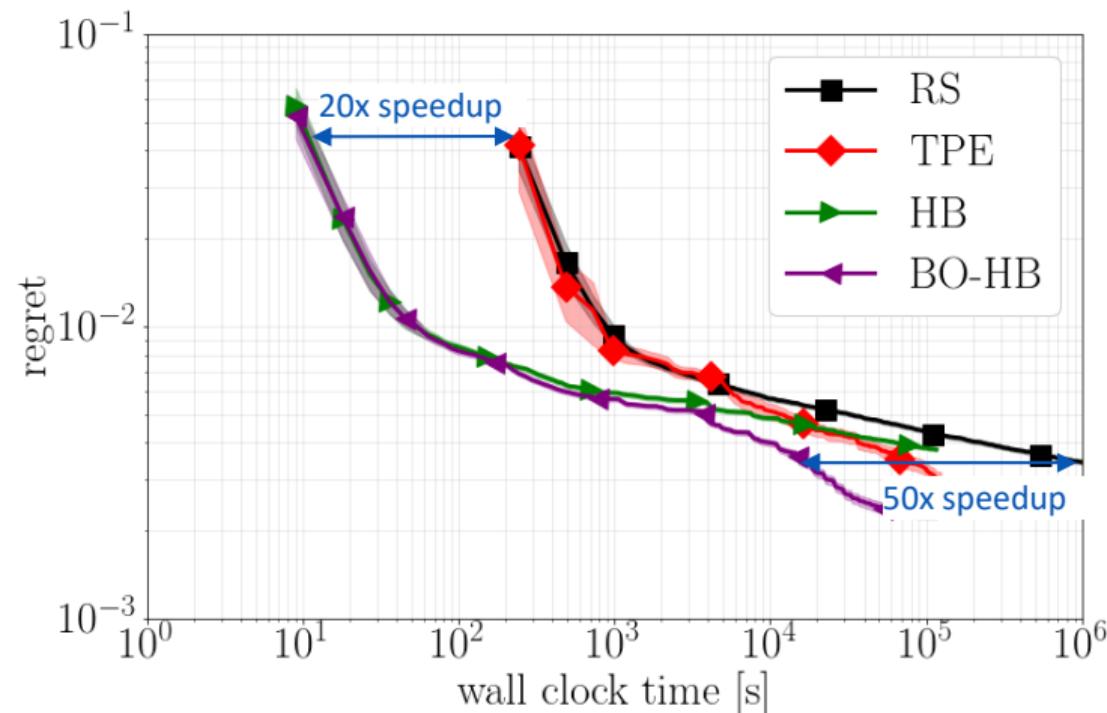


Figure: Performance of RS, TPE, HB and BOHB on Auto-Net on dataset Adult

BOHB: Different number of parallel workers

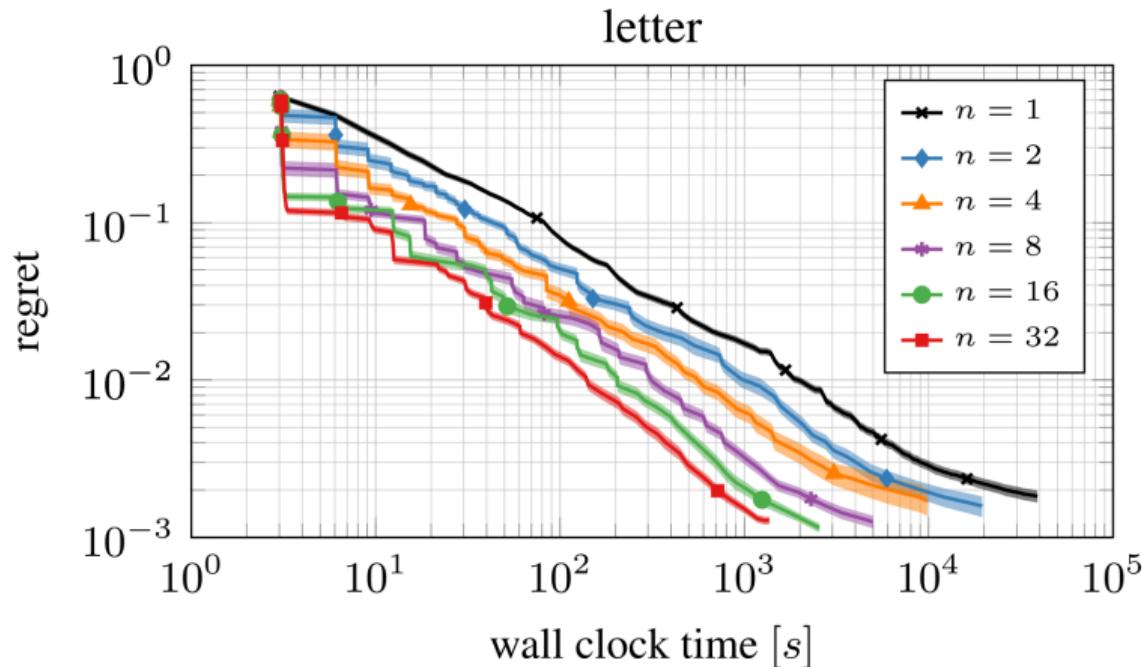


Figure: Performance of BOHB with different number of parallel workers on the letter surrogate benchmark for 128 iterations

BOHB: Optimization of a Bayesian Neural Network

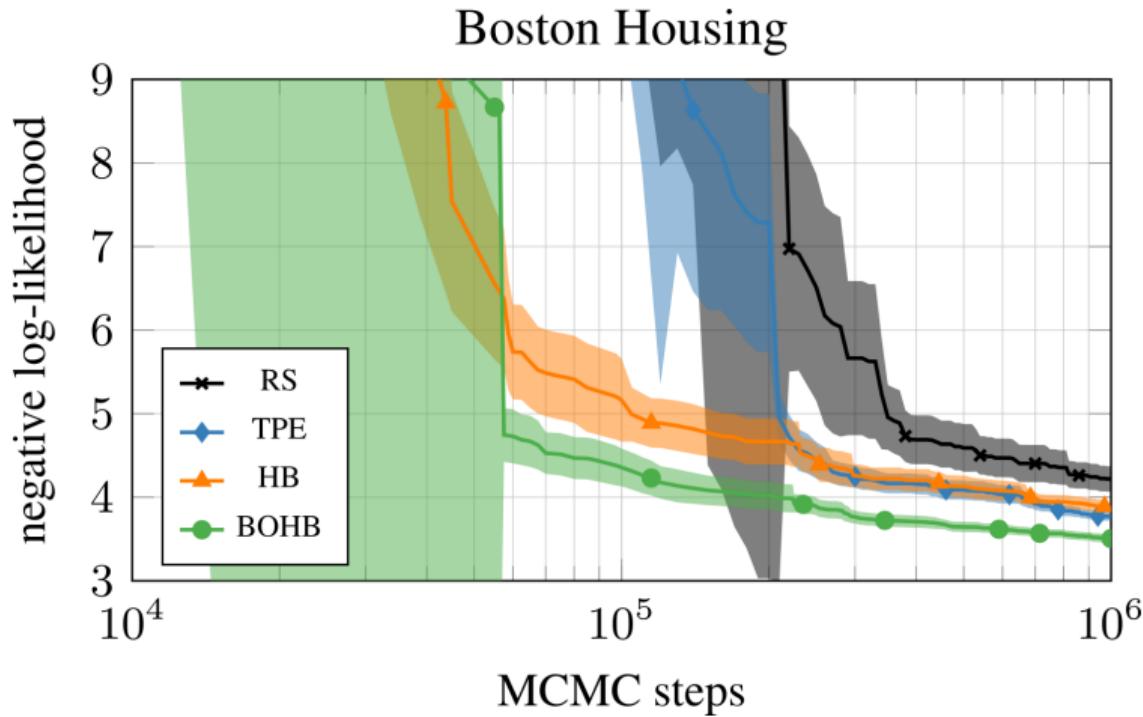


Figure: Optimization of 5 hyperparameters of a Bayesian neural network trained with SGHMC.

BOHB: Optimization of a Reinforcement Learning Agent

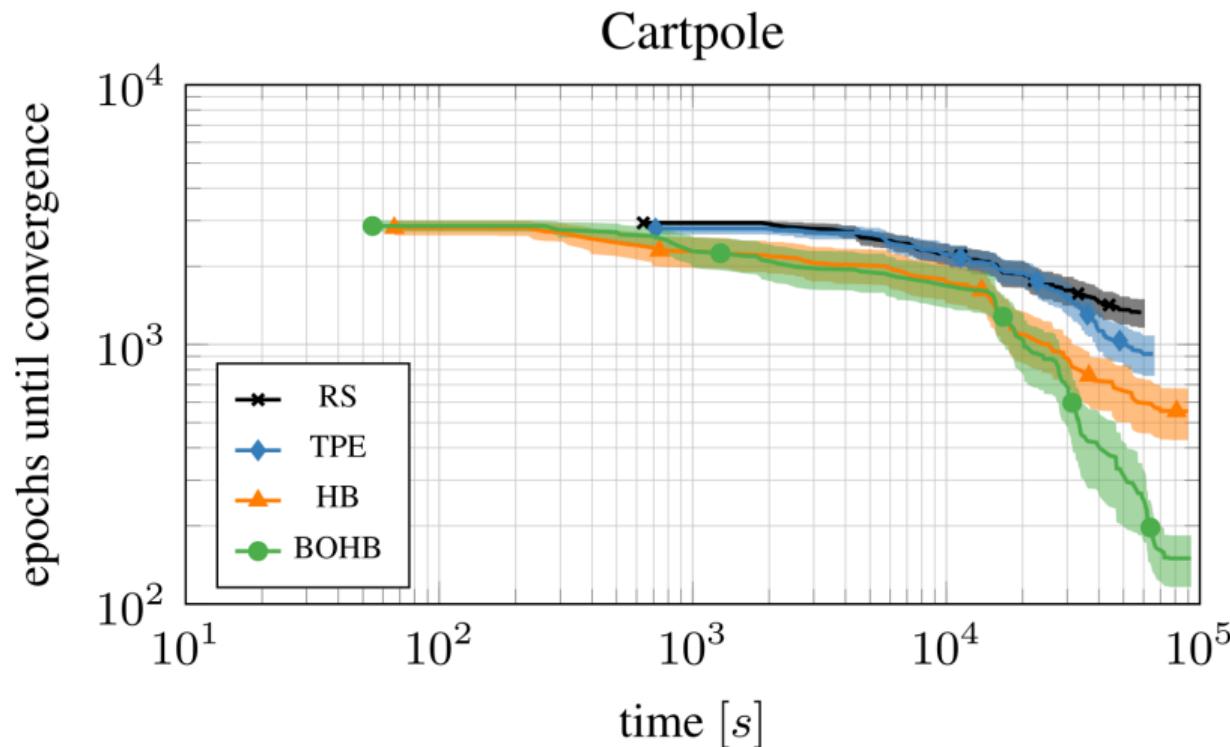


Figure: Hyperparameter optimization of 8 hyperparameters of PPO on the cartpole task.

BOHB: Optimization of an SVM

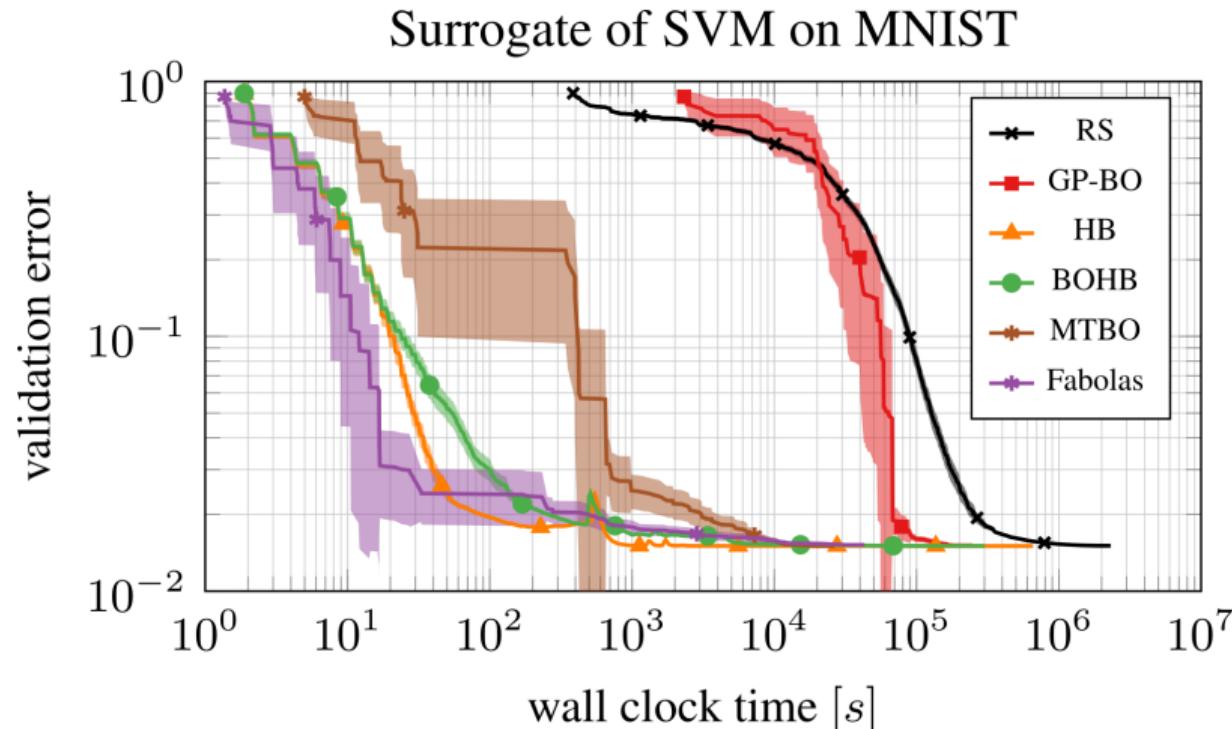


Figure: Comparison on the SVM on MNIST surrogate benchmark

BOHB: Counting Ones

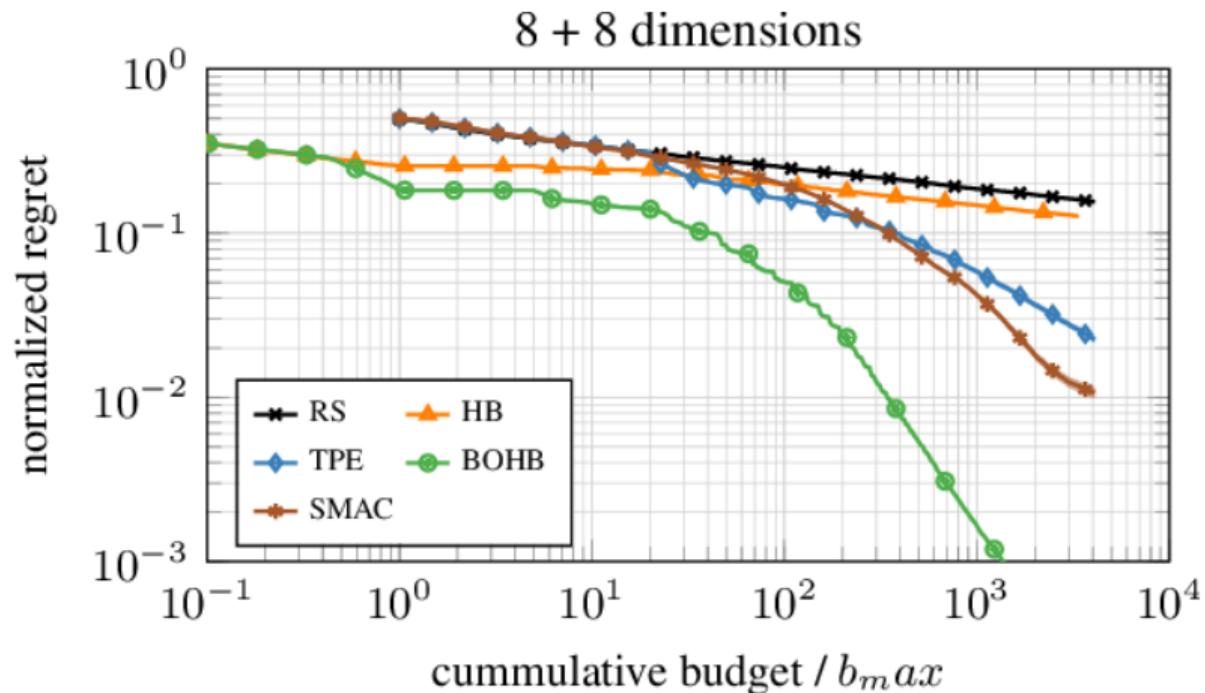


Figure: Results for the counting ones problem in 16 dimensional space with 8 categorical and 8 continuous hyperparameters.

BOHB: Optimization of a Feedforward Network

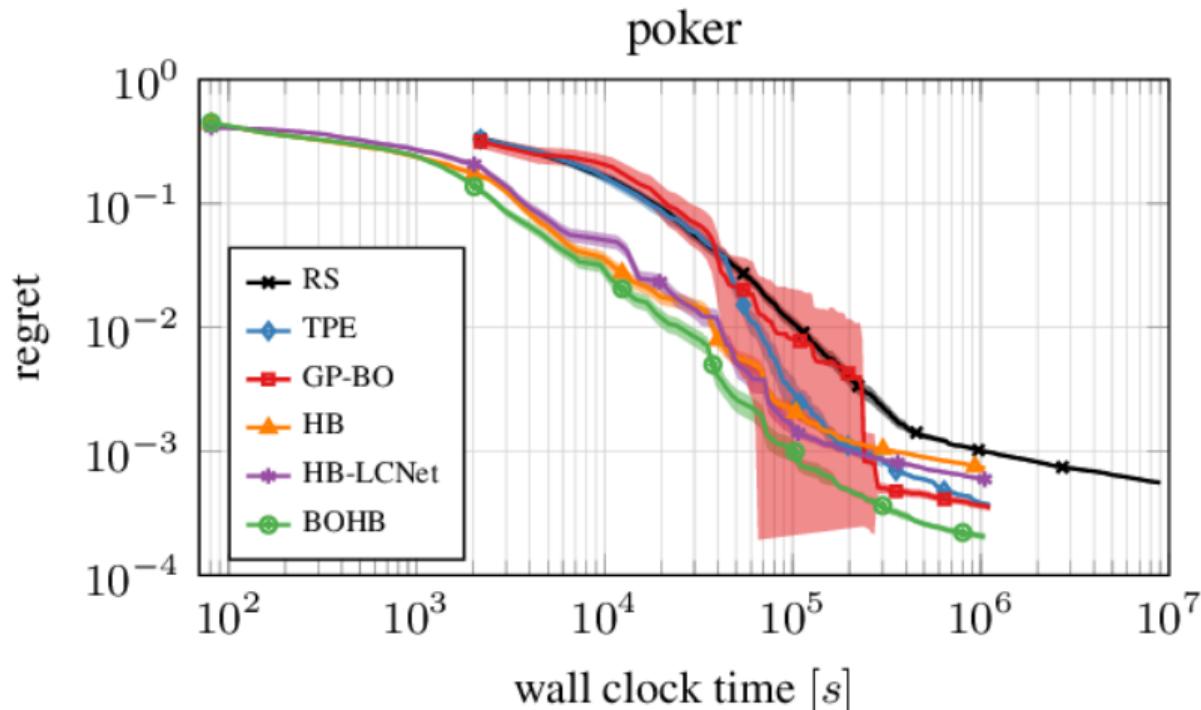


Figure: Optimizing six hyperparameters of a feed-forward neural network on featurized datasets; results are based on surrogate benchmarks.

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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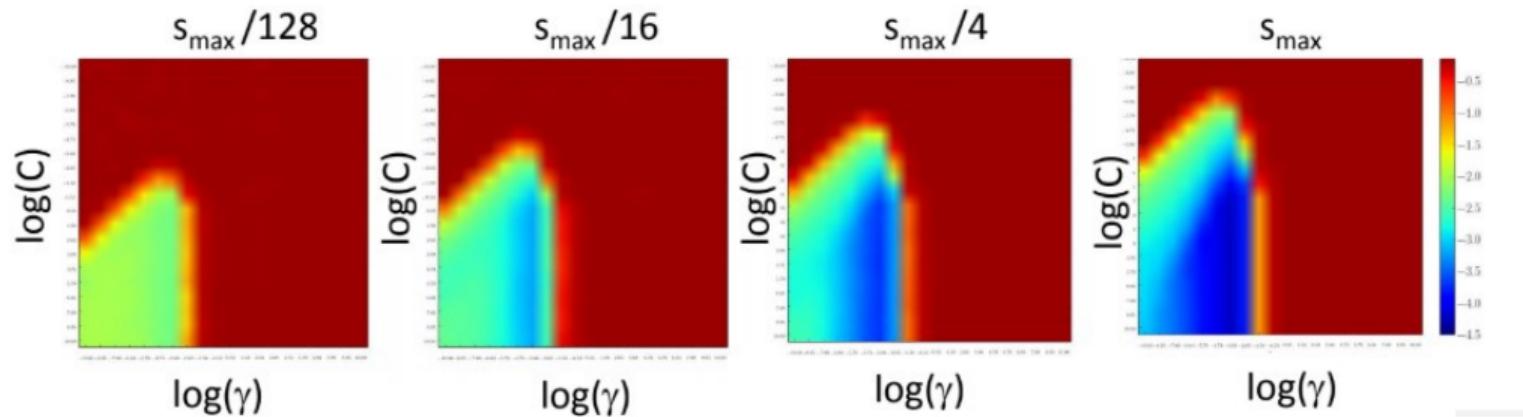
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Multi-fidelity Bayesian optimization

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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, 2017]

- 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:

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

- 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} :

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

- Entropy search [Hennig et al. 2012] aims to minimize the entropy $\mathcal{H}[p_{\min}]$
 - ▶ It aims to be maximally certain about the location of $\boldsymbol{\lambda}^*$
- In a nutshell: select $\boldsymbol{\lambda}$ that maximizes the following acquisition function:

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

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

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

- We still want to minimize the entropy $\mathcal{H}[p_{\min}]$
- 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:

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

- The entire algorithm iterates the following 2 steps until time is up:

- Select (λ, z) by maximizing:

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

- Observe performance $f(\lambda, z)$ and cost $c(\lambda, z)$ 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?

Outline

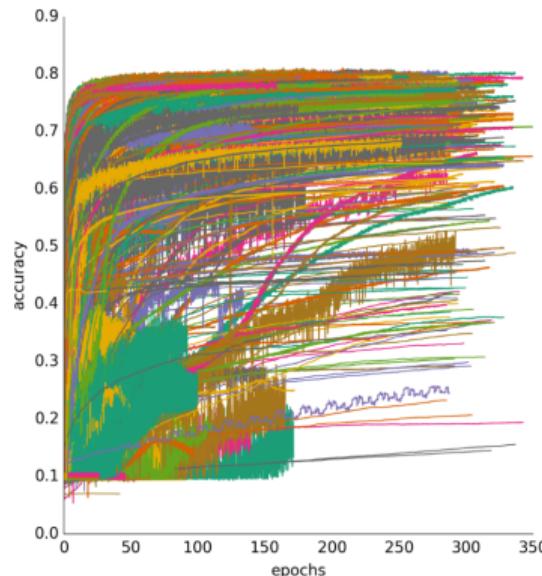
- 1 Overview
- 2 Meta-Learning
- 3 Overview of Multi-Fidelity Optimization
- 4 Hyperband
- 5 BOHB
- 6 Multi-fidelity Bayesian optimization
- 7 Predicting Learning Curves**
- 8 Success Stories and Practical Recommendations

Speedup Techniques for Hyperparameter Optimization

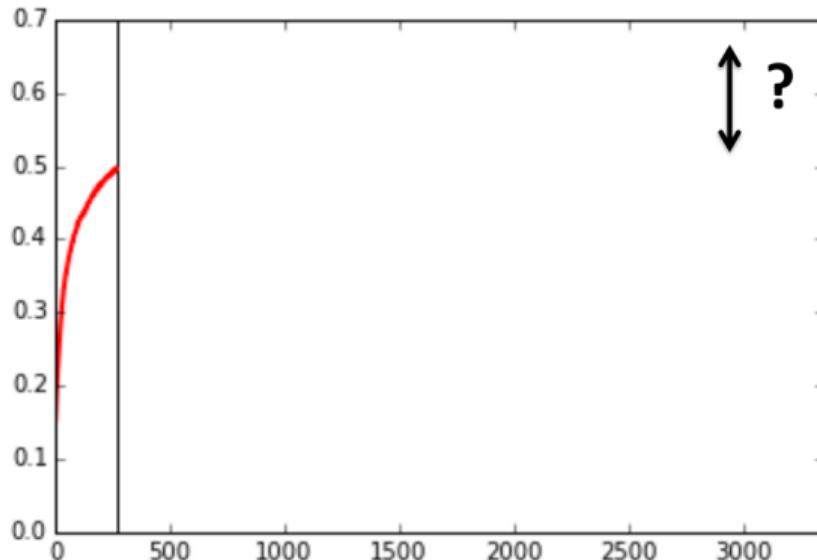
Predicting Learning Curves

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Learning Curves

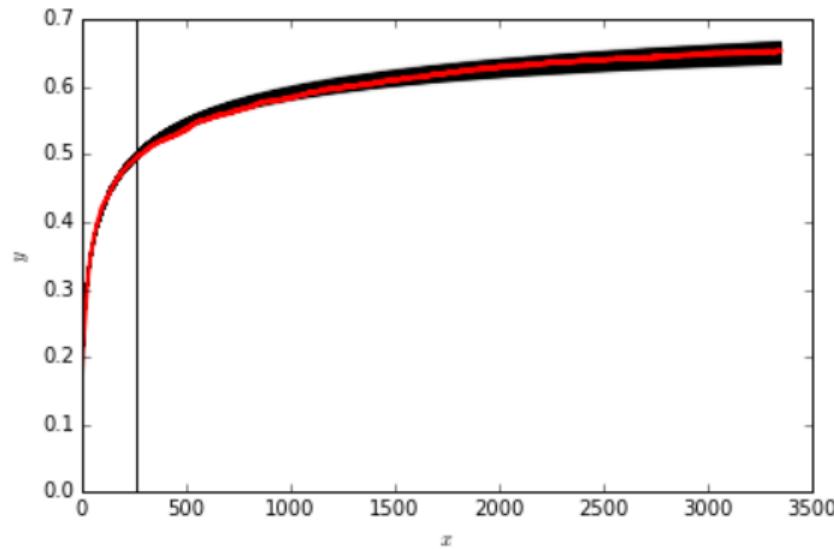


Learning Curve Predictions



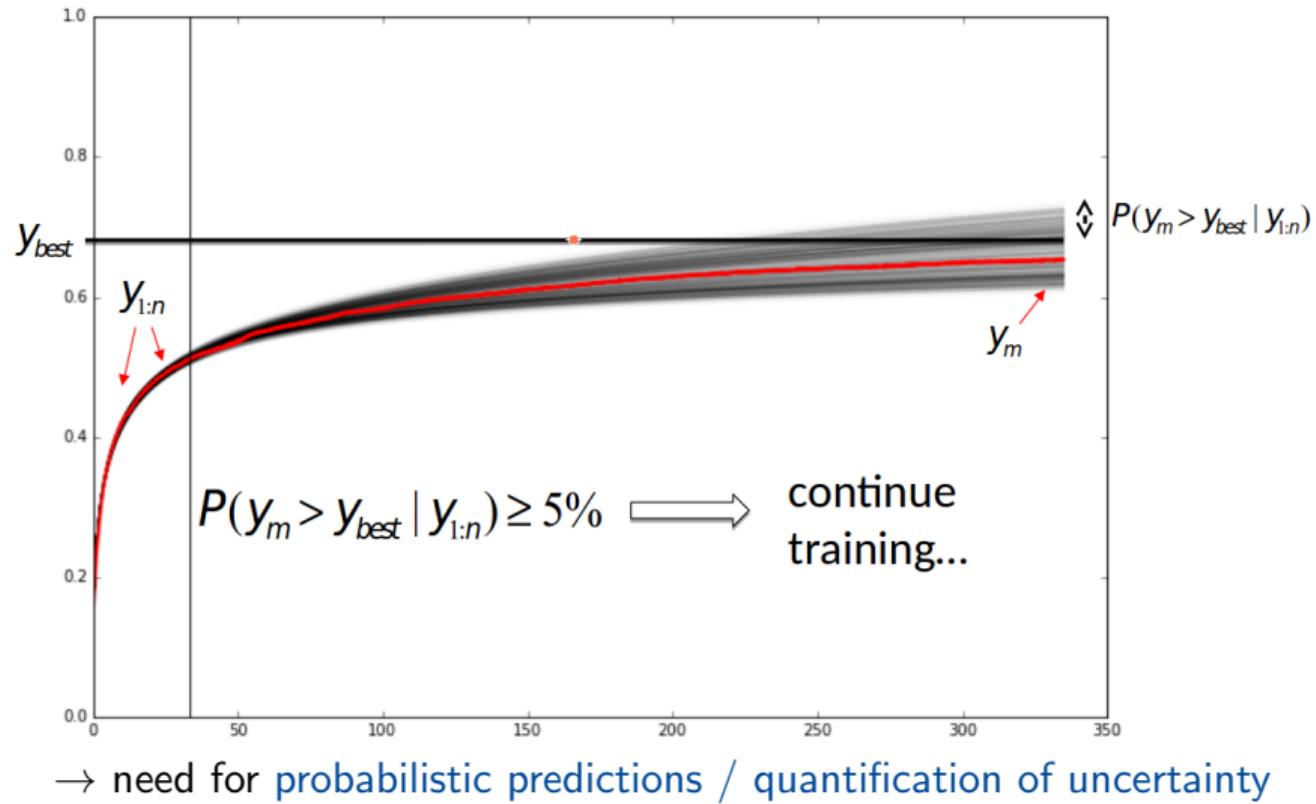
- ① Observe learning curve for the first n steps (here $n = 250$)
- ② **Extrapolation:** fit parametric model on partial learning curve to predict remaining learning curve
 - ▶ Various models can be used (see following slides)

Learning Curve Predictions

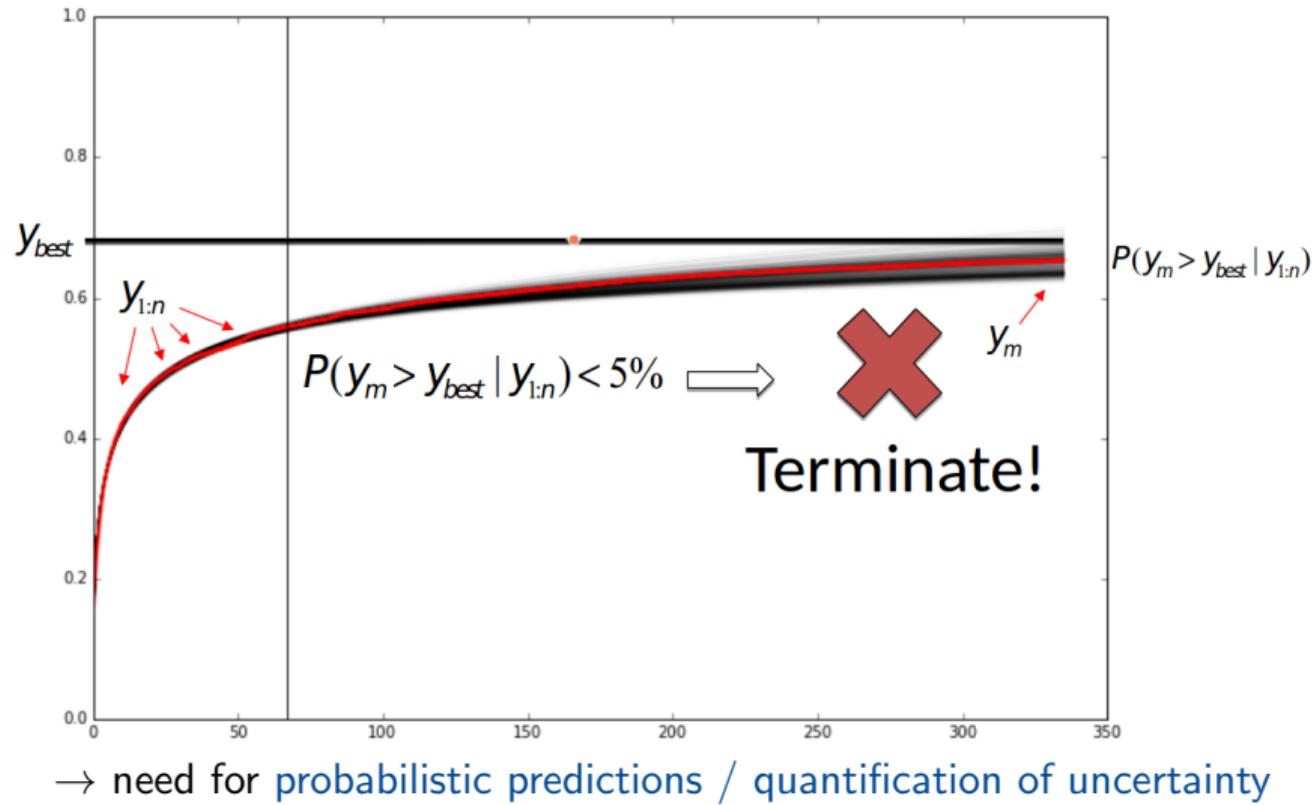


- ① Observe learning curve for the first n steps (here $n = 250$)
- ② **Extrapolation:** fit parametric model on partial learning curve to predict remaining learning curve
 - ▶ Various models can be used (see following slides)

Learning Curves: Early Termination

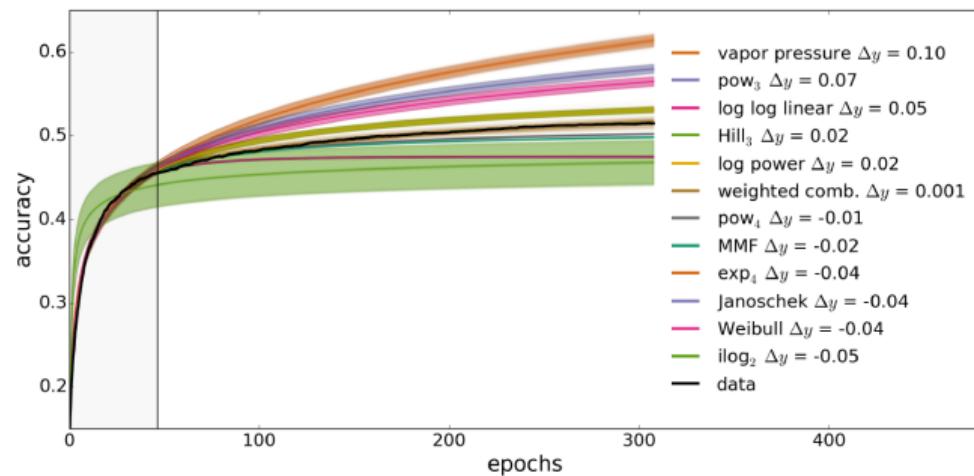


Learning Curves: Early Termination



Parametric Learning Curves [Domhan, Springenberg & Hutter, IJCAI 2015]

- Use a parametric model f_k with parameters θ to model performance at step t as:
 $y_t = f_k(t|\theta) + \epsilon$, with $\epsilon \sim \mathcal{N}(0, \sigma^2)$.
- Linear combination of $K = 11$ parametric types of models:
 $f_{comb}(t|\xi) = \sum_{k=1}^K w_k f_k(t|\theta_k)$, where $\xi = (w_1, \dots, w_K, \theta_1, \dots, \theta_K, \sigma^2)$

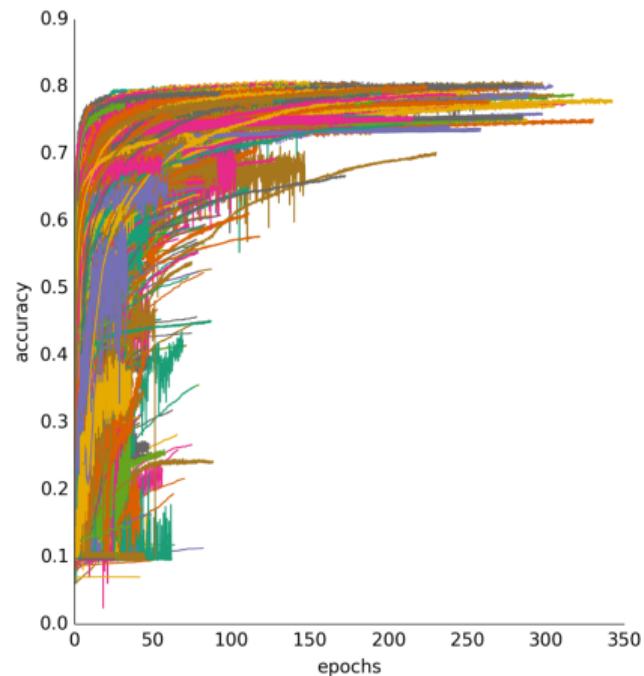
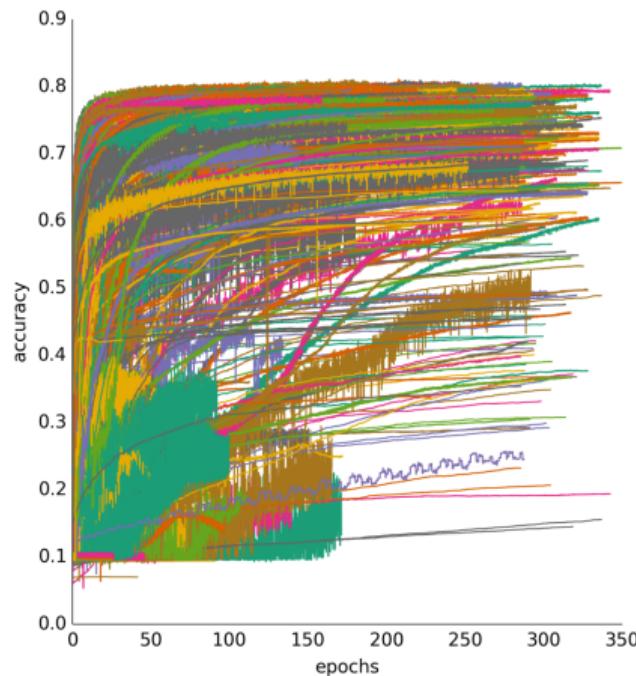


Reference name	Formula
vapor pressure	$\exp(a + \frac{b}{x} + c \log(x))$
pow ₃	$c - ax^{-\alpha}$
log log linear	$\log(a \log(x) + b)$
Hill ₃	$\frac{y_{\max} x^{\eta}}{\kappa^{\eta} + x^{\eta}}$
log power	$\frac{a}{1 + (\frac{x}{e^b})^c}$
pow ₄	$c - (ax + b)^{-\alpha}$
MMF	$\alpha - \frac{\alpha - \beta}{1 + (\kappa x)^{\delta}}$
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

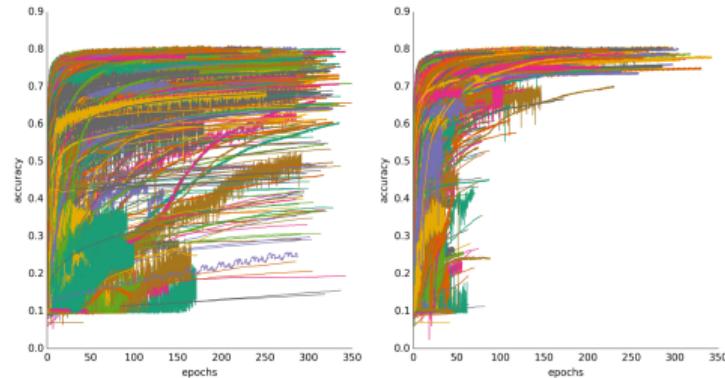
- Use Markov Chain Monte Carlo sampling of ξ to obtain uncertainties

Predictive Termination



All learning curves vs. learning curves with early termination

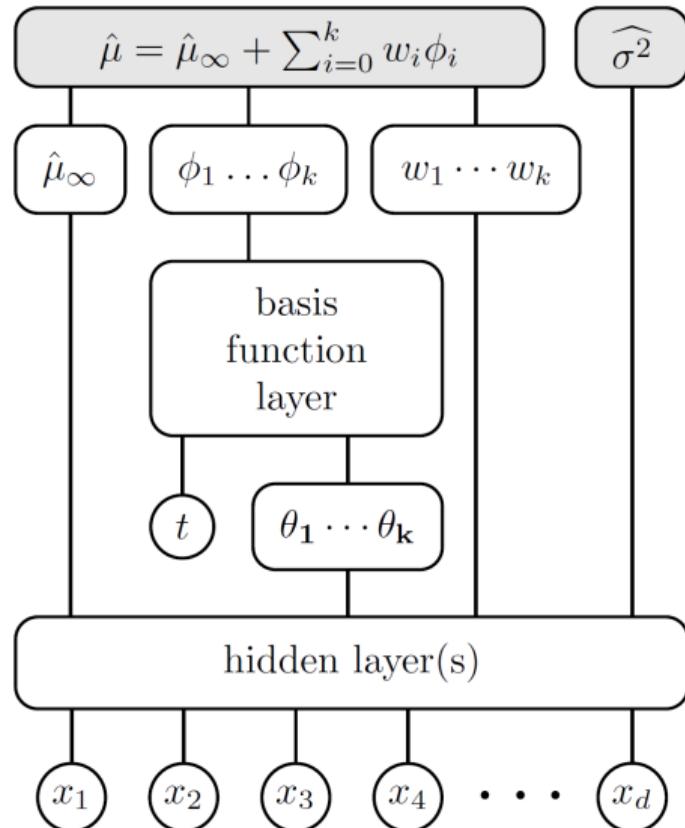
Predictive Termination



All learning curves vs. learning curves with early termination

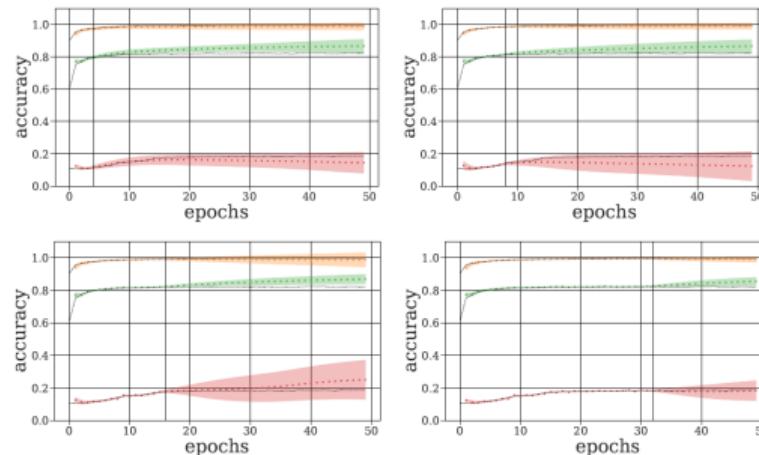
- Disadvantages of this model?
 - ▶ Relies on manually-selected parametric families of curves
 - ▶ Does not take into account hyperparameters used
 - can't learn across hyperparameters

- 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, \dots, 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, AutoML WS 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

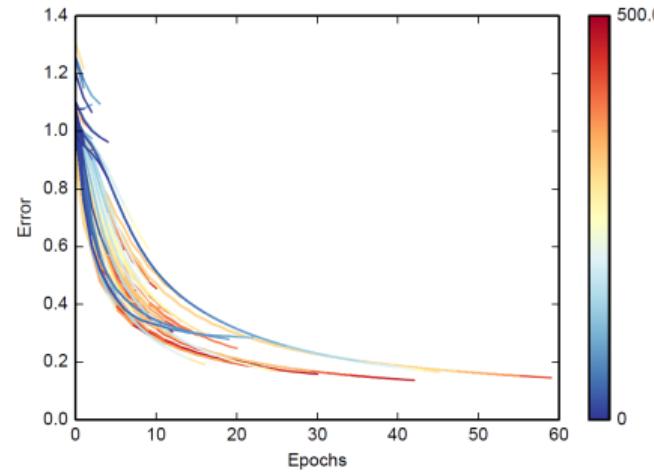
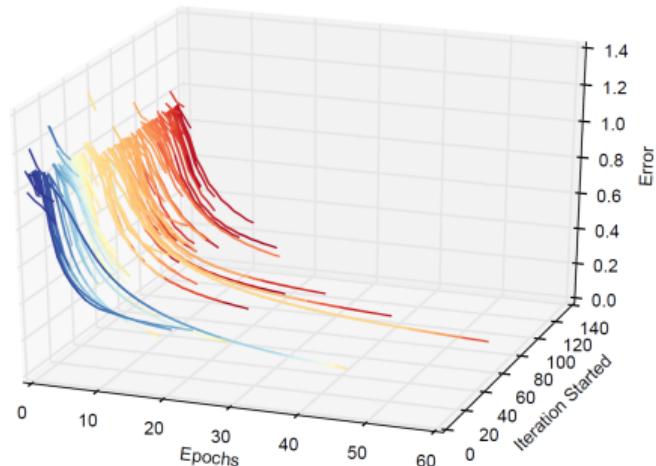
- E.g., a random forest to map from a fixed-size window to the next value

Compare: Baker et al, 2017 [Baker et al, ICLR WS 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? → 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, arXiv 2014]

- Use a Gaussian process with inputs λ 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]

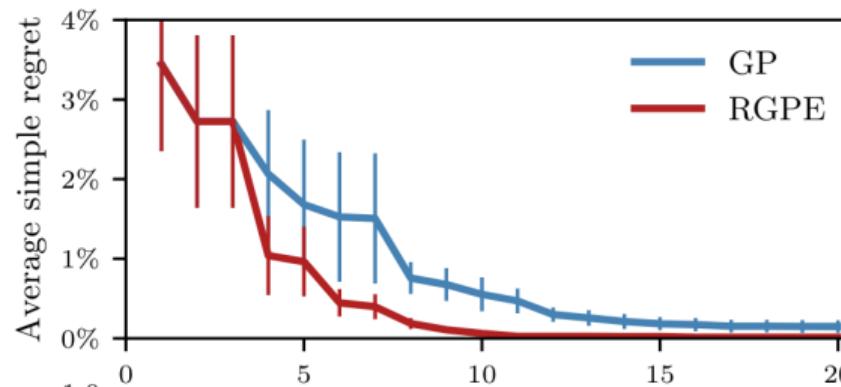
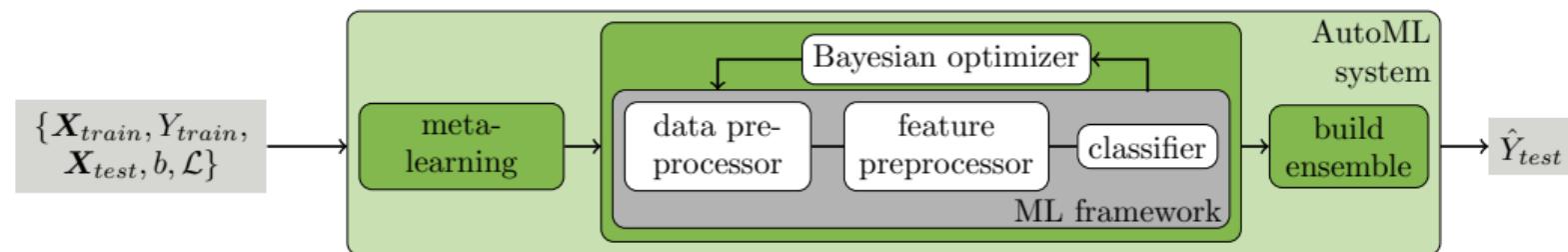


Figure: Bayesian optimization with meta-learning (RGPE) vs. vanilla Bayesian optimization (GP)

Auto-sklearn [Feurer et al, NIPS 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



```
>>> 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, Klein and Hutter, ICML 2018]

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

Cited by 129



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>

 Unwatch ▾

23

 Star

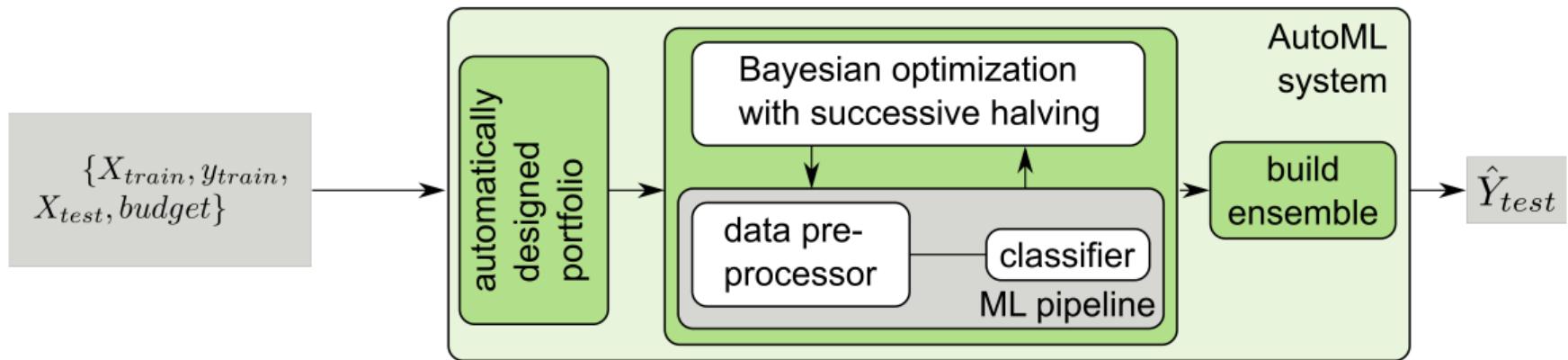
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 Fork

80

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

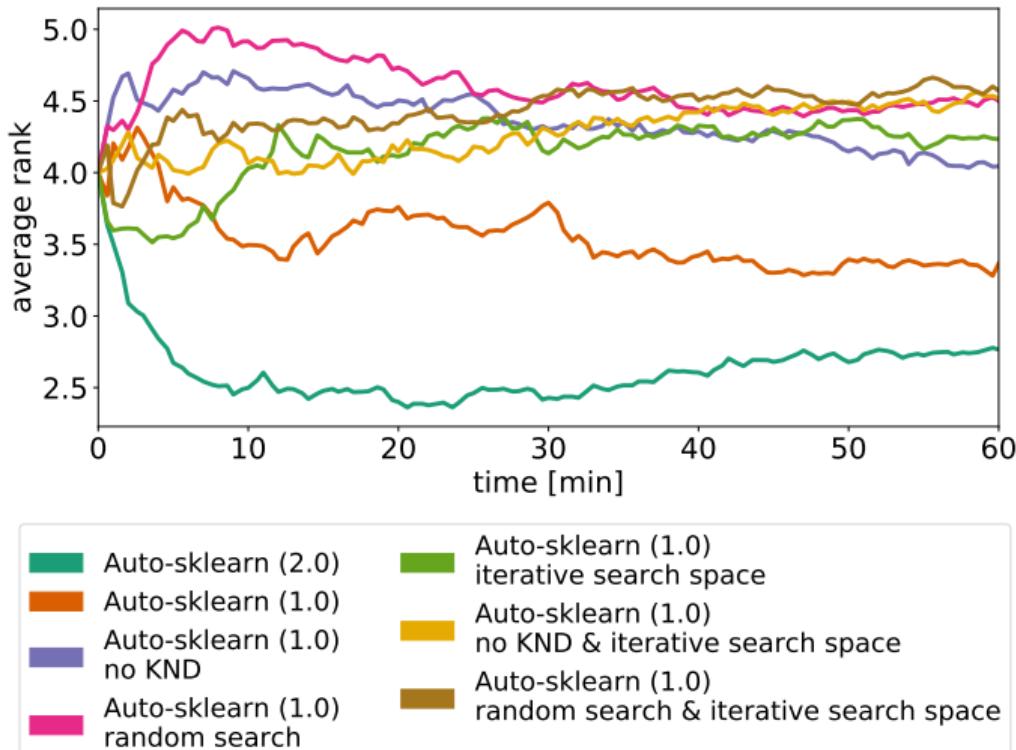
- Idea: automatically choose on a per-dataset basis
 - ▶ holdout or cross-validation
 - ▶ optimization on the full budget or optimization with successive halving

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× reduction of average error
 - ▶ 6× speedup (same performance in 10 minutes as Auto-sklearn 1.0 in 1 hour)



Practical Recommendations Which HPO Method to Use [Feurer & Hutter, 2019]

- If multiple fidelities available: BOHB [Falkner, Klein and Hutter, ICML 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., since 2001]; evaluated for HPO by [Loshchilov & Hutter, ICLR WS 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]