Lecture 9: Algorithm Independent Principles - III

Hyperparameter Optimization, AutoML

Machine Learning, Summer Term 2019

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Lecture Overview

1. Hyperparameter Optimization
2. Automated Machine Learning (AutoML)
3. Grey-Box AutoML

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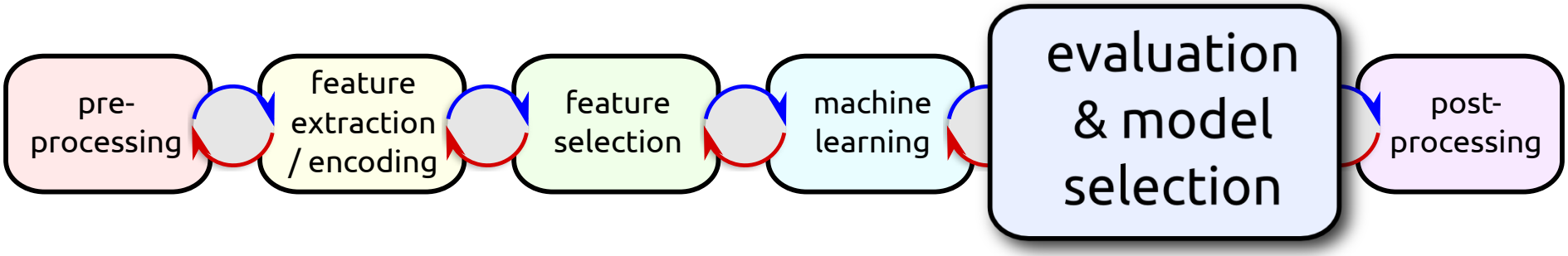
Hyperparameter Optimization in the ML Design Cycle



Part of model selection: how to set free algorithm hyperparameters?

- Hyperparameter optimization is essentially the same problem as model selection, except:
- Many more possible settings to choose from (infinite/exponential)

Parameters vs. Hyperparameters

- Most machine learning algorithms internally optimize parameters
  - E.g., weights in linear regression
  - E.g., split points and leaf predictions in decision trees
  - E.g., deep learning: millions of network weights
- Standard ML approach: min. training loss + $\lambda \times$ regularization loss
  - Using standard gradient-based optimizers
- Hyperparameters: decisions left to the algorithm designer
  - How to set λ?
  - How complex a model to use?
  - How many layers/which structure of deep networks to use?
  - How to set the options of the gradient-based optimizer?

SVM Documentation

Home Installation Documentation Examples

Google Custom Search

Previous sklearn.svm.O... | Next sklearn.svm.SVR | Up API Reference

scikit-learn v0.21.1
Other versions

Please **cite us** if you use the software.

`sklearn.svm`.SVC
Examples using
`sklearn.svm.SVC`

`sklearn.svm`.SVC

class `sklearn.svm.` **SVC** (*C=1.0, kernel='rbf', degree=3, gamma='auto_deprecated', coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None, verbose=False, max_iter=-1, decision_function_shape='ovr', random_state=None*) [source]

C-Support Vector Classification.

The implementation is based on libsvm. The fit time scales at least quadratically with the number of samples and may be impractical beyond tens of thousands of samples. For large datasets consider using `sklearn.linear_model.LinearSVC` or `sklearn.linear_model.SGDClassifier` instead, possibly after a `sklearn.kernel_approximation.Nystroem` transformer.

The multiclass support is handled according to a one-vs-one scheme.

For details on the precise mathematical formulation of the provided kernel functions and how `gamma`, `coef0` and `degree` affect each other, see the corresponding section in the narrative documentation: Kernel functions.

Read more in the User Guide.

Parameters:

C : *float, optional (default=1.0)*
Penalty parameter C of the error term.

kernel : *string, optional (default='rbf')*
Specifies the kernel type to be used in the algorithm. It must be one of 'linear', 'poly', 'rbf', 'sigmoid', 'precomputed' or a callable. If none is given, 'rbf' will be used. If a callable is given it is used to pre-compute the kernel matrix from data matrices; that matrix should be an array of shape `(n_samples, n_samples)`.

degree : *int, optional (default=3)*
Degree of the polynomial kernel function ('poly'). Ignored by all other kernels.

gamma : *float, optional (default='auto')*

Hyperparameter Optimization Method 1: Random Search

- Select configurations uniformly at random (completely uninformed)
- Global search, won't get stuck in a local region
- Parallelizes nicely and is at least better than grid search:

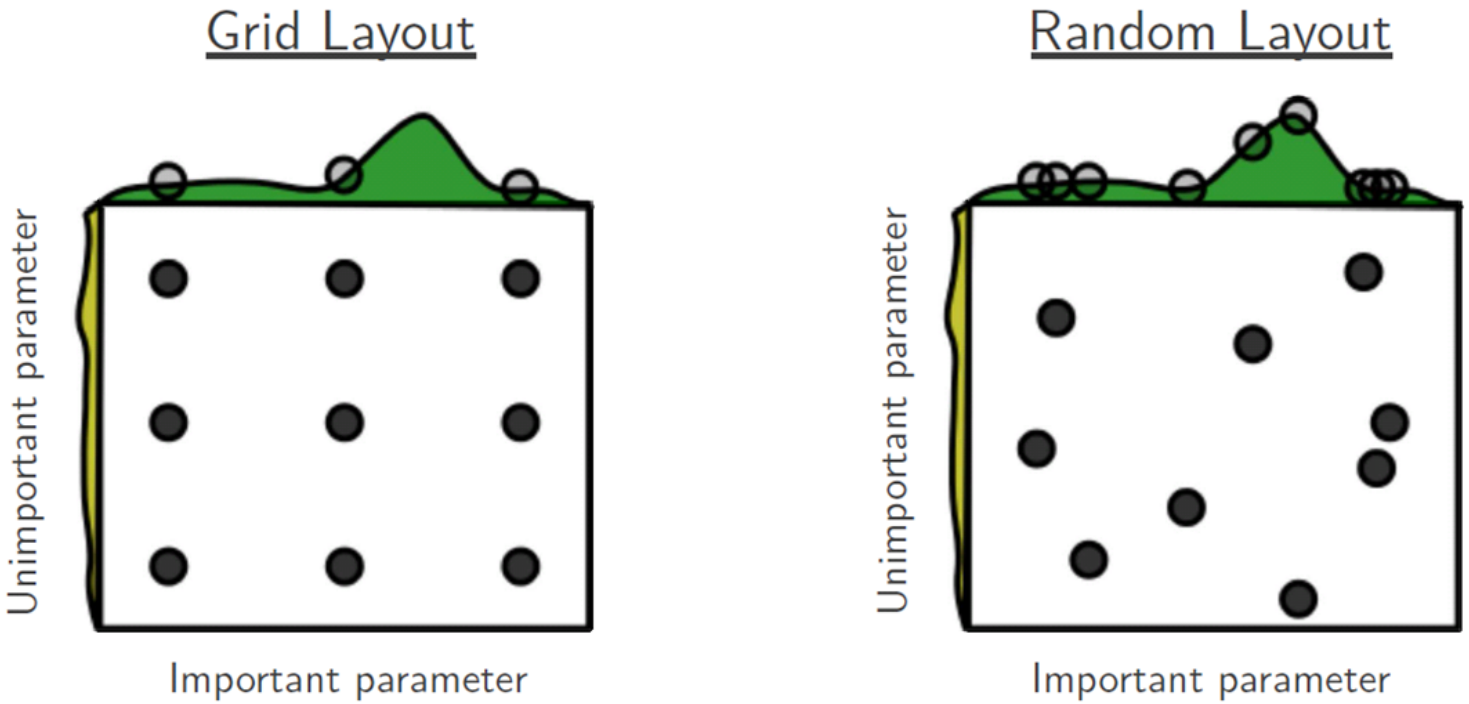


Image source: [Bergstra et al, JMLR 2012]

Hyperparameter Optimization Method 2: Local Search

(also sometimes jokingly called "Graduate Student Descent")

Start with some configuration θ

repeat

  Modify a single hyperparameter

  if *results on benchmark set improve* **then**

    keep new configuration

until *no more improvement possible (or "good enough")*

$\rightsquigarrow$ Manually-executed first-improvement local search

Hyperparameter Opt. Method 3: Bayesian Optimization

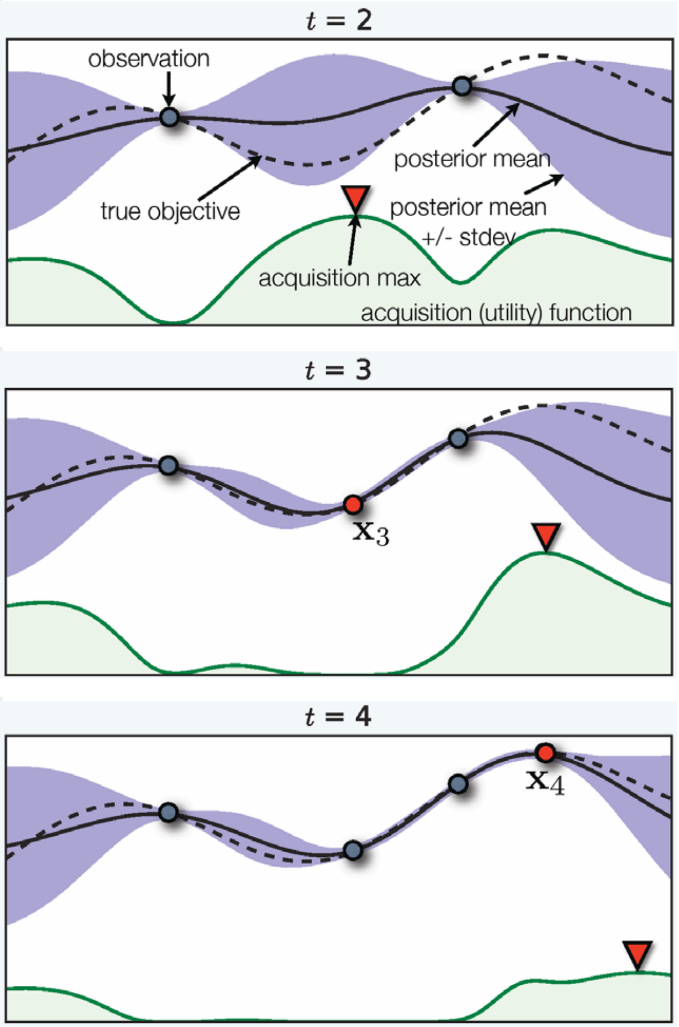
General approach

- Fit a probabilistic model to the collected function samples $\langle \theta, f(\theta) \rangle$
- Use the model to guide optimization, trading off exploration *vs* exploitation

Popular approach in the statistics literature since [Mockus, 1978]

- Efficient in # function evaluations
- Works when objective is nonconvex, noisy, has unknown derivatives, etc
- Recent convergence results

  [Srinivas et al, 2010; Bull 2011; de Freitas et al, 2012; Kawaguchi et al, 2015]



Bayesian Optimization Algorithm

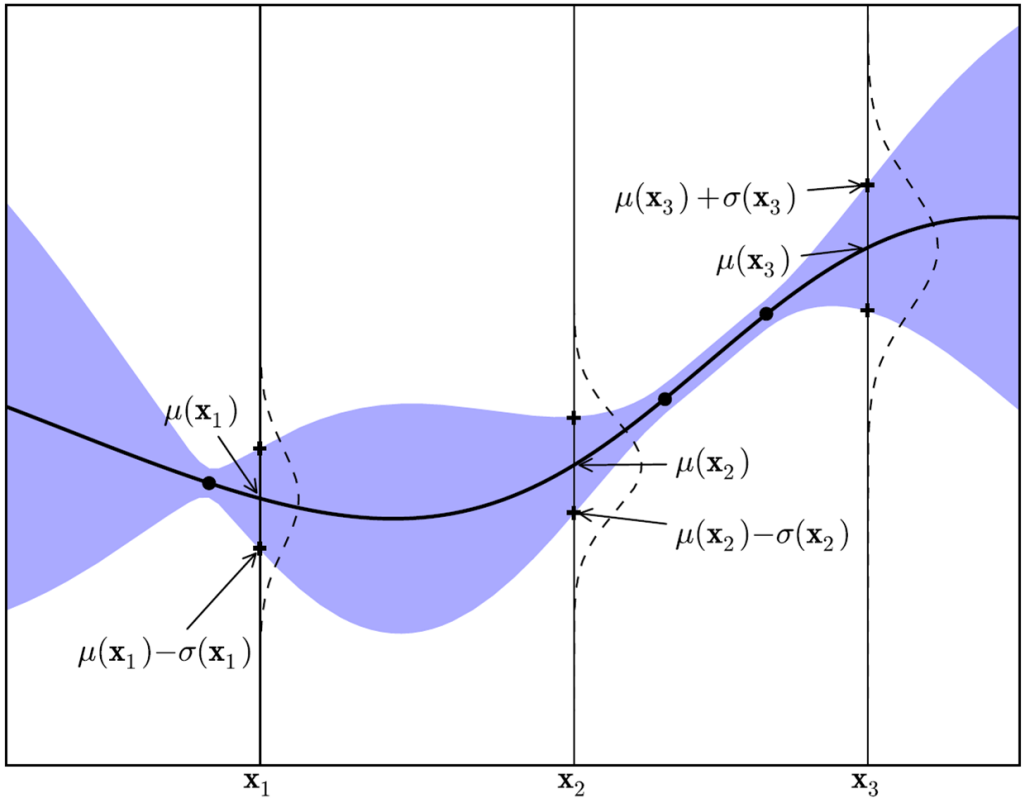
Algorithm 1: Bayesian Optimization (BO)

Input : Search Space $\mathcal{X}$, black box function f, acquisition function α, maximal number of function evaluations m

$\mathcal{D}_0 \leftarrow$ initial_design($\mathcal{X}$);
for $n = 1, 2, \ldots m - |D_0|$ **do**
    $\hat{m} : \theta \mapsto y \leftarrow$ fit predictive model on $\mathcal{D}_{n-1}$;
    select x_n by optimizing $x_n \in \arg\max_{x \in \mathcal{X}} \alpha(x; \mathcal{D}_{n-1}, \hat{m})$;
    Query $y_n := f(x_n)$;
    Add observation to data $D_n := D_{n-1} \cup \{\langle x_n, y_n \rangle\}$;
return *Best* x *according to* D_m

Acquisition Function: Upper Confidence Bound

- $\text{UCB}(\theta) = \mu(\theta) + \kappa_t \sigma(\theta)$, with exploration parameter κ
  - for maximizing f!



- Which point would we pick next with UCB and $\kappa = 1$?
- κ_t increases over time

Range Transformations of Hyperparameters

- Several hyperparameters naturally lay on a logarithmic scale
  - E.g., learning rate between 10^{-5} and 10^{0}
- Transform these to a linear scale
  - E.g., instead work with $\log_{10}(\text{lr})$, with values between -5 and 0
- Good rule of thumb: transform the space to the one you would want to sample from uniformly
  - E.g., uniform sampling from $[10^{-5}, 10^{0}]$ would have 90% samples greater than 10^{-1}

Conditional Hyperparameters

- Some hyperparameters h are only active if other hyperparameters p take certain values
  - E.g., weight initialization for layer k is only active if the hyperparameter number of layers is at least k
- We call these hyperparameters conditional with parents p
- You can always ignore such conditionality, but exploiting it can dramatically simplify the problem

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Automated Machine Learning

Machine Learning is very successful in many applications.

- But it still requires human machine learning experts to
  - Preprocess the data
  - Select / engineer features
  - Select a model family
  - Optimize hyperparameters
  - Construct ensembles
  - ...
- AutoML: taking the human expert out of the loop
- Deep learning helps to automatically learn features
  - But it is even more sensitive to hyperparameters

Automated Machine Learning

The AutoML approach introduced by Auto-WEKA [Thornton et al, 2013]

- Expose the choices in a machine learning framework
  - Algorithms, hyperparameters, preprocessors, ...
  - Highly conditional hyperparameter space
  - Combined algorithm selection and hyper-parameter optimization
    $\rightarrow$ defined in detail on the next slide
- Optimize CV performance using Bayesian optimization

$\rightsquigarrow$ Obtain a true push-button solution for machine learning

Extended in Auto-sklearn [Feurer et al, 2015]

CASH Problem [Thornton et al. 2013]

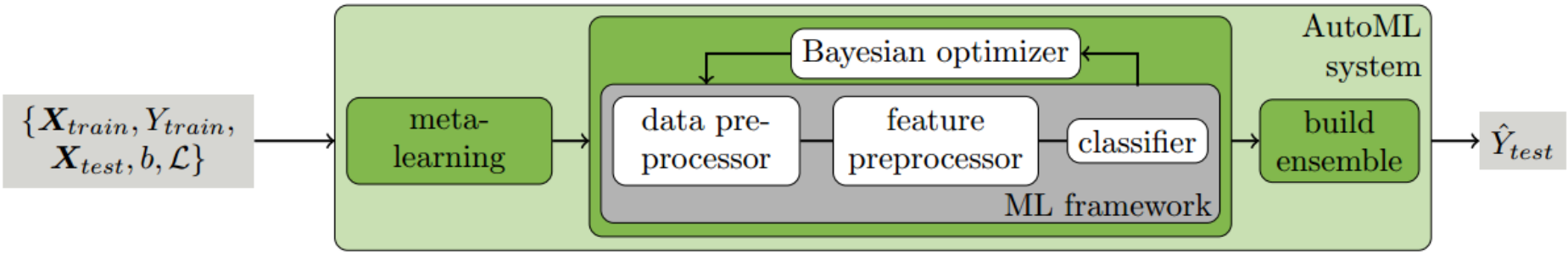
Let

- $\mathcal{A} = A^{(1)}, \ldots, A^{(J)}$ be a set of algorithms,
- the hyper-parameters of each algorithm $A^{(j)}$ have domain $\Lambda^{(j)}$,
- $D_{train} = \{(x_1, y_1), ..., (x_n, y_n)\}$ be a training set which is split into K cross-validation folds $\{D^{(1)}_{valid}, \ldots, D^{(K)}_{valid}\}$ and $D^{(i)}_{train} = D_{train} - D^{(i)}_{valid}$ for $i = 1, \ldots, K$,
- $\mathcal{L}(A^{(j)}_{\lambda}, D^{(i)}_{train}, D^{(i)}_{valid})$ denote the loss of $A^{(j)}_{\lambda}$ trained on $D^{(i)}_{train}$ and evaluated on $D^{(i)}_{valid}$.

The *CASH* problem is to find the joint algorithm and hyper-parameter setting that minimizes this loss across the K folds:

$$A^*, \lambda^* \in \underset{A^{(j)} \in \mathcal{A}, \lambda \in \Lambda^{(j)}}{\arg\min} \frac{1}{K} \sum_{i=1}^{K} \mathcal{L}(A^{(j)}_{\lambda}, D^{(i)}_{train}, D^{(i)}_{valid})$$

Auto-sklearn [Feurer et al. 2015]



- Winner of ChaLearn Automatic Machine Learning Challenge
  - Performed better than 150 teams of human experts
  - Searches over ≈15 classifiers & preprocessors (110 hyperparameters)
- Trivial to use even for novices in machine learning:

```
import autosklearn.classification as cls
automl = cls.AutoSklearnClassifier()
automl.fit(X_train, y_train)
y_hat = automl.predict(X_test)
```

Availabe online: `https://github.com/automl/auto-sklearn`

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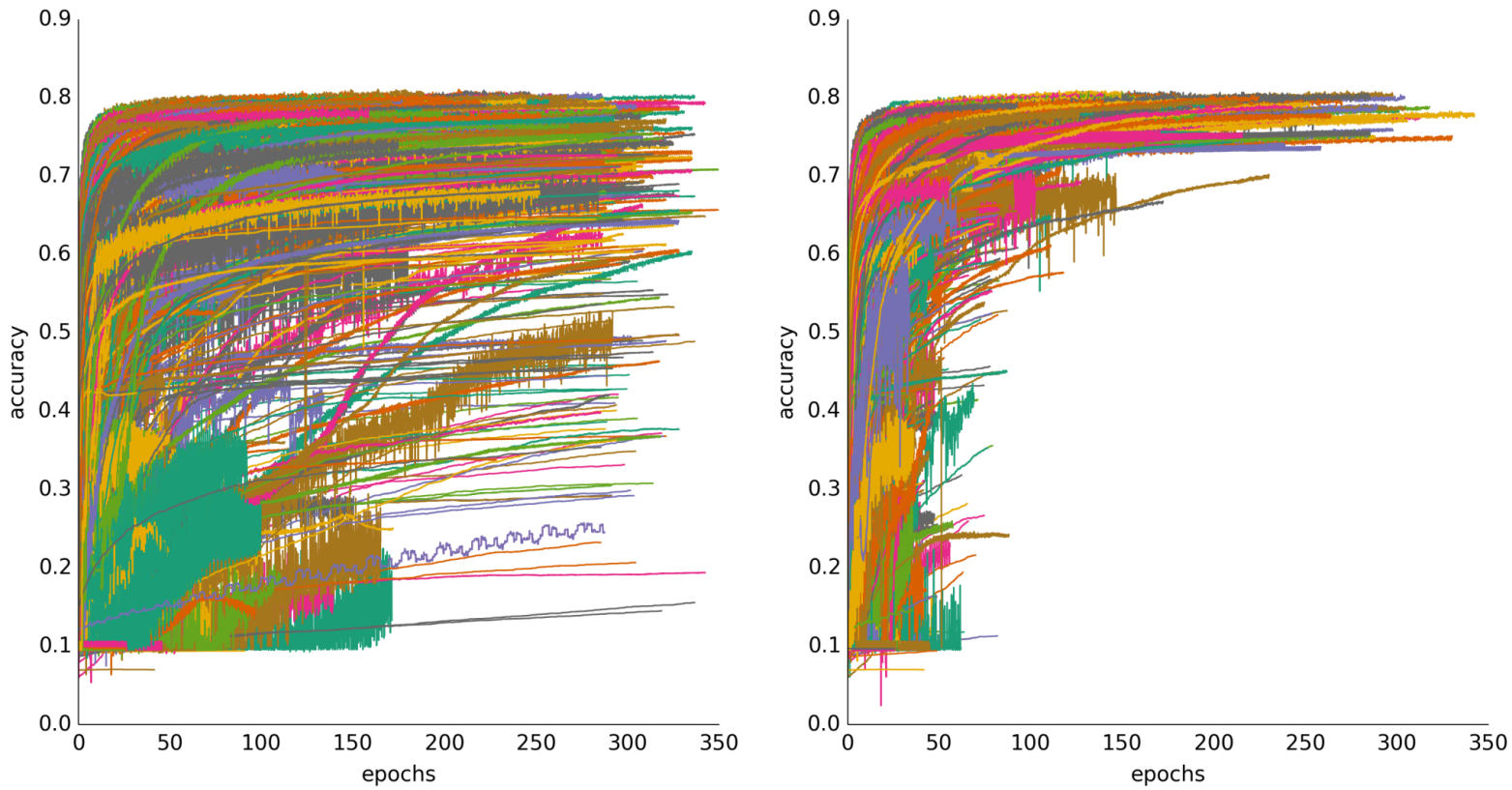
Speeding up Hyperparameter Optimization Methods

- If we use k-fold cross-validation
  - We can reject poor hyperparameter settings after few folds
- If we use iterative ML algorithms
  - We can stop poor runs early
- If runs on smaller datasets are faster (almost always)
  - We can quickly select decent models based on data subsets

Learning Curve Tuning



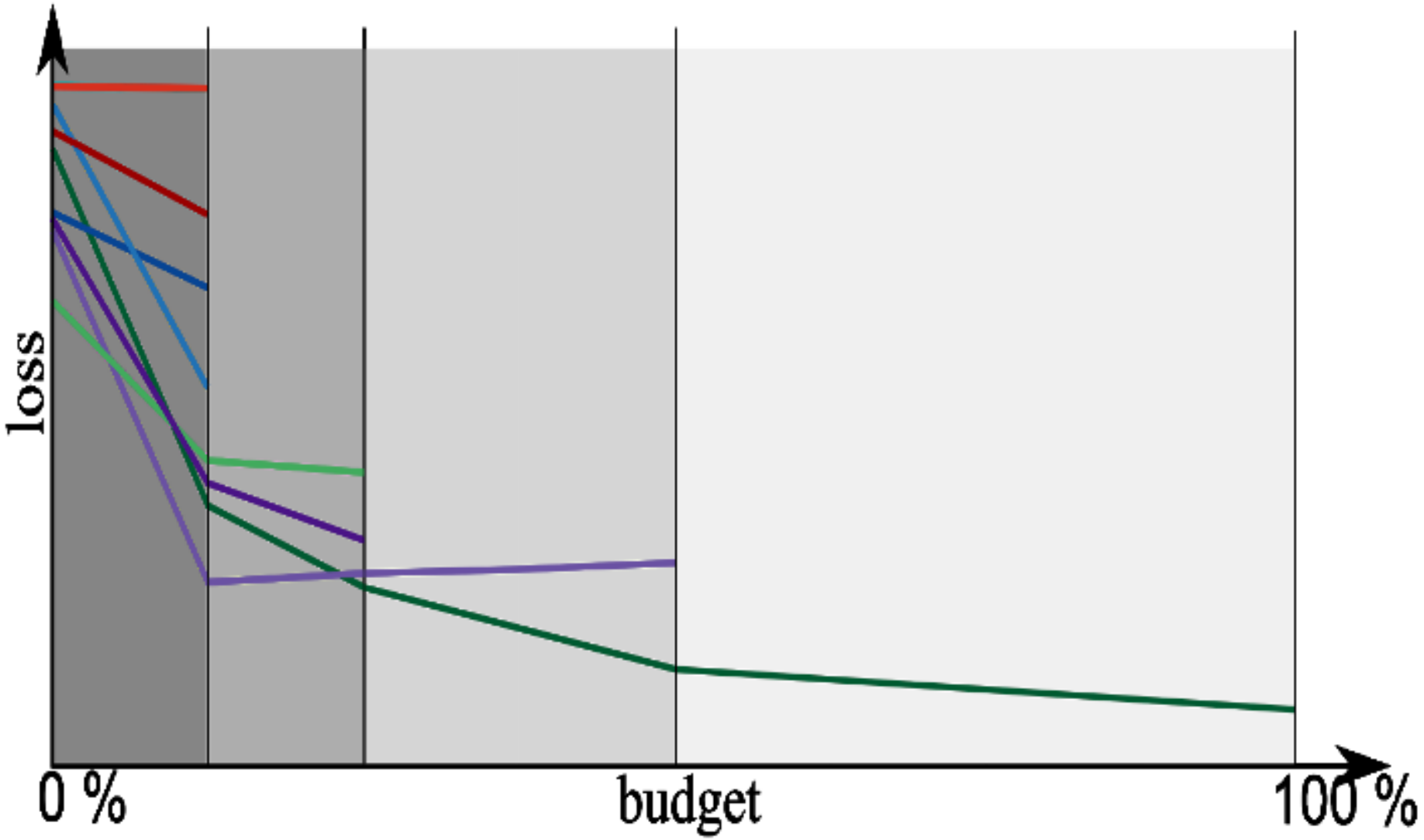
⇝ We only want to train the best learning curves until the end

Successive Halving [Jamieson and Talwalkar 2015]

Successive Halving

- Ideas:
  - Invest only resources in promising configurations
  - $\rightsquigarrow$ aggressive dropping of poor configurations
  - Model-free — (more or less assumption free)
- Algorithm Outline:
  - Input: n (randomly sampled) configurations and budget B
  1. Run remaining configurations with some resource allocation (depending on B)
  2. Sort configurations by cost (e. g., validation loss)
  3. Throw away lower half of configurations
  4. Repeat
- Resource allocation can correspond to
  - partial learning curves
  - subset of training data

Successive Halving: Illustration

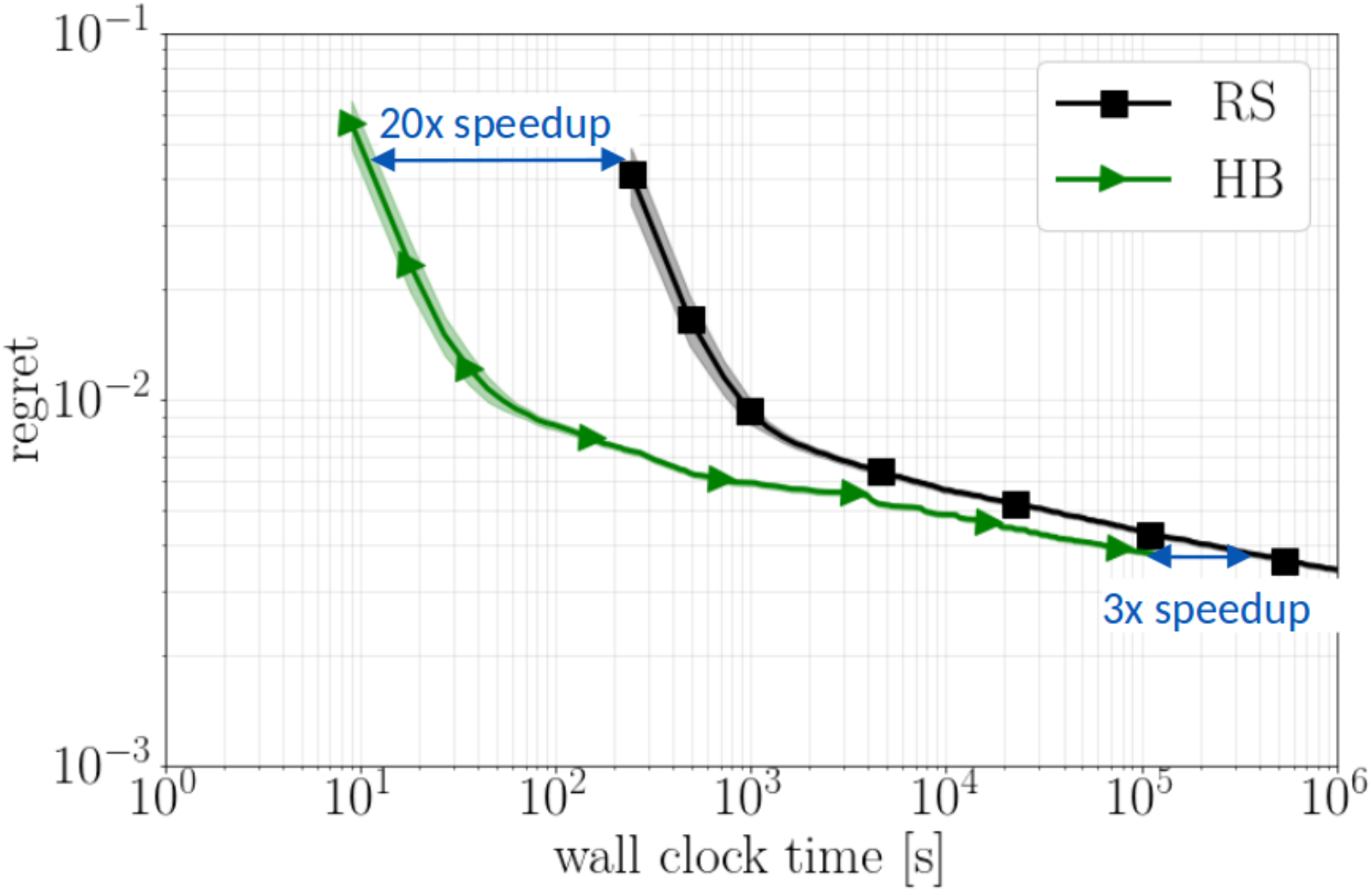


Hyperband [Li et al. 2016]

Hyperband

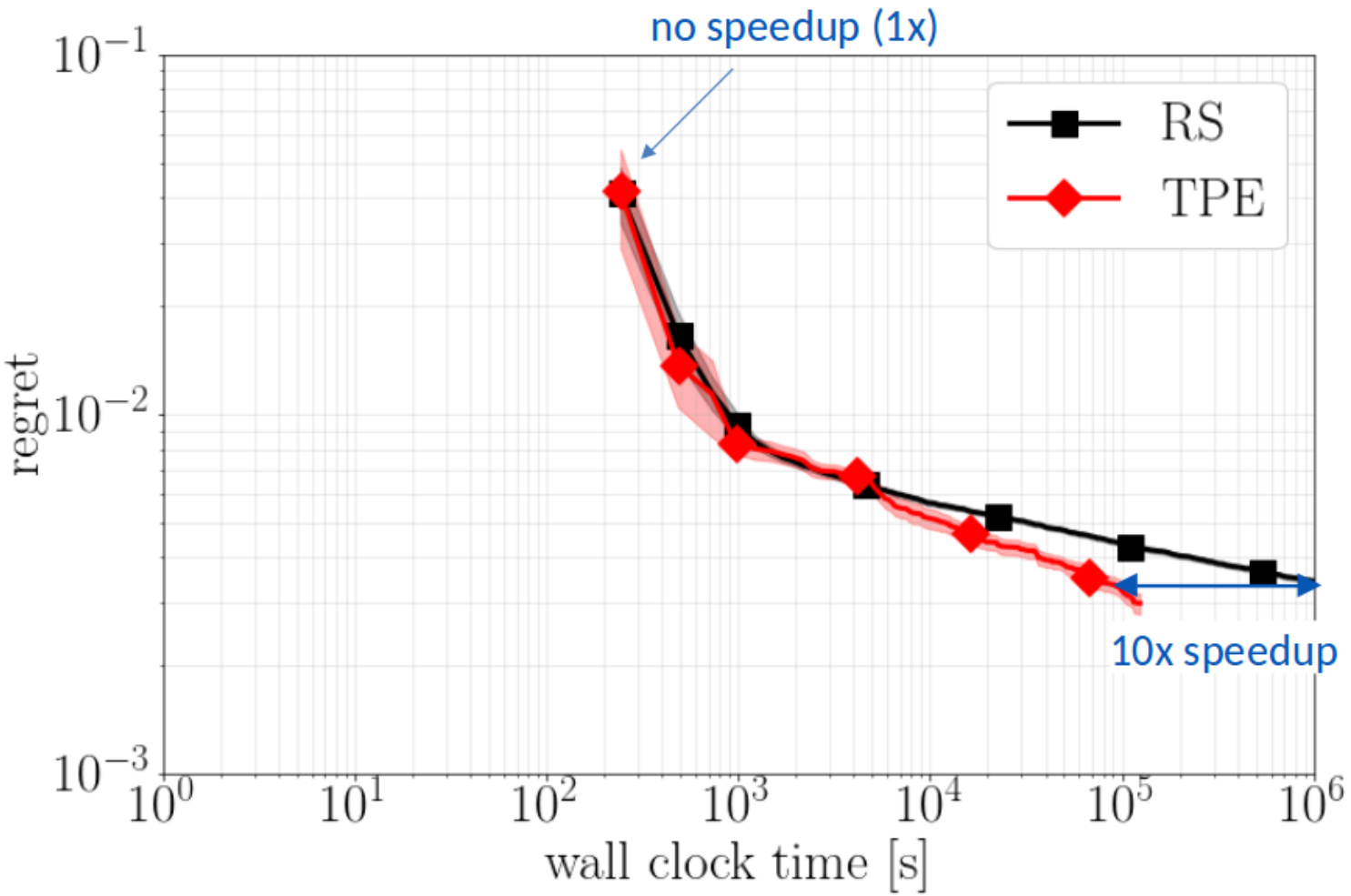
- Issue of successive halving (for a fixed B):
  Do you want to run many configurations with aggressive rejection?
  Or: Do you want to run few configurations with non-aggressive rejection?
- Ideas:
  - Add an outer loop to try different trade-offs between #configurations and budget
  - Add further parameter: proportion of configurations discarded in each round of successive halving
- Starts with many configurations that gets aggressively rejected
- In later iterations, few configurations with more budget each
- Returns: configuration with the smallest intermediate loss seen so far.

Random Search vs. Hyperband



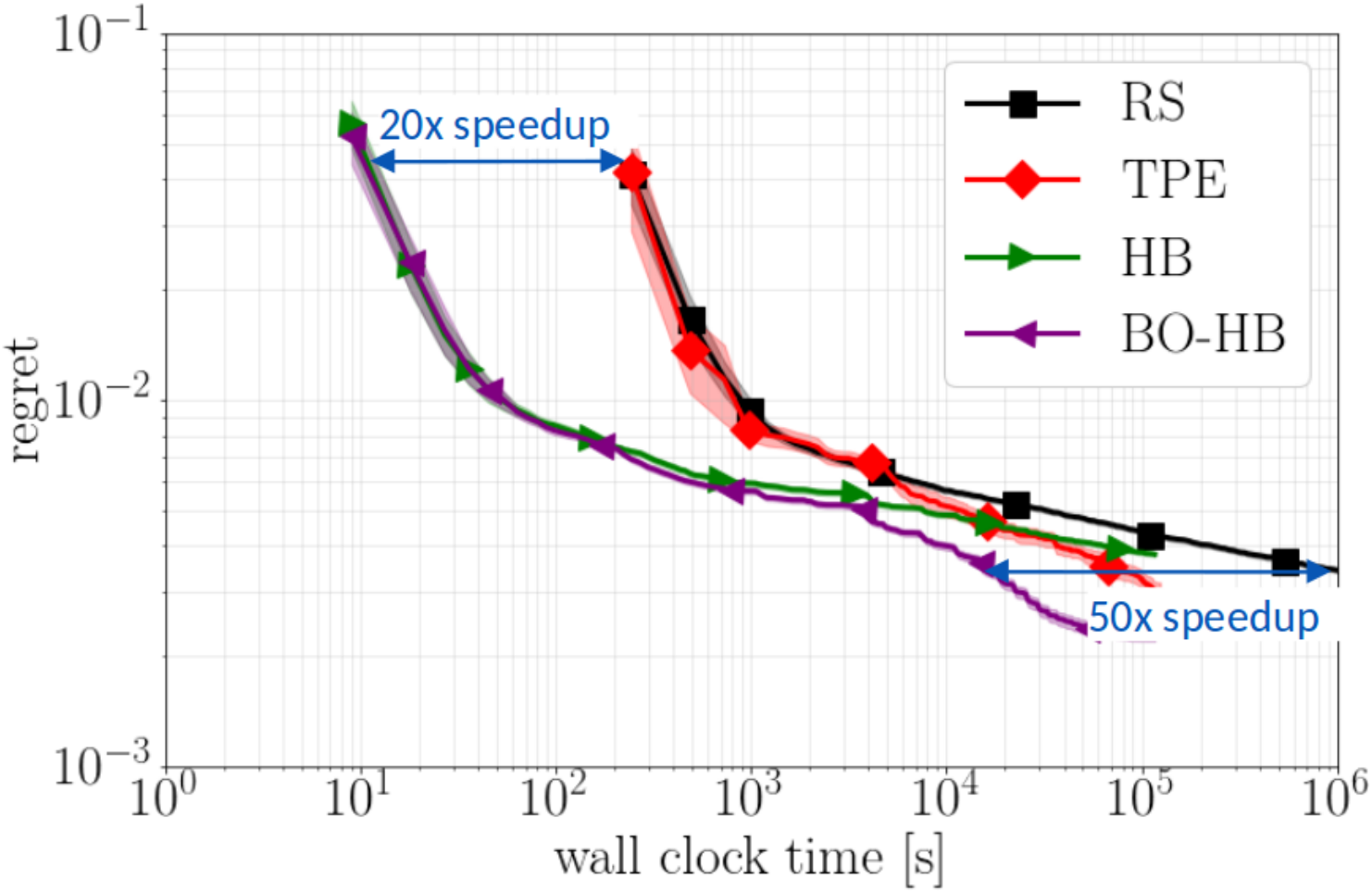
$\rightsquigarrow$ Hyperband performs well early on

Random Search vs. Bayesian Optimization



$\rightsquigarrow$ Bayesian optimization performs well later on

Random Search vs. Bayesian Optimization vs. Hyperband



$\rightsquigarrow$ A combination of Bayesian Optimization and Hyperband performs well overall

BOHB: a Robust & Efficient Framework for Hyperparameter Optimization

- BOHB: Bayesian Optimization & HyperBand
  - Bayesian optimization for selecting configurations
  - Hyperband for implementing the speedup techniques, using the concept of a budget (size of data subsets, #epochs, #CV folds, etc)
  - Currently one of the best available approach for robust & efficient hyperparameter optimization
- You can use this for optimizing your own hyperparameters `https://github.com/automl/HpBandSter`

Summary by learning goals

Having heard this lecture, you can now . . .

- Describe the difference between parameters and hyperparameters
- Give some examples of hyperparameters of various algorithms
- Describe the ideas behind random search and Bayesian optimization
- Explain methods to speedup hyperparameter optimization by using grey-box approaches

Further Reading

- Random search: [Bergstra et al, 2012]
- Bayesian optimization: [Mockus, 1978]; [Brochu et al, 2010]
- BOHB: [Falkner et al, 2019]