Introduction Automated Machine Learning

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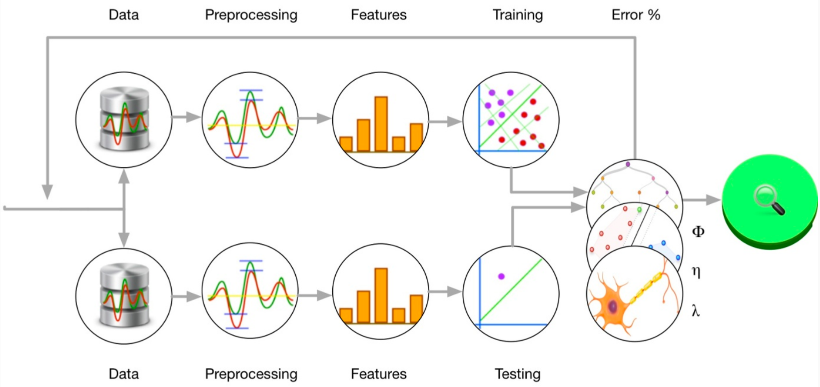
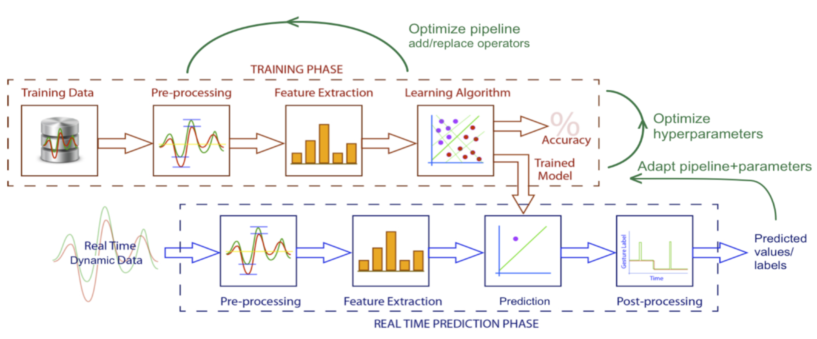
Machine Learning Pipeline

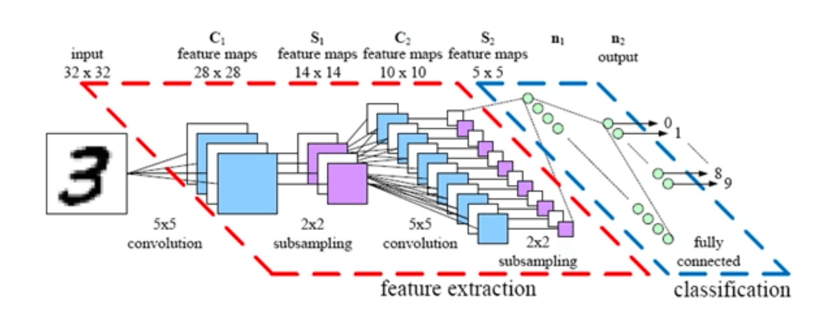


(Image Courtesy Joaquin Vanschoren)

Automated Machine Learning



(Image Courtesy Joaquin Vanschoren)



(Image Courtesy Joaquin Vanschoren)

Neural Architecture Search

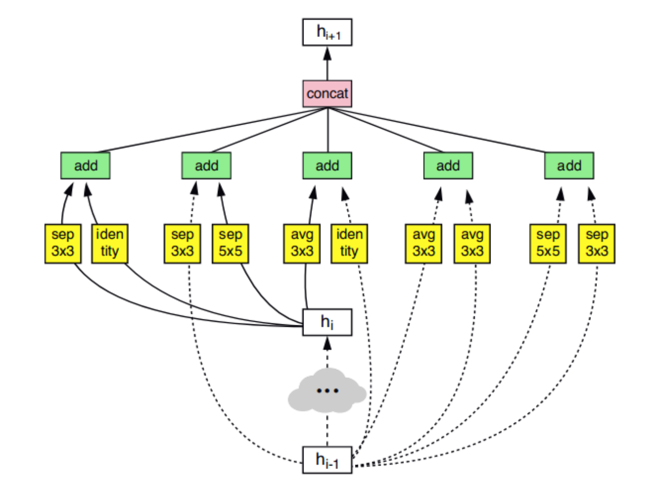


Image from [Zoph et al., 2018]

Hyperparameter Optimization

Finding the right hyperparameters for a machine learning algorithm A can be defined as an optimization problem:

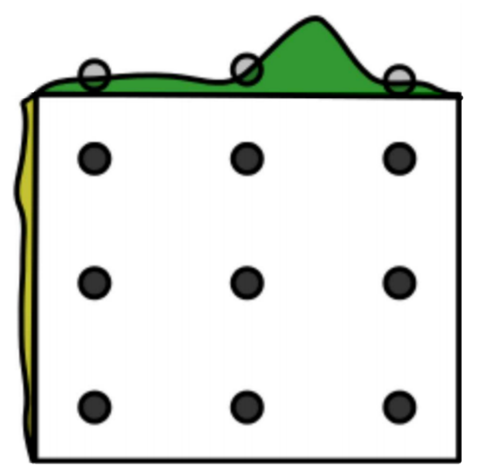
$$\boldsymbol{x}_\star \in \arg\min_{\boldsymbol{x} \in \mathbb{X}} f(\boldsymbol{x})$$

- $\boldsymbol{x}$ denotes all hyperparameters that should be optimized
- $\mathbb{X}$ is the configuration space which specifies the domain for each hyperparameter
- f measures the error of training A with hyperparameters $\boldsymbol{x}$, e. g. validation error
- we assume f to be noisy, i. e. we only observe $y(\boldsymbol{x}) = f(\boldsymbol{x}) + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, \sigma_{noise})$

Configspace

	Name	Range	Default	log scale	Type	Conditional
Network hyperparameters	batch size	$[32, 4096]$	32	✓	float	-
	number of updates	$[50, 2500]$	200	✓	int	-
	number of layers	$[1, 6]$	1	-	int	-
	learning rate	$[10^{-6}, 1.0]$	10^{-2}	✓	float	-
	L_2 regularization	$[10^{-7}, 10^{-2}]$	10^{-4}	✓	float	-
	dropout output layer	$[0.0, 0.99]$	0.5	✓	float	-
	solver type	{SGD, Momentum, Adam, Adadelta, Adagrad, smorm, Nesterov }	smorm3s	-	cat	-
	lr-policy	{Fixed, Inv, Exp, Step}	fixed	-	cat	-
Conditioned on solver type	β_1	$[10^{-4}, 10^{-1}]$	10^{-1}	✓	float	✓
	β_2	$[10^{-4}, 10^{-1}]$	10^{-1}	✓	float	✓
	ρ	$[0.05, 0.99]$	0.95	✓	float	✓
	momentum	$[0.3, 0.999]$	0.9	✓	float	✓
Conditioned on lr-policy	γ	$[10^{-3}, 10^{-1}]$	10^{-2}	✓	float	✓
	k	$[0.0, 1.0]$	0.5	-	float	✓
	s	$[2, 20]$	2	-	int	✓
Per-layer hyperparameters	activation-type	{Sigmoid, TanH, ScaledTanH, ELU, ReLU, Leaky, Linear}	ReLU	-	cat	✓
	number of units	$[64, 4096]$	128	✓	int	✓
	dropout in layer	$[0.0, 0.99]$	0.5	-	float	✓
	weight initialization	{Constant, Normal, Uniform, Glorot-Uniform, Glorot-Normal, He-Normal, He-Uniform, Orthogonal, Sparse}	He-Normal	-	cat	✓
	std. normal init.	$[10^{-7}, 0.1]$	0.0005	-	float	✓

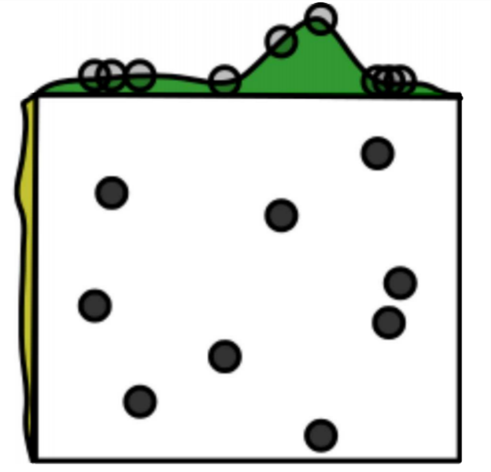
Grid Search



Grid Search

- easy to implement and to parallelize
- in continuous spaces unlikely to find the global optimum

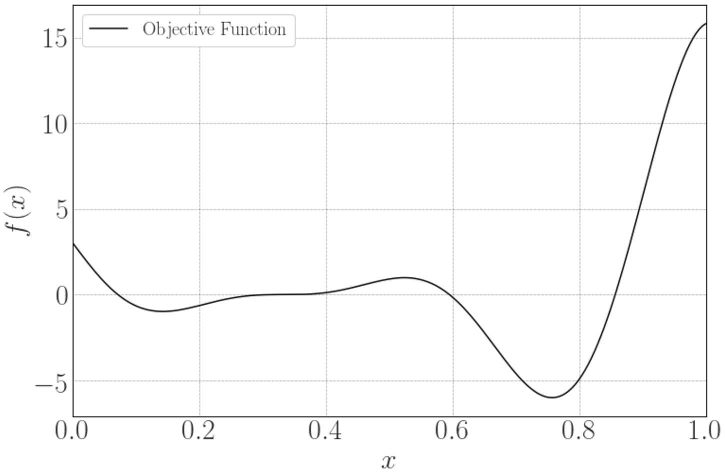
Random Search



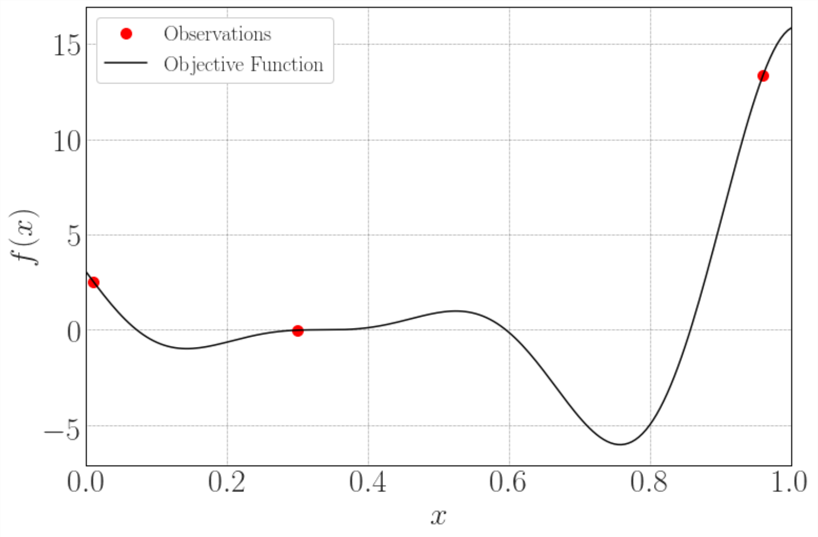
Random Search

- also easy to implement and to parallelize
- if all hyperparameters have non-zero probability, random search is guaranteed to converge to the global optimum
- cannot exploit knowledge obtain from previous function evaluations

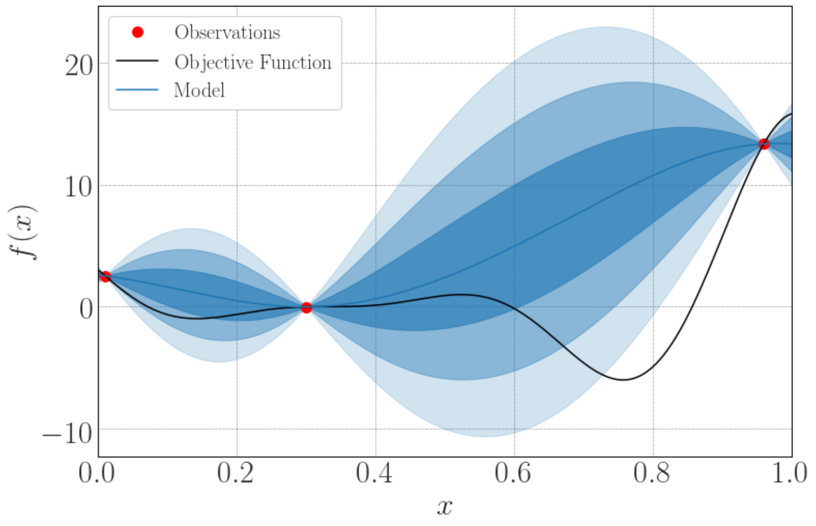
Bayesian optimization



Bayesian optimization



Bayesian optimization



Gaussian Process

We can model the objective function $f(\boldsymbol{x})$ with a Gaussian process [Rasmussen and Williams, 2006]:

$$f(\boldsymbol{x}) \sim \mathrm{GP}(\mu(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}'))$$

A Gaussian process is fully defined by:

- a mean function $\mu(\boldsymbol{x})$ which is usually set to $\mu(\boldsymbol{x}) = 0$
- a kernel function $k(\boldsymbol{x}, \boldsymbol{x}')$ which measures the similarity between two points $\boldsymbol{x}$ and $\boldsymbol{x}'$. For example the RBF kernel:

  $$k(x, x') = \theta_0 \cdot \exp\left(-\frac{\|x - x'\|^2}{\theta_1}\right)$$

  where θ_0 and θ_1 are hyperparameters.

Given new observed data D we can compute the posterior mean $\mu(\boldsymbol{x}|\theta, D)$ and variance $\sigma^2(\boldsymbol{x}|\theta, D)$ analytically.

Gaussian Process

Pros:

- smooth and reliable uncertainty estimates
- priors can easily be incorporated

Cons:

- not easily applicable in discrete or conditional spaces
- scales cubically with the number of data points
- sensitive to its own hyperparameters

Random Forest

Consists of T regression trees where each tree splits the input space into disjoint regions $S_0, \ldots S_{L-1}$ where L is the number of leafs. Tree prediciation for unseen points:

$$\tilde{\mu}(\boldsymbol{x}_\star) = \sum_{l=1}^{L} c_l \cdot \mathbb{I}(\boldsymbol{x}_\star \in S_i) \tag{1}$$

with $\mathbb{I}$ as the indicator function that returns 1 if $\boldsymbol{x}_\star \in S_i$ and 0 otherwise.

For unseen test points we can compute the predictive distribution by:

$$\mu(\boldsymbol{x}_\star) = \frac{1}{T} \sum_{t=1}^{T} \tilde{\mu}_t(\boldsymbol{x}_\star) \tag{2}$$

$$\sigma^2(\boldsymbol{x}_\star) = \frac{1}{T} \sum_{t=1}^{T} (\tilde{\mu}_t(\boldsymbol{x}_\star) - \mu(\boldsymbol{x}_\star))^2 \tag{3}$$

Random Forest

Pros:

- scales much better with data
- can easily handle categorical, continuous and discrete spaces
- fairly robust against its own hyperparameters

Cons:

- the uncertainty estimates are often poor
- do not extrapolate well
- priors cannot easily be incorporated

Bayesian Neural Networks

Bayesian neural networks use a Bayesian treatment of neural network weight to obtain uncertainty estimates (see [Springenberg et al., 2016, Snoek et al., 2015])

Pros:

- scales much better with data
- can easily handle categorical, continuous and discrete spaces
- given enough network samples obtain nice and smooth uncertainty estimates

Cons:

- need usually more data than Gaussian processes
- brittle against its own hyperparameters.

DNGO [Snoek et al., 2015]

- fit simple 3-layer feed forward neural network with linear output layer on $\boldsymbol{X}, \boldsymbol{y}$
- after training, remove output layer
- use features of last layer as basis functions for Bayesian linear regression to get uncertainty estimates

Recap Bayesian Linear Regression

Given some data points $\boldsymbol{X} \in \mathbb{R}^{N\times D}$ with targets $\boldsymbol{y} \in \mathbb{R}^{N}$ we model:

$$y_i = x_i \boldsymbol{w} + \varepsilon_i \tag{4}$$

where we assume that $\varepsilon_i \sim \mathcal{N}(0, \frac{1}{\beta})$

Recap Bayesian Linear Regression

By assuming a Gaussian prior $p(\boldsymbol{w} \mid \alpha) = \mathcal{N}(\boldsymbol{w} \mid 0, \alpha^{-1}\mathbb{I})$ we can compute the posterior in closed form $p(\boldsymbol{w} \mid \mathbf{m}, \mathbf{K})$ after observing some data $\boldsymbol{X}$, $\boldsymbol{y}$, where:

$$\mathbf{m} = \beta \mathbf{K}^{-1} \boldsymbol{X} \boldsymbol{y} \tag{5}$$

$$\mathbf{K} = \beta \boldsymbol{X}^T \boldsymbol{X} + \alpha \mathbb{I} \tag{6}$$

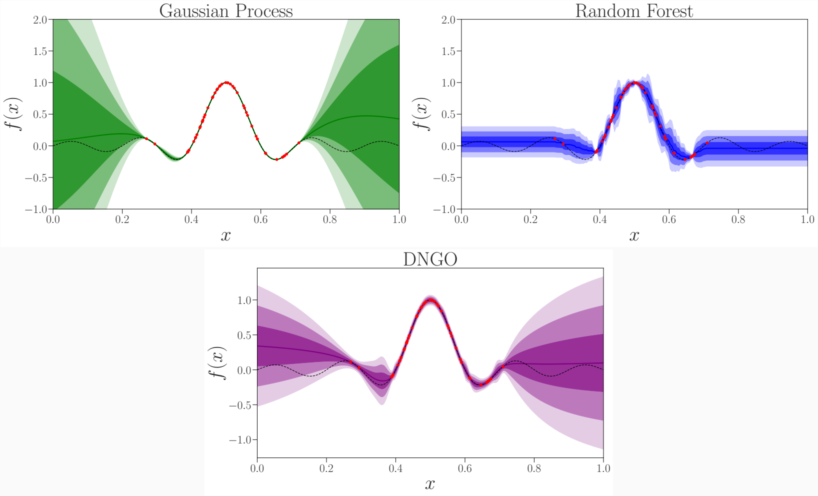
Recap Bayesian Linear Regression

For unseen test points $\boldsymbol{x}_\star$ the predictive distribution is a Gaussian $p(y_\star \mid \boldsymbol{x}_\star, \boldsymbol{X}, \boldsymbol{y}, \alpha, \beta) = \mathcal{N}(y_\star \mid m_\star, \sigma_\star^2)$:

$$m_\star = \mathbf{m}^T \boldsymbol{x}_\star \tag{7}$$

$$\sigma_\star = \frac{1}{\beta} + \boldsymbol{X}^T \mathbf{K} \boldsymbol{X} \tag{8}$$

Model Comparison



Exploitation vs Exploration

Given our model m and some data $D = \{(\boldsymbol{x}_0, y_0), \ldots (\boldsymbol{x}_n, y_n)\}$ how do we **decide** which hyperparameter configuration $\boldsymbol{x}_{n+1}$ we shall evaluate next?

Exploitation vs Exploration

Given our model m and some data $D = \{(\boldsymbol{x}_0, y_0), \ldots (\boldsymbol{x}_n, y_n)\}$ how do we **decide** which hyperparameter configuration $\boldsymbol{x}_{n+1}$ we shall evaluate next?

Naive solution: simply optimize $\mu(\boldsymbol{x})$, however, that would only pick points around the best observed point.

Exploitation vs Exploration

Given our model m and some data $D = \{(\boldsymbol{x}_0, y_0), \ldots (\boldsymbol{x}_n, y_n)\}$ how do we **decide** which hyperparameter configuration $\boldsymbol{x}_{n+1}$ we shall evaluate next?

Naive solution: simply optimize $\mu(\boldsymbol{x})$, however, that would only pick points around the best observed point.

We have to trade off between:

- **exploring** in regions of the configuration space where our model is uncertain
- however, since our ultimate goal is to locate the global optimum $\boldsymbol{x}_\star$, we also want to **exploit** in the good regions of the configuration space

Acquisition Functions

We use an acquisition function $a(\boldsymbol{x})$ that automatically trades off exploration and exploitation.

To find the next point $\boldsymbol{x}_{n+1}$ we numerically optimize $a(\boldsymbol{x})$:

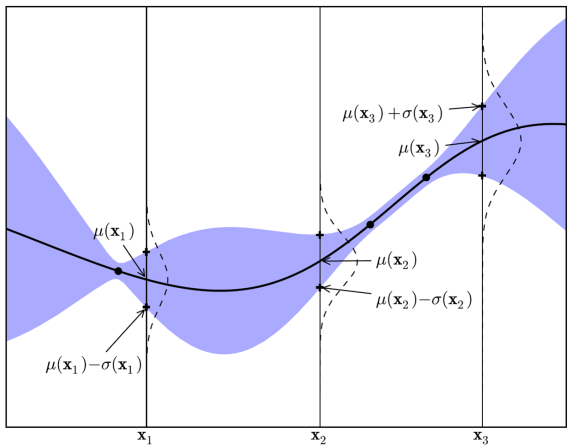
$$\boldsymbol{x}_{n+1} \in \arg\max_{\boldsymbol{x} \in \mathbb{X}} a(\boldsymbol{x})$$

Since the acquisition function only depends on our model, it is cheap to evaluate and often provides gradient information.

Common ways to optimize the acquisition function:

- Gradient Ascent
- Evolutionary Algorithms
- Local Search
- Random Search

Upper Confidence Bound



Upper Confidence Bound [Srinivas et al., 2010]

Computes the acquisition function by:

$$a(\boldsymbol{x}) = \mu(\boldsymbol{x}) + \beta\sigma(\boldsymbol{x})$$

- β is a hyperparameter that controls exploration and exploitation
- under some assumptions, you can proof that UCB converges to the global optimum

Expected Improvement [Jones et al., 1998]

Probably the most often used acquisition function is expected improvement, which computes:

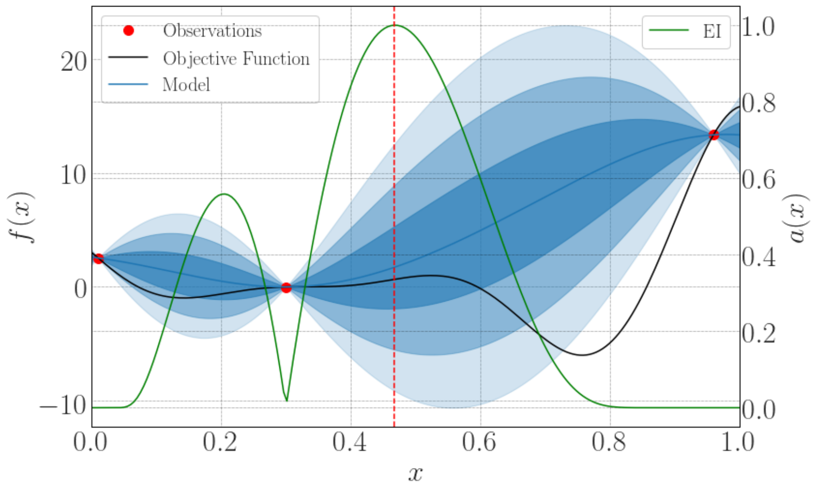
$$a(\boldsymbol{x}) = E_{p(f|D)}[\max(y_\star - f(\boldsymbol{x}), 0)].$$

where $y_\star \in \arg\min\{y_0, \ldots, y_n\}$. Assuming $p(f|D)$ to be a Gaussian, we can compute EI in closed form by:

$$a(\boldsymbol{x}) = \sigma(\boldsymbol{x})(\gamma(\boldsymbol{x})\Phi(\gamma(\boldsymbol{x})) + \phi(\gamma(\boldsymbol{x})))$$

here $\gamma(\boldsymbol{x}) = \frac{y_\star - \mu(\boldsymbol{x})}{\sigma(\boldsymbol{x})}$ and Φ is the CDF and ϕ is the PDF of a standard normal distribution.

Acquisition Functions



Bayesian Optimization [Jones et al., 1998]

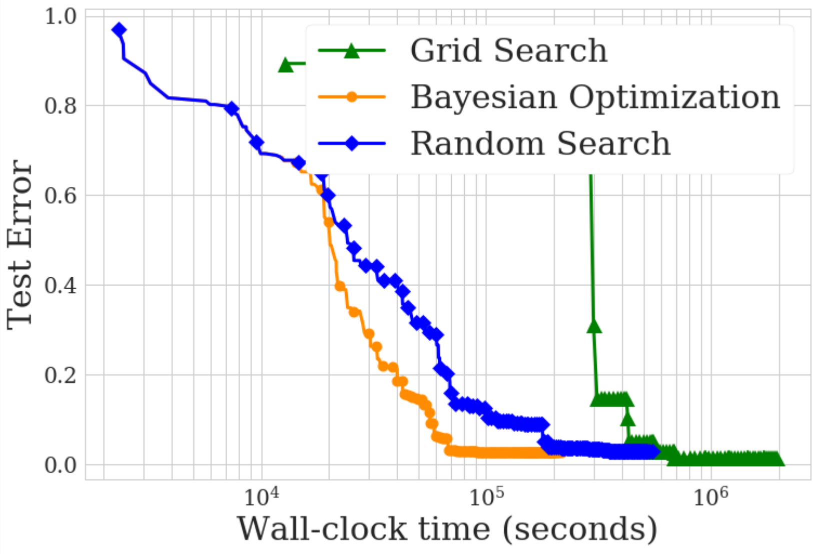
Algorithm 1 Bayesian Optimization

```
Initialize data $D_0$ using an initial design.
for $t = 1, 2, \ldots$ do
    Fit probabilistic model for $f(\boldsymbol{x})$ on data $D_{t-1}$
    Choose $\boldsymbol{x}_t$ by maximizing the acquisition function $a(\boldsymbol{x})$
    Evaluate $y_t \sim f(\boldsymbol{x}_t) + \mathcal{N}(0, \sigma^2)$, and augment the data: $D_t = D_{t-1} \cup \{(\boldsymbol{x}_t, y_t)\}$
    Choose incumbent $\hat{\boldsymbol{x}}_t \leftarrow \arg\min\{y_1, \ldots y_t\}$
```

Bayesian optimization

- uses a probabilistic model to guide the search towards the global optimum
- under some assumptions converges to the global optimum
- more tricky to implement, especially in a parallel setting

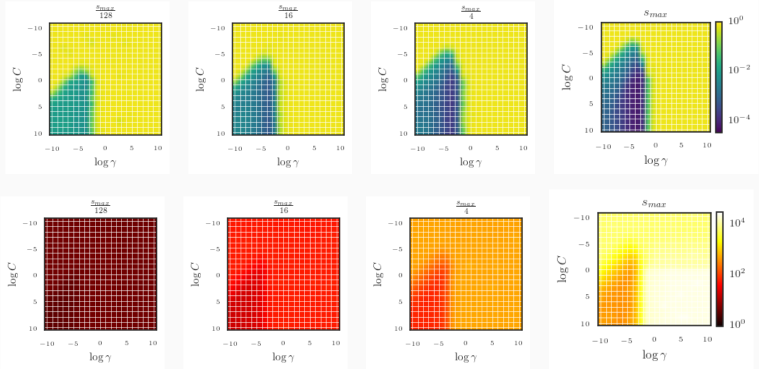
Bayesian Optimization



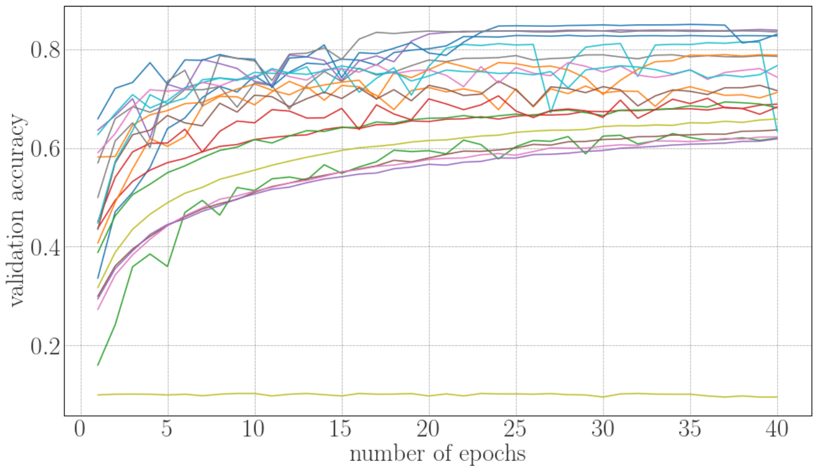
Multi-fidelity Optimization

- Even though Bayesian optimization is *sample efficient*, it still requires tens to hundreds of function evaluations.
- We often have access to *cheap-to-evaluate* approximations $\tilde{f}(\cdot, b)$ of of the true objective function $f(\cdot)$, so called **fidelities**.
- Each fidelity is parameterized by a so-called *budget* $b \in [b_{min}, b_{max}]$.
  - if $b = b_{max}$: then $\tilde{f}(\cdot, b_{max}) = f(\cdot)$
  - if $b < b_{max}$: then $\tilde{f}(\cdot, b)$ is only an approximation of $f(\cdot)$ whose quality typically increases with b.

Dataset Subsets [Klein et al., 2017]



Learning Curves



Successive Halving [Jamieson and Talwalkar, 2016]

Algorithm 2 Successive Halving

Require: initial budget b_0, maximum budget b_{max}, set of n configurations $C = \{c_1, c_2, \dots c_n\}$

```
b = b_0
while b ≤ b_max do
    L = {f̃(c, b) : c ∈ C}
    C = top_k(C, L, ⌊|C|/η)⌋
    b = η · b
```

$b = b_0$

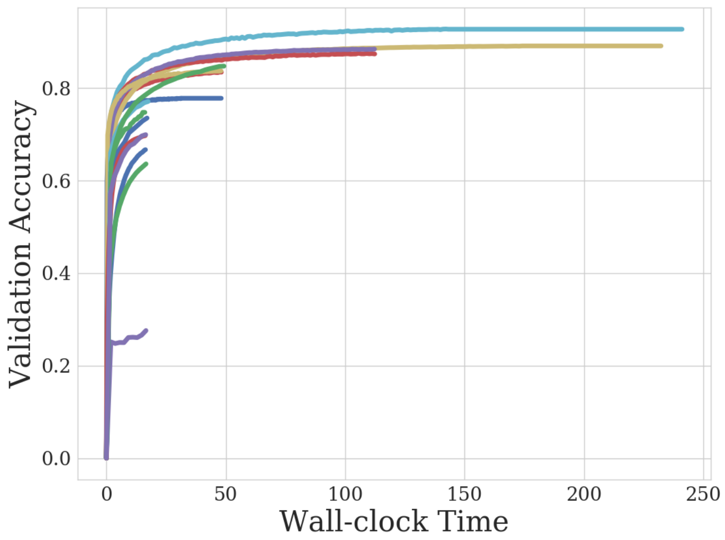
while $b \leq b_{max}$ **do**

$\quad L = \{\tilde{f}(c, b) : c \in C\}$

$\quad C = \mathrm{top_k}(C, L, \lfloor |C|/\eta)\rfloor$

$\quad b = \eta \cdot b$

Successive Halving



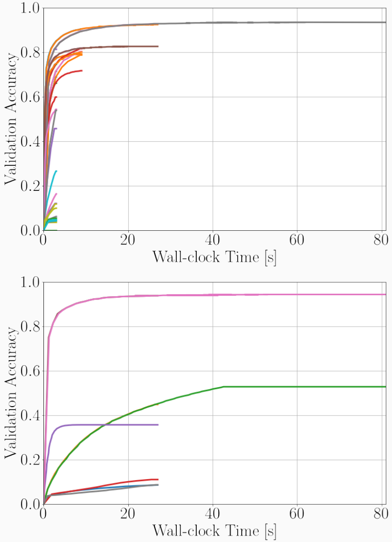
Hyperband [Li et al., 2017]

Algorithm 3 Hyperband

Require: budgets b_{min} and b_{max}, η

$s_{max} = \lfloor \log_\eta \frac{b_{max}}{b_{min}} \rfloor$
for $s \in \{s_{max}, s_{max} - 1, \ldots, 0\}$ **do**
  sample $n = \lceil \frac{s_{max}+1}{s+1} \cdot \eta^s \rceil$ configurations
  run SH on them with $\eta^s \cdot b_{max}$ as initial budget

Hyperband


Validation Accuracy
Wall-clock Time [s]
0.0
0.2
0.4
0.6
0.8
1.0
0
20
40
60
80

Hyperband vs. Bayesian Optimization [Falkner et al., 2018]

Hyperband:

- very efficient in terms of anytime performance
- due to the random sampling, cannot reuse previously gain knowledge and take a long time to converge

Bayesian optimization:

- in its standard form it cannot exploit fidelites (however, several extensions exist)
- in the most cases converges faster than random search

Can we combine both methods?

Tree of Parzen Estimators [Bergstra et al., 2011]

We fit two kernel density estimator for the good and bad configurations:

$$l(\boldsymbol{x}) = p(y < \alpha | \boldsymbol{x}, D)$$
$$g(\boldsymbol{x}) = p(y > \alpha | \boldsymbol{x}, D)$$

To select a new candidate $\boldsymbol{x}_{new}$ to evaluate, it maximizes the ratio $\frac{l(\boldsymbol{x})}{g(\boldsymbol{x})}$, which is equivalent of optimizing expected improvement.

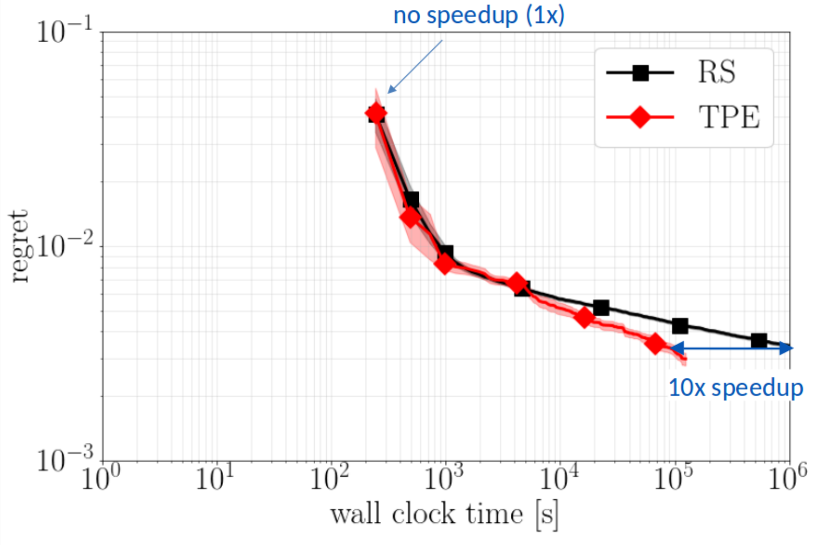
BOHB [Falkner et al., 2018]

Algorithm 4 Pseudocode for sampling in BOHB

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

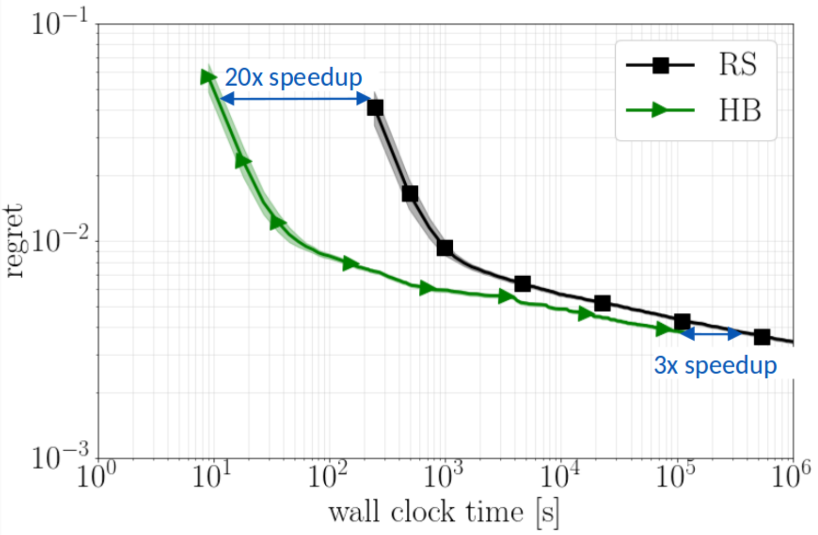
if rand() $\leq \rho$ **then**
    return random configuration
$b = \arg\max \left\{ D_b : |D_b| \geq N_{min} + 2 \right\}$
if $b = \emptyset$ **then**
    return random configuration
fit KDEs as in TPE but for each budget b
draw N_s samples according to $l'(\boldsymbol{x})$
return sample with highest ratio $l(\boldsymbol{x})/g(\boldsymbol{x})$

BOHB



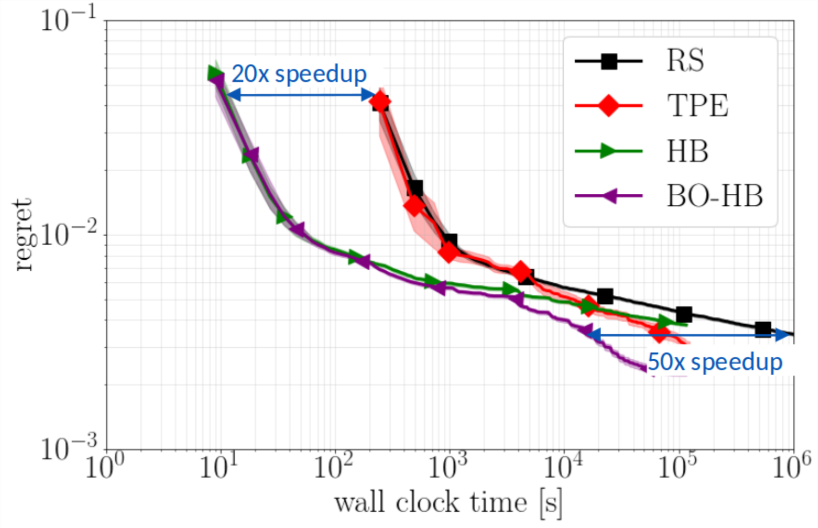
no speedup (1x)
RS
TPE
10x speedup
regret
10^{-1}
10^{-2}
10^{-3}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
wall clock time [s]

BOHB



RS
HB
20x speedup
3x speedup
10^{-1}
10^{-2}
10^{-3}
regret
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
wall clock time [s]

BOHB

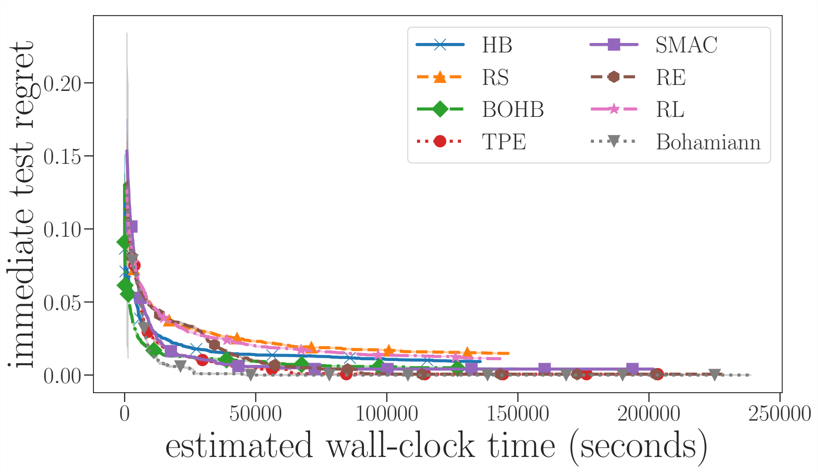


regret
10^{-1}
10^{-2}
10^{-3}
10^0
10^1
10^2
10^3
10^4
10^5
10^6
wall clock time [s]
RS
TPE
HB
BO-HB
20x speedup
50x speedup

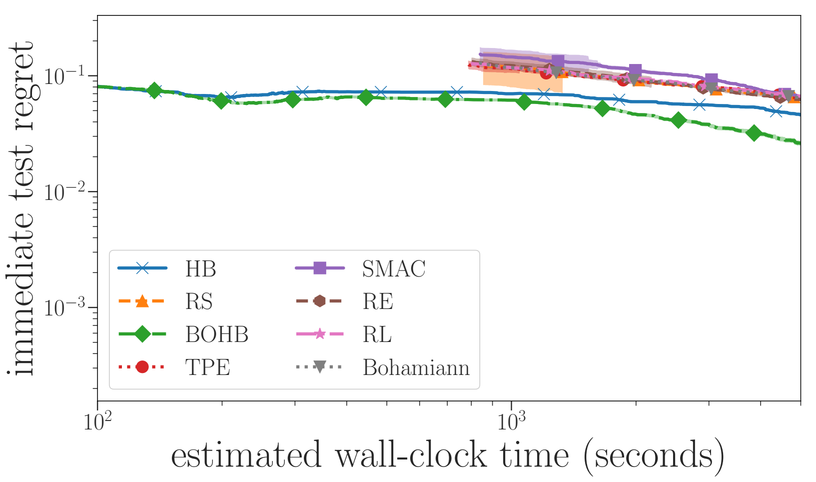
Benchmarking

- Benchmarking is important to make further progress in the field
- Large computational demands make thorough benchmarking extremely expensive
- In practice this slows down development of new methods

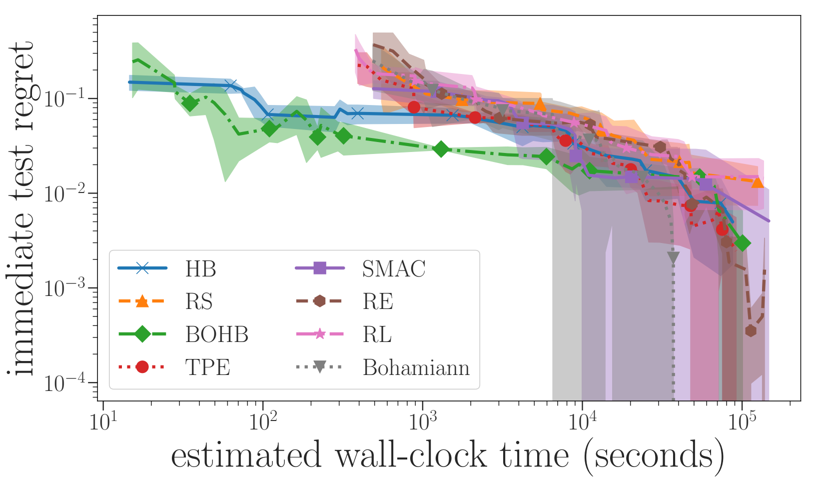
Benchmarking Pitfalls



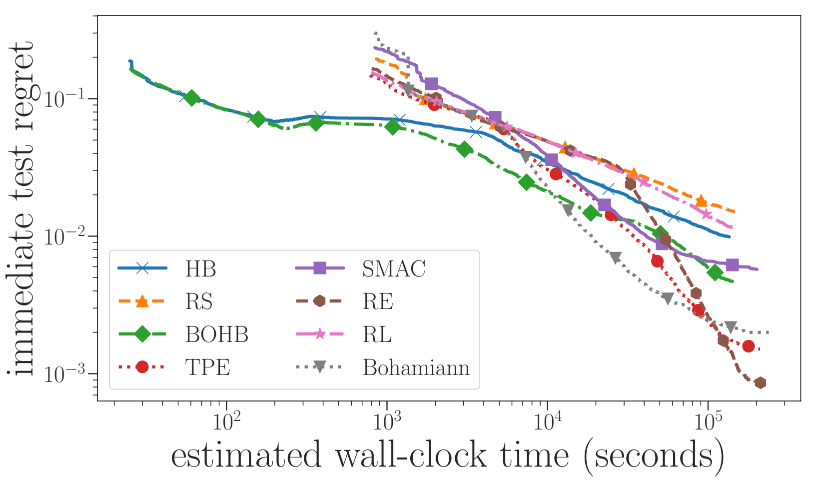
Benchmarking Pitfalls



Benchmarking Pitfalls



Benchmarking Pitfalls



Pro Tips for Benchmarking

- Almost all optimizers are **randomized**, i.e depend on the seed, thus, we need a sufficent amount of independent runs to getter a better estimate of a optimizer's performance
- Run all optimizers **sufficiently long**, since in the beginning the most methods do not work better than random
- Plot the **performance over time** rather than just the final performance
- Use **log-scales** and learn how to read them

Conclusions

- Bayesian optimization is an efficient strategy for hyperparameter optimization
- By using fidelities of the objective function we can speed up the optimization procedure
- Hyperband is an extension of random search that exploits multi-fidelity of the objective function,
- BOHB combines Hyperband with Bayesian optimization to combine the strengths of both methods
- Benchmarking plays an important role in developing new methods

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