AutoML: Dynamic Configuration & Learning

Learning to Learn: Supervised

Bernd Bischl Frank Hutter Lars Kotthoff
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- First idea: learn weight updates of a neural network

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[Andrychowicz et al. 2016]

Weight updates (note: θ denote DNN weights):

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Even more general:

$$\theta^{(t+1)} = \theta^{(t)} + g^{(t)}(\nabla f(\theta^{(t)}), \phi)$$

where g is the optimizer and ϕ are the parameters of the optimizer g.

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$\rightsquigarrow$ Goal: Optimize f wrt θ by learning g (resp. ϕ)

Learning to Learn: Objective [Andrychowicz et al. 2016]

$$L(\phi) = \mathbb{E}\left[f(\theta^*(f, \phi))\right]$$

where L is a loss function and $\theta^*(f, \phi)$ are the optimized weights θ^* by using the optimizer parameterized with ϕ on function f.

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$$\theta^{(t+1)} = \theta^{(t)} + g^{(t)}$$

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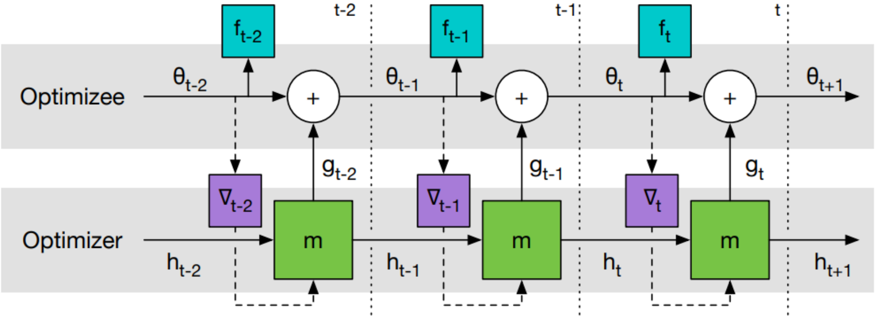
$\rightsquigarrow$ "Learning to learn gradient descent by gradient descent"

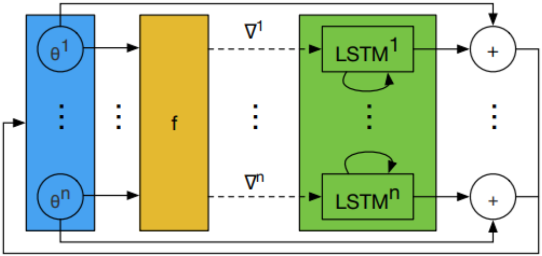
Learning to Learn: LSTM approach [Andrychowicz et al. 2016]

Optimizee Target network to be trained

Optimizer LSTM with hidden state h_t that predicts weight updates g_t



Learning to Learn: Coordinatewise LSTM optimizer [Andrychowicz et al. 2016]



- One LSTM for each coordinate (i.e., weight)
- All LSTMs have shared parameters ϕ
- Each coordinate has its own separate hidden state

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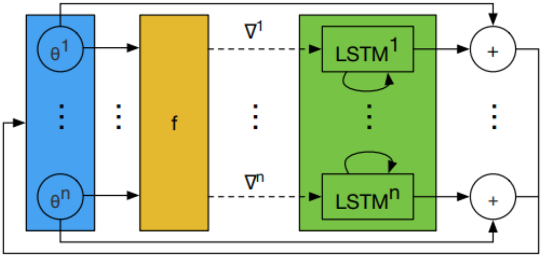

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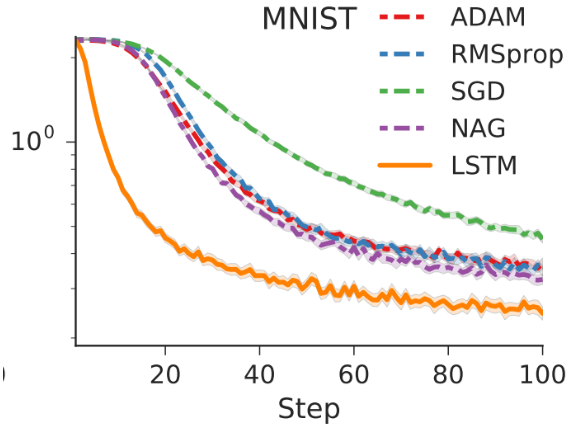
$\rightsquigarrow$ We can train the LSTM on k weights and apply it larger DNNs with k' weights, where $k \leq k'$

Learning to Learn with LSTM: Results [Andrychowicz et al. 2016]



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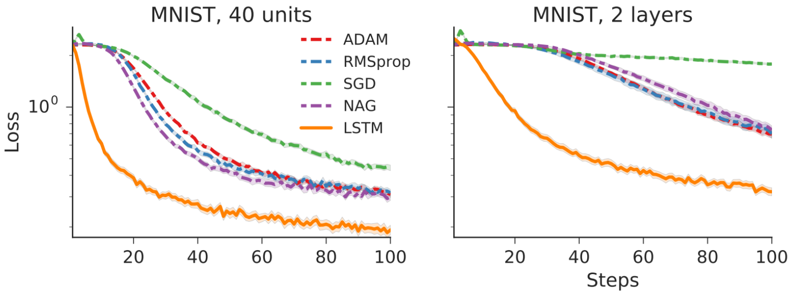
Changing the original architecture of the DNN:



⇝ learnt optimizer is robust against some architectural changes

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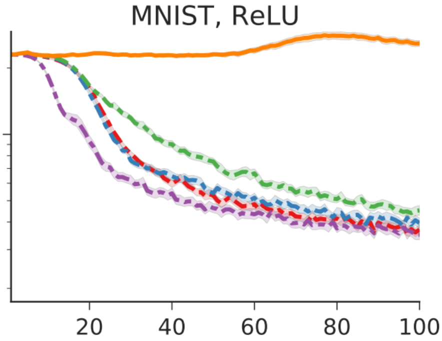
Changing the activation function to ReLU:



$\rightsquigarrow$ fails on other activation functions

Learning Black-box Optimization [Chen et al. 2017]

Black Box Optimization Setting

$$\mathbf{x}^* \in \arg\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

1. Given the current state of knowledge $h^{(t)}$ propose a query point $\mathbf{x}^{(t)}$
2. Observe the response $y^{(t)}$
3. Update any internal statistics to produce $h^{(t+1)}$

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Learning Black Box Optimization

Essentially, a similar idea as before:

$$\begin{aligned} h^{(t)}, \mathbf{x}^{(t)} &= \mathsf{RNN}_\phi(h^{(t-1)}, \mathbf{x}^{(t-1)}, y^{(t)}) \\ y^{(t)} &\sim p(y|\mathbf{x}^{(t)}) \end{aligned}$$

- Using recurrent neural network (RNN) to predict next x_t.
- $h^{(t)}$ is the internal hidden state

Learning Black-box Optimization: Loss Functions [Chen et al. 2017]

- Sum loss: Provides more information than final loss

$$L_{\text{sum}}(\phi) = \mathbb{E}_{f,y^{(1:T-1)}}\left[\sum_{t=1}^{T} f(\mathbf{x}^{(t)})\right]$$

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  - requires model (e.g., GP)

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- Observed Improvement Loss:

$$L_{\mathsf{OI}}(\phi) = \mathbb{E}_{f,y^{(1:T-1)}}\left[\sum_{t=1}^{T} \min\left\{f(\mathbf{x}^{(t)}) - \min_{i<t}(f(\mathbf{x}^{(i)})), 0\right\}\right]$$

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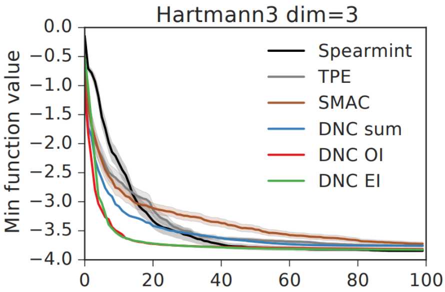

- Hartmann3 is an artificial function with 3 dimensions

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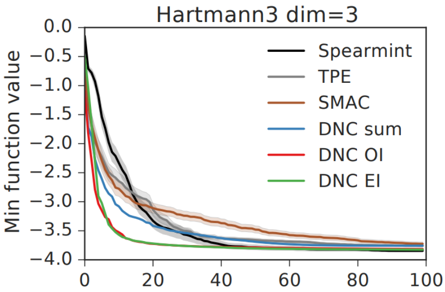

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⇝ L_{OI} and L_{EI} perform best

⇝ L_{OI} easier to compute than L_{EI}
because we need a predictive model to compute EI

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Learning to Learn: Reinforcement Learning

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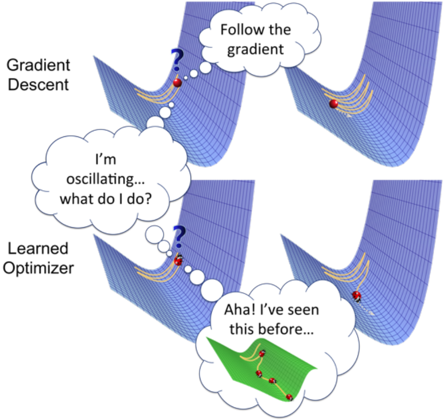
Learning to Optimize via Reinforcement Learning [Li and Malik. 2017]



Source: `https://bair.berkeley.edu/blog/2017/09/12/learning-to-optimize-with-rl/`

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Reinforcement Learning for Learning to Optimize

State current location, objective values and gradients evaluated at the current and past locations

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Cost/Reward Objective value at the current location

- Since the RL agent will optimize the cumulative cost, this is equivalent to L_{sum} [Chen et al. 2017] $(\gamma = 0)$
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Training Set randomly generated objective functions

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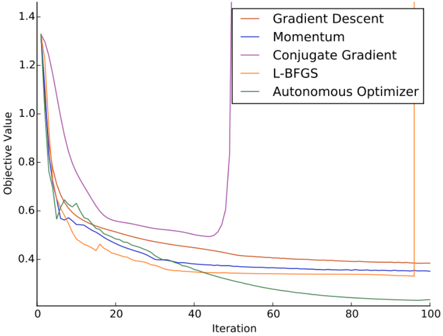

- 2-layer DNN with ReLUs
- Training datasets for training RL agent:
  four multivariate Gaussians and sampling 25 points from each
  - $\rightsquigarrow$ hard toy problem

Learning Acquisition Functions [Volpp et al. 2019]

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- Idea: Learn a *neural acquisition function* from data

$\rightsquigarrow$ Replace acquisition function

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 T

$\mathcal{D}^{(0)} \leftarrow$ initial_design($\mathcal{X}$);
for $t = 1, 2, \dots T - |D_0|$ **do**
  $\hat{c} : \mathbf{x} \mapsto c(\mathbf{x}) \leftarrow$ fit predictive model on $\mathcal{D}^{(t-1)}$;
  select $\mathbf{x}^{(t)}$ by optimizing $\mathbf{x}^{(t)} \in \arg\max_{\mathbf{x} \in \mathcal{X}} \alpha(\mathbf{x}; \mathcal{D}^{(t-1)}, \hat{c})$;
  Query $y^{(t)} := f(\mathbf{x}^{(t)})$;
  Add observation to data $D^{(t)} := D^{(t-1)} \cup \{\langle \mathbf{x}^{(t)}, y^{(t)} \rangle\}$;
return *Best* $\mathbf{x}$ *according to* D *or* $\hat{c}$

Neural Acquisition Function [Volpp et al. 2019]

Although the acquisition function α depends on the history $\mathcal{D}^{(t-1)}$ and the predictive model $\hat{c}$, α mainly makes use of the predictive mean μ and variance σ^2.

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Neural acquisition function (AF):

$$\alpha_\theta(\mathbf{x}) = \alpha_\theta(\mu^{(t)}(\mathbf{x}), \sigma^{(t)}(\mathbf{x}), \mathbf{x}, t, T)$$

where θ are the parameters of a neural network, and μ, σ, $\mathbf{x}$, t, T are its inputs.

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Policy π_θ: Neural acquisition function α_θ

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Reward $r^{(t)}$: negative simple regret: $r^{(t)} = f(\mathbf{x}^*) - f(\hat{\mathbf{x}})$

- assumes that we can estimate the optimal $\mathbf{x}^*$ for *training* functions

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Transition probability : Noisy evaluation of f and the predictive model update

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- $\alpha_\theta(\xi_i)$ are interpreted as the logits of categorical distribution, s.t.

$$\pi_\alpha(\cdot \mid s^{(t)}) = \mathsf{Cat}\left[\alpha_\theta(\xi_1), \ldots, \alpha_\theta(\xi_N)\right]$$

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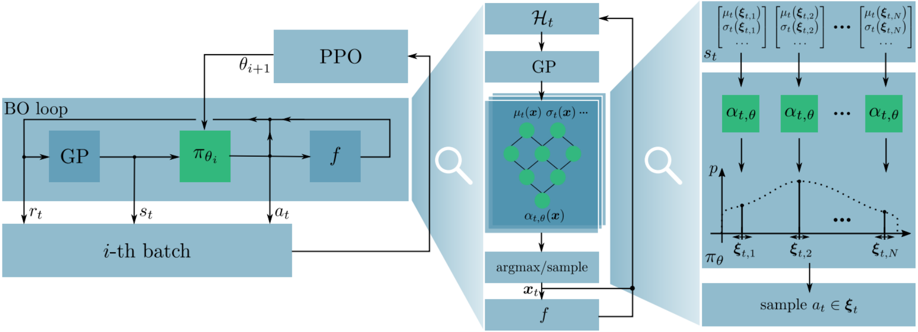
- Due to curse of dimensionality, we need a two step approach for $\xi^{(t)}$
  1. sample ξ_{global} using a coarse Sobol grid
  2. sample ξ_{local} using local optimization starting from the best samples in ξ_{global}

$\rightsquigarrow$ $\xi^{(t)} = \xi_{\text{global}} \cup \xi_{\text{local}}$

Learning Acquisition Functions: Overview [Volpp et al. 2019]

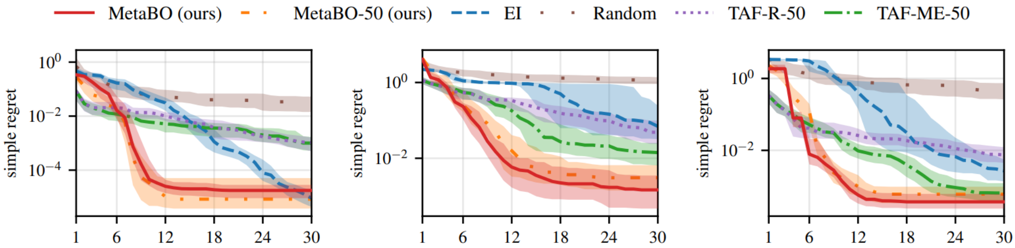


MetaBO Training Loop

Neural AF in the BO loop

Policy architecture

Results on Artificial Functions [Volpp et al. 2019]



(a) Branin ($D = 2$) (b) Goldstein-Price ($D = 2$) (c) Hartmann-3 ($D = 3$)

- Approach by [Volpp et al. 2019] called MetaBO
- MetaBO performs better than other acquisition functions (EI, GP-UCB, PI) and other baselines (Random, TAF)

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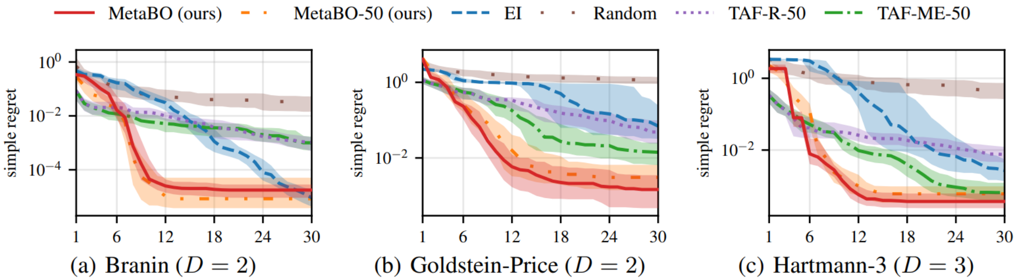

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Assumption: You have a family of functions at hand that resembles your target function.

AutoML: Dynamic Configuration & Learning

Learning to Adjust Learning Rates

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Learning Problem [Daniel et al. 2016]

- Optimization of a function:

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$$F(\mathbf{X}; \theta) = \frac{1}{N} \sum_{i=1}^{N} f(\mathbf{x}^{(i)}; \theta)$$

Learning Step Size Policies [Daniel et al. 2016]

- Idea: Learn the hyperparameters of the weight update (short notation)

$$\theta^{(t+1)} = \theta^{(t)} - \alpha^{(t)} \nabla F(\theta^{(t)})$$
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- Note(ii): later we denote the learnt hyperparameters as λ

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- Idea: Learn the hyperparameters of the weight update (short notation)

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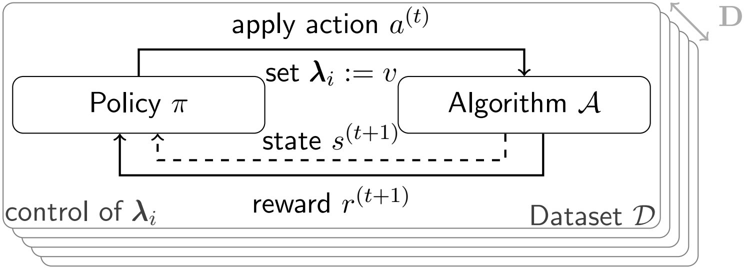
$$\nabla F(\theta^{(t)}) = \frac{1}{N} \sum_{i=1}^{N} \nabla f_i(\theta^{(t)})$$

- For SGD, this would be for example the learning rate α
- Note (i): α have to be adapted in the course of the training
  - similar to learning rate schedules (e.g., cosine annealing)
- Note(ii): later we denote the learnt hyperparameters as λ
- Idea: Use reinforcement learning to learn a policy $\pi : s \mapsto a$ to control the learning rate (or other adaptive hyperparameters)

Recap: Reinforcement Learning for Dynamic Algorithm Configuration



To apply that, we need to define:

1. State description
2. Action space
3. Reward function

RL for Step Size Policies: State [Daniel et al. 2016]

Predictive change in function value:

$$s_1 = \log\left(\mathsf{Var}(\Delta\tilde{f}_i)\right)$$

$$\Delta\tilde{f}_i = \tilde{f}(\mathbf{x}^{(i)};\theta+\delta\theta) - f(\mathbf{x}^{(i)};\theta)$$

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Uncertainty Estimate (noise level):

$$s_{K+i} \leftarrow \gamma s_{K+i} + (1 - \gamma)(s_i - \hat{s}_i)^2$$

RL for Step Size Policies: Learning [Daniel et al. 2016]

Reward (average loss improvement over time):

$$r = \frac{1}{T-1} \sum_{t=2}^{T} \left(\log(L^{(t-1)}) - \log(L^{(t)}) \right)$$

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- can be learnt for example via Relative Entropy Policy Search (REPS) [Peter et al. 2010]

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- Goal: obtain robust policies,
  i.e., good performance for many different DNN architectures
  - $\rightsquigarrow$ Sample architectures e.g., with different numbers of filters and layers
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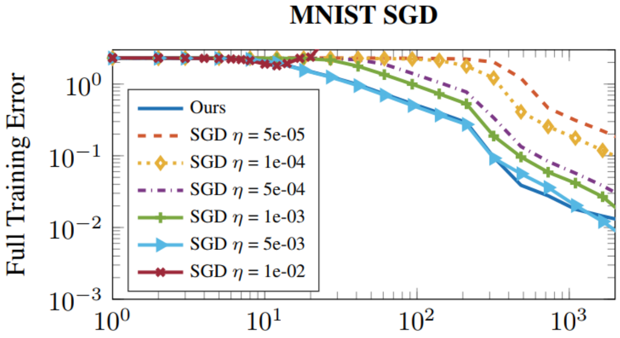

"Ours" refers to the approach by [Daniel et al. 2016] and η is the learning rate

AutoML: Dynamic Configuration & Learning

Dynamic Configuration

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

Iterative Optimization Heuristics

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  1. the algorithm's behavior changes over time
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- other examples: restart probability of search, mutation rate of evolutionary algorithms, ...

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- Still not guaranteed that optimal setting of e.g. learning rate schedules will lead to optimal learning behavior
  - Learning rate schedules are only heuristics

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- So far, we assumed that an algorithm runs with static settings
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the *dynamic algorithm configuration problem* is to obtain a policy $\pi^* : s_t \times \mathcal{D} \mapsto \boldsymbol{\lambda}$ by optimizing its cost across a distribution of datasets:

$$\pi^* \in \arg\min_{\pi \in \mathbf{\Pi}} \int_{\mathbf{D}} p(\mathcal{D}) c(\pi, \mathcal{D}) \, \mathrm{d}\mathcal{D}$$

Dynamic Algorithm Configuration as Contextual MDP [Biedenkapp et al. 2020]

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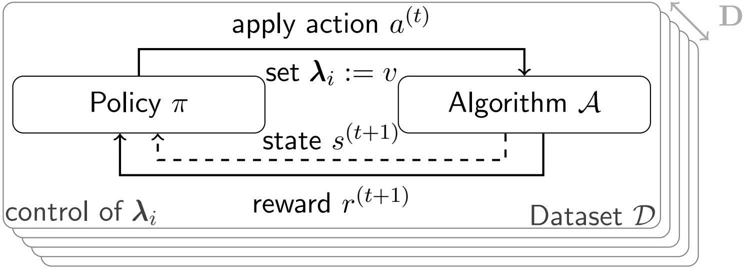
Context $\mathcal{D}$	A given dataset (or task)



Solving Dynamic Algorithm Configuration

Solve unknown MDP by using reinforcement learning (RL):

$$\mathcal{V}_{\mathcal{D}}^{\pi}(s^{(t)}) = \mathbb{E}\left[\sum_{k=0}^{\infty} \gamma^k r_{\mathcal{D}}^{(t+k+1)} | s^{(t)} = s\right]$$

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$$\max_{\pi, \mathbf{v}} \mathcal{C}(\pi, \mathbf{v}, K) = \sum_{i=1}^{|\mathbf{D}|} \mathbf{v}_i \mathcal{R}_i(\pi) - \frac{1}{K} \sum_{i=1}^{|\mathbf{D}|} \mathbf{v}_i$$

with θ being the agent's policy parameters and
$\mathbf{v}$ being a masking vector for choosing the tasks at hand.

AutoML: Dynamic Configuration & Learning

Overview

Bernd Bischl   Frank Hutter   Lars Kotthoff
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Black vs. Grey vs. White Box

- Often we treat AutoML as a black-box problem
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$\rightsquigarrow$ Goal: Replace algorithm components by learned policies

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- Main component is the heuristic for proposal mechanism of new solution candidates

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Learning to Learn: L2L

The goal of L2L is to learn a proposal mechanism from data.

AutoML: Dynamic Configuration & Learning

Population-based Training

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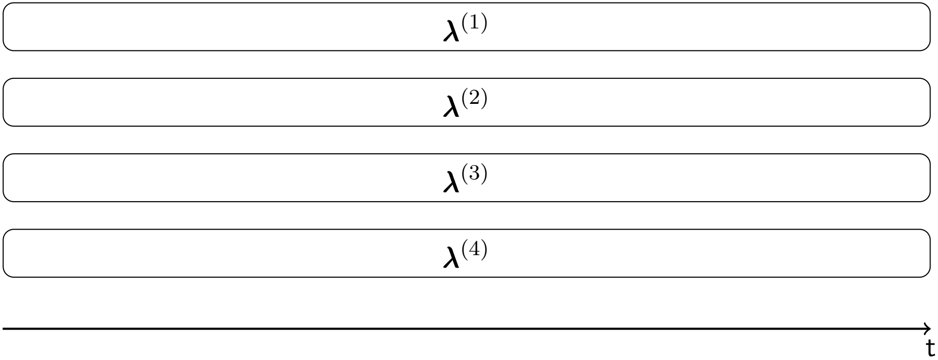
$\rightsquigarrow$ Try to figure out best hyperparameter settings on the fly

Massively parallelized Random Search



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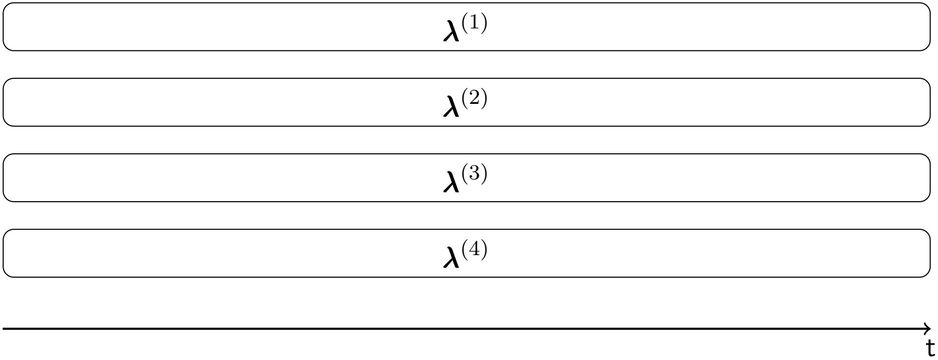

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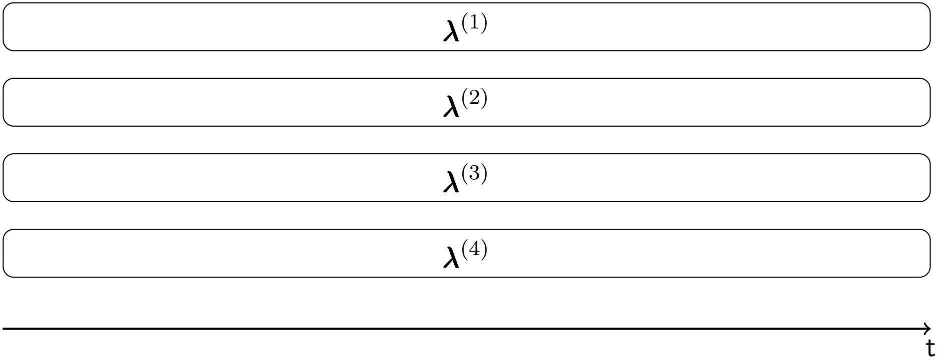

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Population-based Training [Jaderberg et al. 2017]

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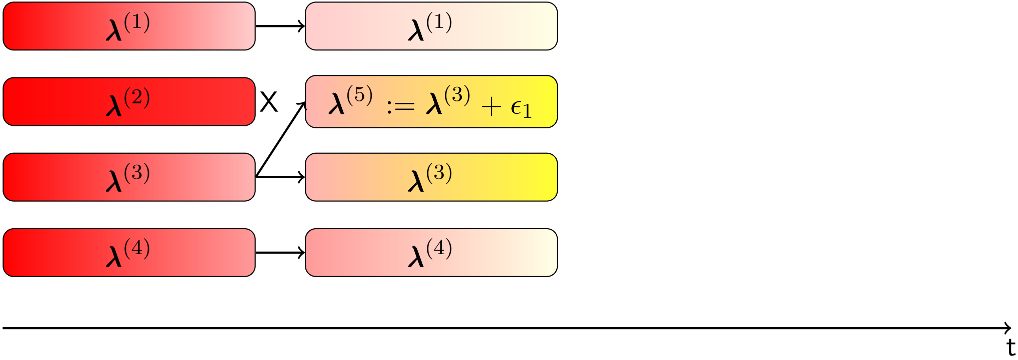

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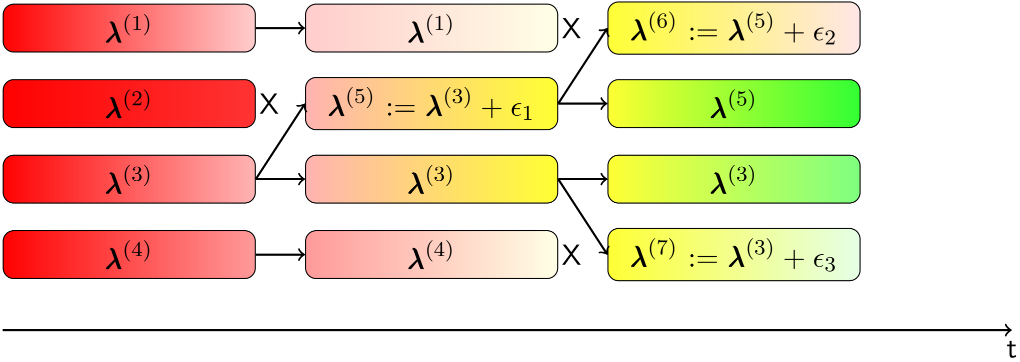

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Population-based Training [Jaderberg et al. 2017; Liang et al. 2020]

General workflow of PBT:

1. Sample initial population
   - Each population member is a combination of hyperparameter setting $\boldsymbol{\lambda}$ and (partially trained) model

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- Since hyperparameter settings changes while training the models,
  PBT relates to dynamic algorithm configuration
- Since each population member (i.e., model) can be trained independently,
  PBT can be efficiently parallelized
  - $\rightsquigarrow$ Drawback: requires substantial parallel compute resources

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PBT + BO: Outline

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  - Hallucinate performance of other hyperparameter settings in optimistically, pessimistically or in expectation of the current surrogate model

PBT + BO: Parallel Evaluation [Parker-Holder et al. 2020]

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- Remark: Also add $c^{(t-1)}$ as an input to the BO-surrogate model to ease the task of predicting the improvement