AutoML: Dynamic Configuration & Learning

Overview

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

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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

Dynamic Configuration

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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
- However, settings, such as learning rate, have to be adapted over time

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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]

State $s^{(t)}$ are described by statistics gathered in the algorithm run

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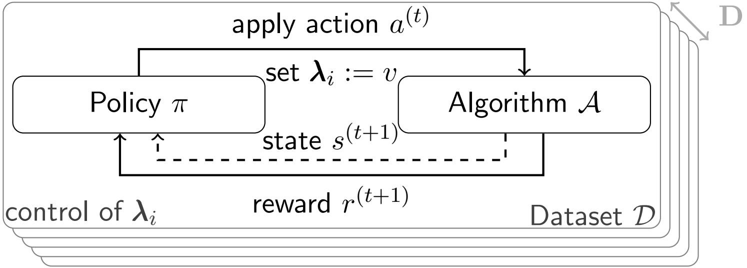
Context $\mathcal{D}$ A given dataset (or task)



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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$$\pi^* \in \arg\max_{\pi \in \mathbf{\Pi}} \int_{\mathbf{D}} p(\mathcal{D}) \int_{\mathcal{S}^{(0)}} \Pr(s^{(0)}) \cdot \mathcal{V}^{\pi}_{\mathcal{D}}(s^{(0)}) \, \mathrm{d}s^{(0)} \, \mathrm{d}\mathcal{D}$$

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$\rightsquigarrow$ equivalent to Dynamic Algorithm Configuration definition

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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.

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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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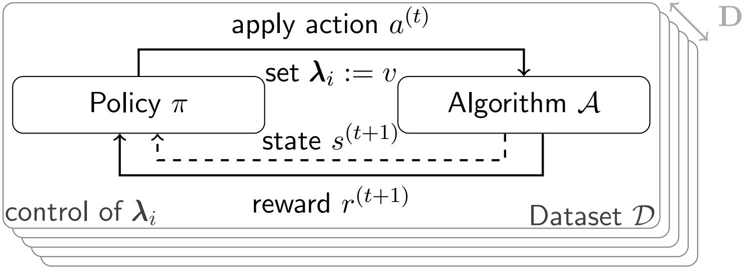
- Idea: Use reinforcement learning to learn a policy $\pi : s \mapsto a$ to control the learning rate (or other adaptive hyperparameters)

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):

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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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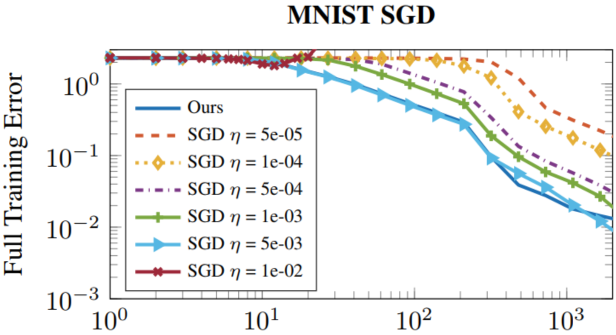

"Ours" refers to the approach by [Daniel et al. 2016] and η is the learning rate

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Population-based Training

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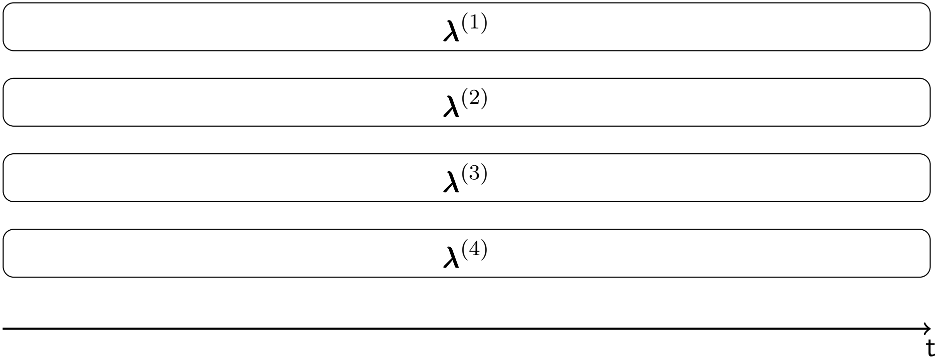
$\rightsquigarrow$ Try to figure out best hyperparameter settings on the fly

Massively parallelized Random Search



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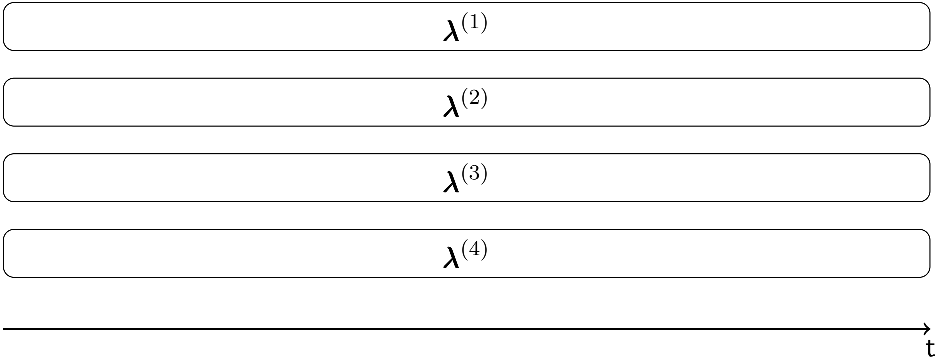

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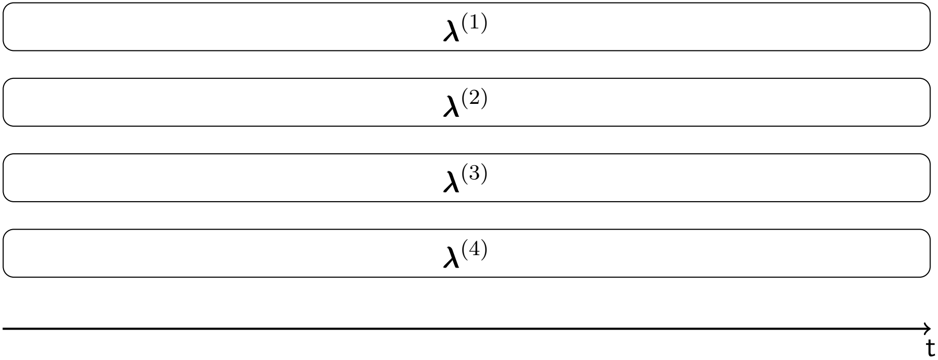

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Population-based Training [Jaderberg et al. 2017]

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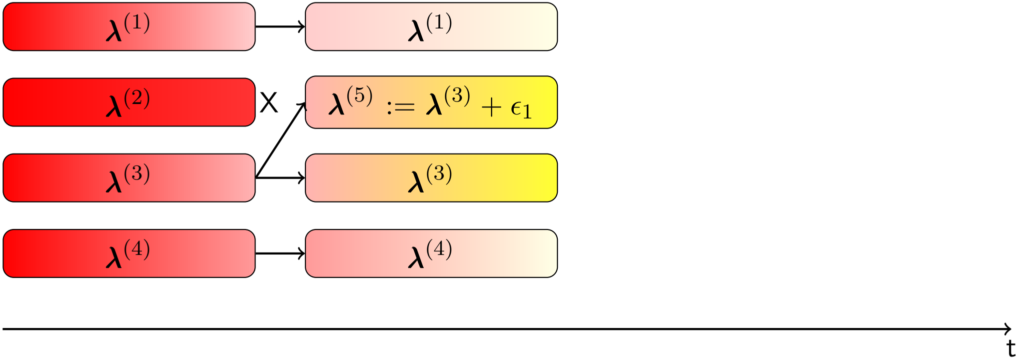

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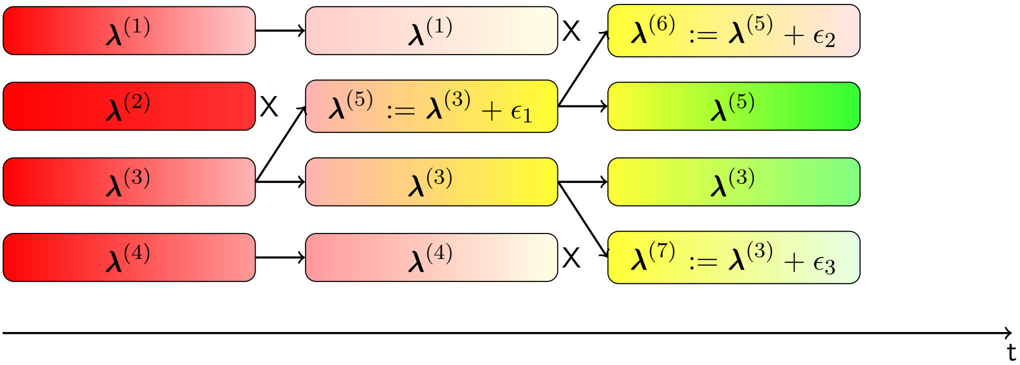

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- Since each population member (i.e., model) can be trained independently,
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  - $\leadsto$ Drawback: requires substantial parallel compute resources

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PBT + BO: Outline

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

AutoML: Dynamic Configuration & Learning

Learning to Learn: Supervised

Bernd Bischl Frank Hutter Lars Kotthoff
Marius Lindauer Joaquin Vanschoren

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Idea

- Learn algorithms directly, e.g., how to search in the weight space
- First idea: learn weight updates of a neural network

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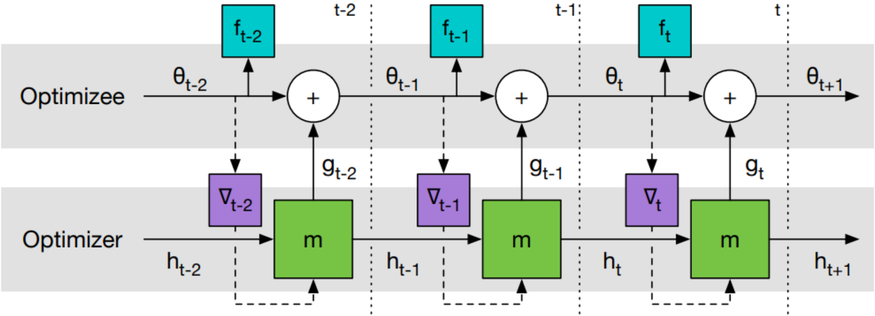
$\rightsquigarrow$ "Learning to learn gradient descent by gradient descent"

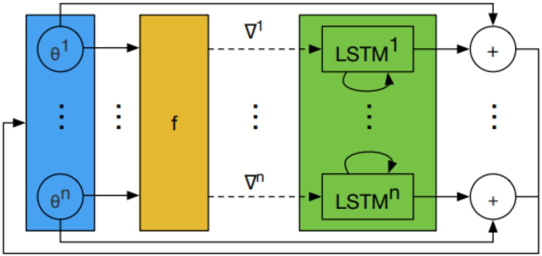
Learning to Learn: LSTM approach [Andrychowicz et al. 2016]

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]



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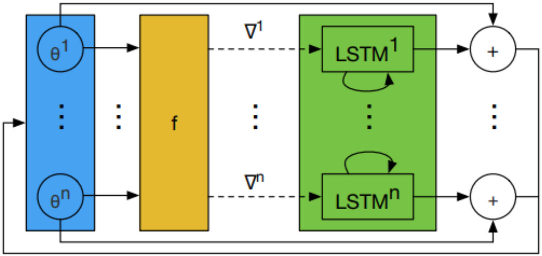

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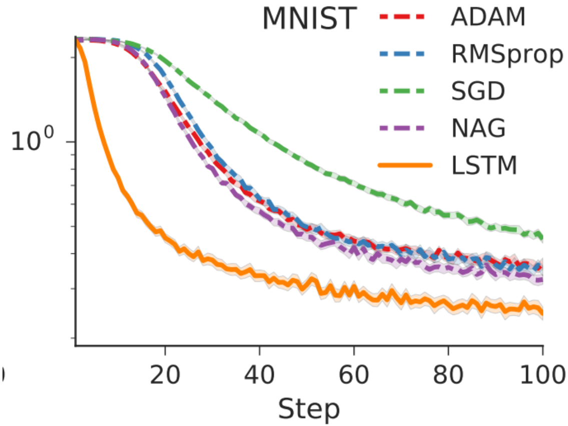
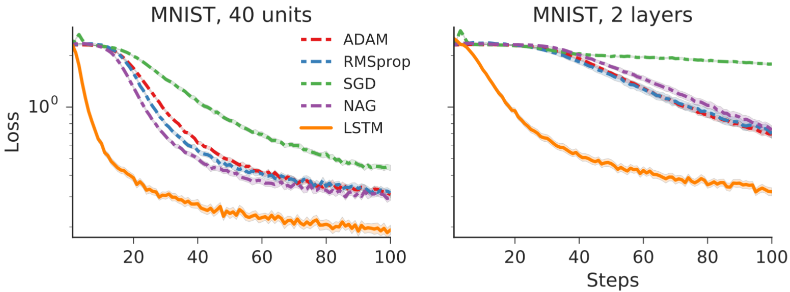
$\leadsto$ We can train the LSTM on k weights and apply it larger DNNs with k' weights, where $k \leq k'$

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



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

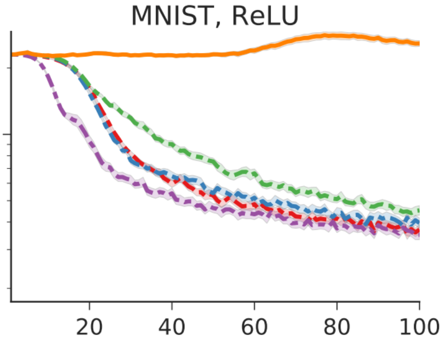
Changing the original architecture of the DNN:



⇝ learnt optimizer is robust against some architectural changes

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

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 $h^{(t+1)}$

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

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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- 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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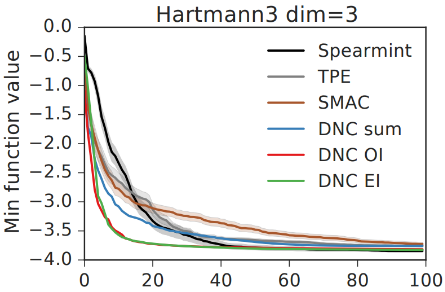

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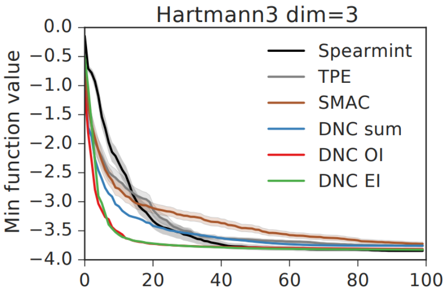

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⇝ L_{OI} and L_{EI} perform best

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

AutoML: Dynamic Configuration & Learning

Learning to Learn: Reinforcement Learning

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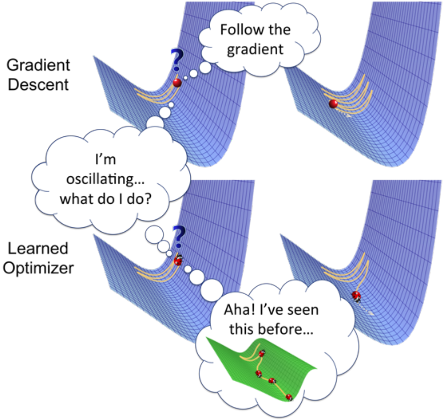
Learning to Optimize via Reinforcement Learning [Li and Malik. 2017]



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

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Reinforcement Learning for Learning to Optimize

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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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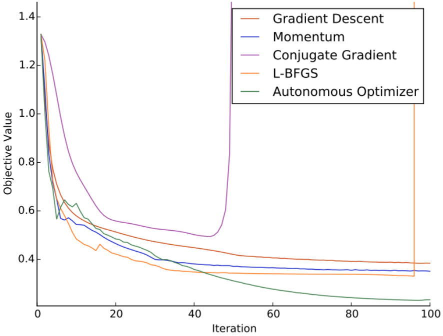

- 2-layer DNN with ReLUs
- Training datasets for training RL agent:
  four multivariate Gaussians and sampling 25 points from each
  - $\rightsquigarrow$ hard toy problem

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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 $t = 1, 2, \ldots T - |D_0|$ **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]

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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.

RL to train Neural AF [Volpp et al. 2019]

Policy π_θ: Neural acquisition function α_θ

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

Policy [Volpp et al. 2019]

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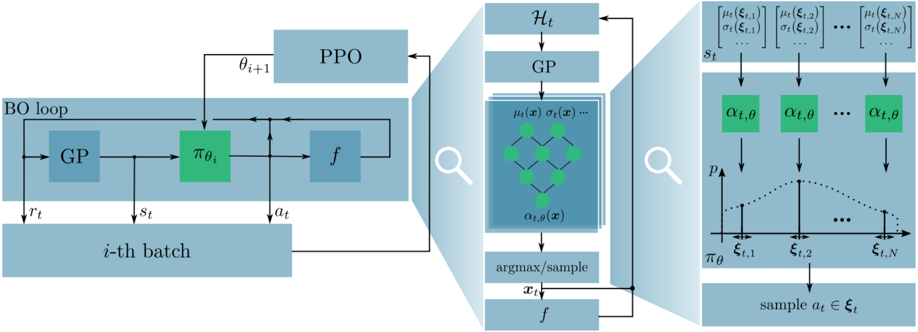
- Due to curse of dimensionality, we need a two step approach for $\xi^{(t)}$
  1. sample ξ_{global} using a coarse Sobol grid
  2. sample ξ_{local} using local optimization starting from the best samples in ξ_{global}

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

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

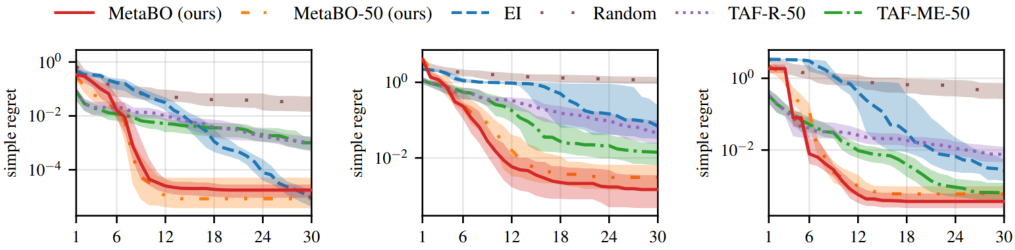


MetaBO Training Loop

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
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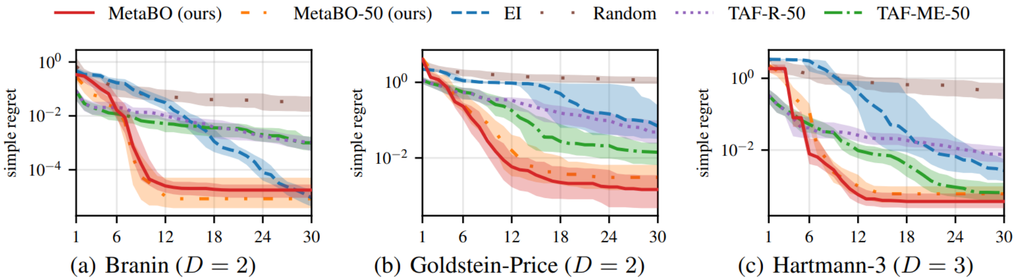

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Assumption: You have a family of functions at hand that resembles your target function.