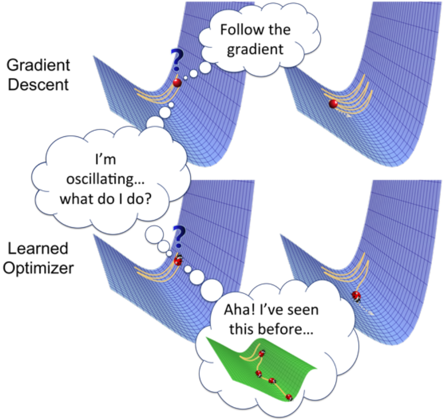
AutoML: Dynamic Configuration & Learning

Learning to Learn: Reinforcement Learning

Bernd Bischl   Frank Hutter   Lars Kotthoff
Marius Lindauer   Joaquin Vanschoren

Learning to Optimize via Reinforcement Learning [Li and Malik'17]



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

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

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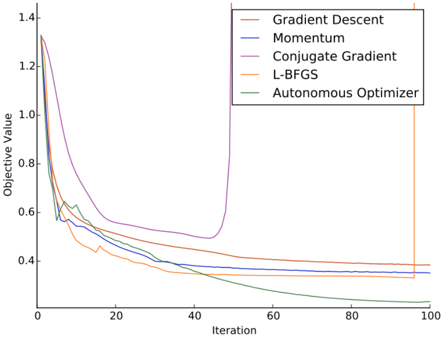
Training Set randomly generated objective functions

Learning to Optimize via Reinforcement Learning Results [Li and Malik'17]



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

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    - probability of improvement (PI)
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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.'19]

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

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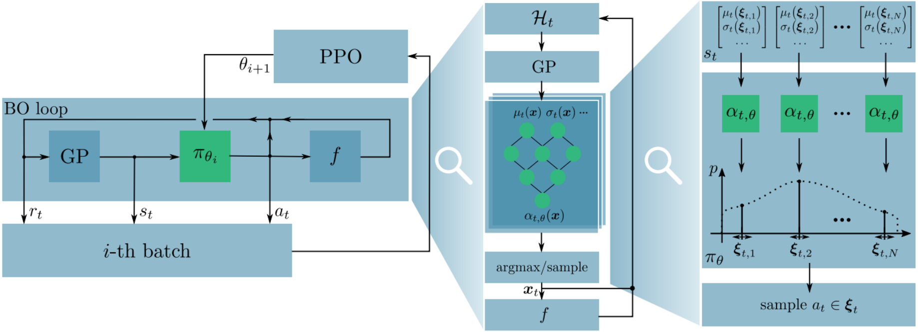
- Due to curse of dimensionality, we need a two step approach for $\xi^{(t)}$
  1. sample ξ_{global} using a coarse Sobol grid
  2. sample ξ_{local} using local optimization starting from the best samples in ξ_{global}

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

Learning Acquisition Functions: Overview [Volpp et al.'19]

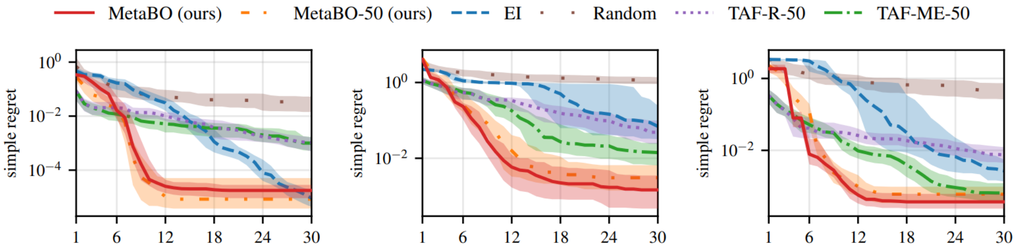


MetaBO Training Loop

Neural AF in the BO loop

Policy architecture

Results on Artificial Functions [Volpp et al.'19]



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

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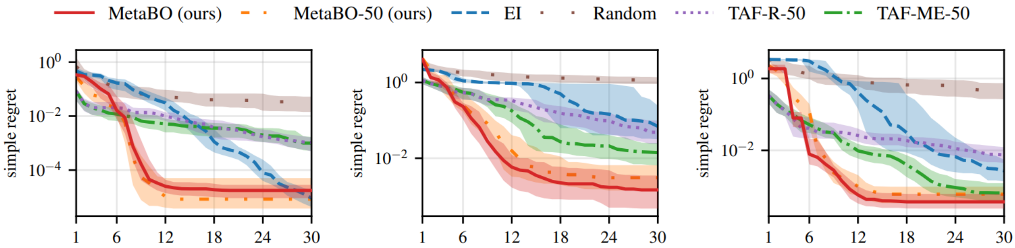

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Assumption: You have a family of functions at hand that resembles your target function.