AutoML: Dynamic Configuration & Learning

Learning to Learn: Supervised

Bernd Bischl Frank Hutter Lars Kotthoff <u>Marius Lindauer</u> Joaquin Vanschoren

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- First idea: learn weight updates of a neural network

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Learning to learn by gradient descent by gradient descent

[Andrychowicz et al'16]

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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)

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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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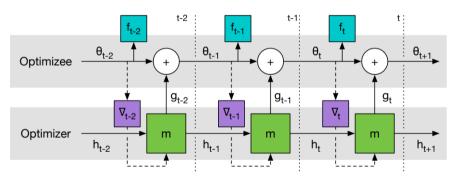
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- → "Learning to learn gradient descent by gradient descent"

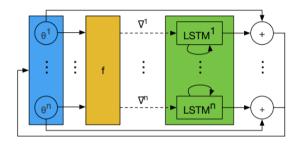
Learning to Learn: LSTM approach [Andrychowicz et al'16]

Optimizee Target network to be trained

Optimizer LSTM with hidden state h_t that predicts weight updates g_t

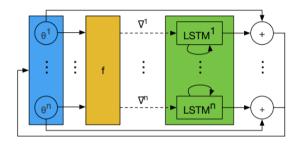


Learning to Learn: Coordinatewise LSTM optimizer [Andrychowicz et al'16]



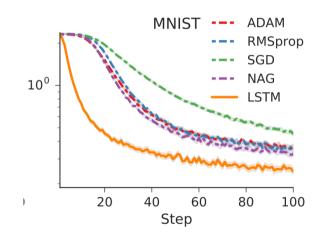
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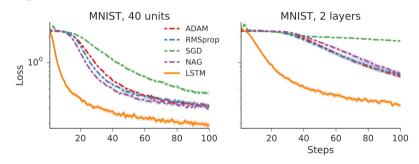
- One LSTM for each coordinate (i.e., weight)
- \bullet All LSTMs have shared parameters ϕ
- Each coordinate has its own separate hidden state
- We can train the LSTM on k weights and apply it larger DNNs with k' weights, where $k \leq k'$

Learning to Learn with LSTM: Results [Andrychowicz et al'16]



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Changing the original architecture of the DNN:

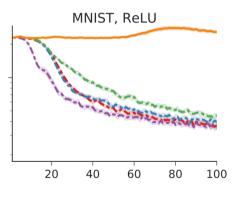


→ learnt optimizer is robust against some architectural changes

Learning to Learn with LSTM: Results

[Andrychowicz et al'16]

Changing the activation function to ReLU:



→ fails on other activation functions

Learning Black-box Optimization [Chen et al'17]

Black Box Optimization Setting

$$\mathbf{x}^* \in \operatorname*{arg\,min}_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

- **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'17]

Learning Black Box Optimization

Essentially, a similar idea as before:

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

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

Learning Black-box Optimization: Loss Functions

[Chen et al'17]

• Sum loss: Provides more information than final loss

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

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- El loss: Try to learn behavior of Bayesian optimizer based on expected improvement (El)
 - requires model (e.g., GP)

$$L_{\mathsf{EI}}(\phi) = -\mathbb{E}_{f,y^{(1:T-1)}}\left[\sum_{t=1}^T \mathsf{EI}(\mathbf{x}^{(t)}|y^{(1:t-1)})
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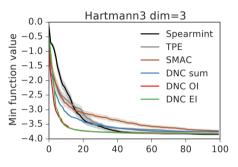
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Observed Improvement Loss:

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

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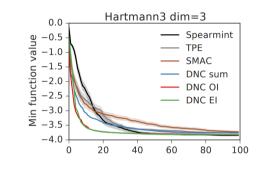
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• Hartmann3 is an artificial function with 3 dimensions

Learning Black-box Optimization: Results

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- Hartmann3 is an artificial function with 3 dimensions
- \leadsto L_{OI} and L_{EI} perform best
- \sim $L_{
 m OI}$ easier to compute than $L_{
 m EI}$ because we need a predictive model to compute EI