# 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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 $\rightsquigarrow$  Goal: Optimize f wrt  $\theta$  by learning g (resp.  $\phi$ )

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

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

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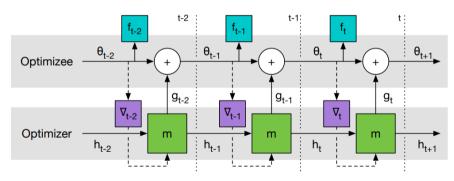
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- → "Learning to learn gradient descent by gradient descent"

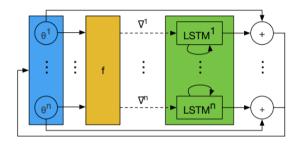
# Learning to Learn: LSTM approach [Andrychowicz et al. 2016]

Optimizee Target network to be trained

Optimizer LSTM with hidden state  $h_t$  that predicts weight updates  $g_t$ 

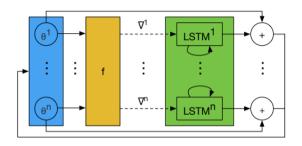


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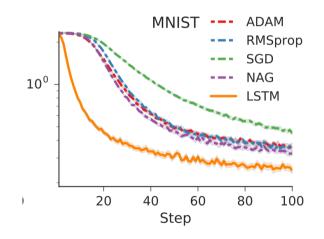
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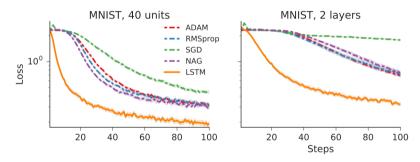
- One LSTM for each coordinate (i.e., weight)
- $\bullet$  All LSTMs have shared parameters  $\phi$
- Each coordinate has its own separate hidden state
- We can train the LSTM on k weights and apply it larger DNNs with k' weights, where  $k \leq k'$

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



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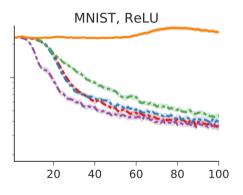
Changing the original architecture of the DNN:



→ learnt optimizer is robust against some architectural changes

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

Changing the activation function to ReLU:



→ fails on other activation functions

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

#### 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. 2017]

#### 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. 2017]

• 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)})
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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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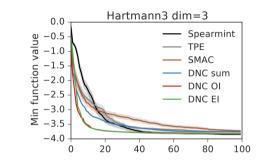
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Observed Improvement Loss:

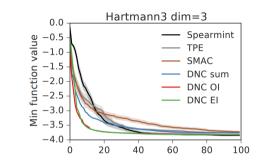
$$L_{\mathsf{OI}}(\phi) = \mathbb{E}_{f, y^{(1:T-1)}} \left[ \sum_{t=1}^{T} \min \left\{ f(\mathbf{x}^{(t)}) - \min_{i < t} (f(\mathbf{x}^{(i)})), 0 \right\} \right]$$

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- Hartmann3 is an artificial function with 3 dimensions
- $\rightarrow$   $L_{OI}$  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