AutoML: Dynamic Configuration & Learning

Population-based Training

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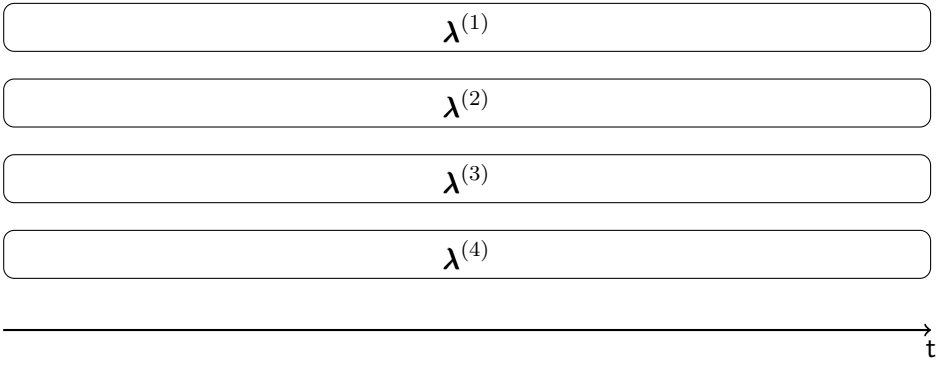
⇝ Try to figure out best hyperparameter settings on the fly

Massively parallelized Random Search



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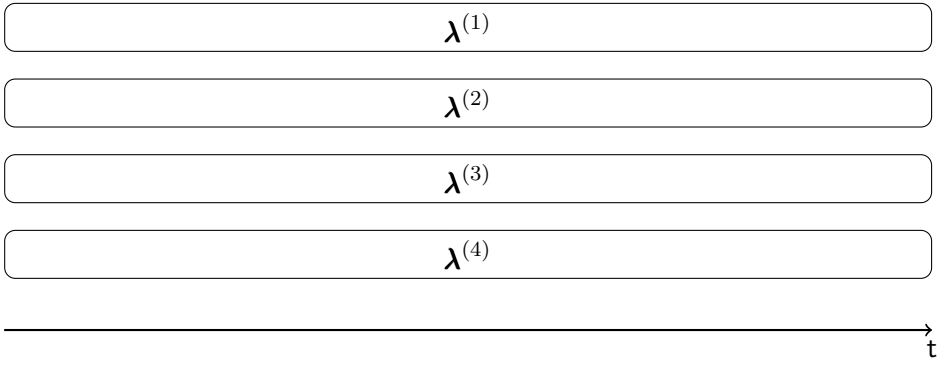

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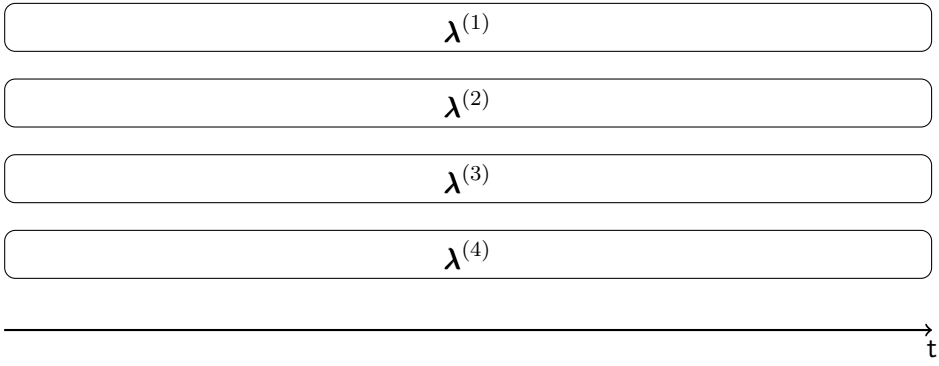

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- Pure exploration on a large population of configurations
- No dynamic adaptation

Population-based Training [Jaderberg et al. 2017]

- The color indicates the performance over time

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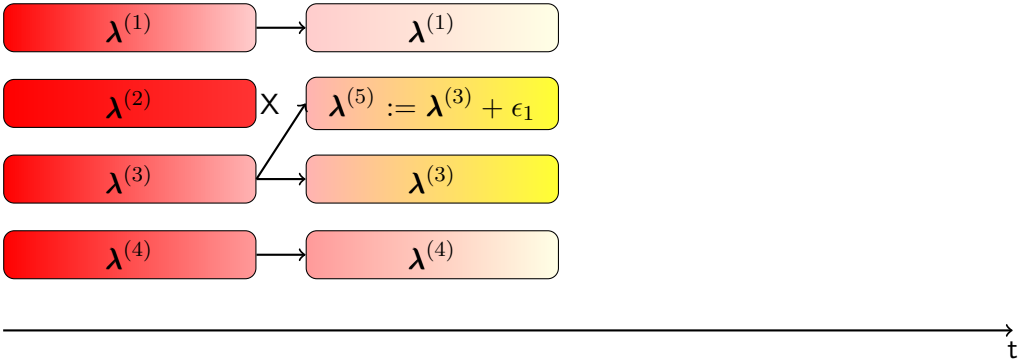

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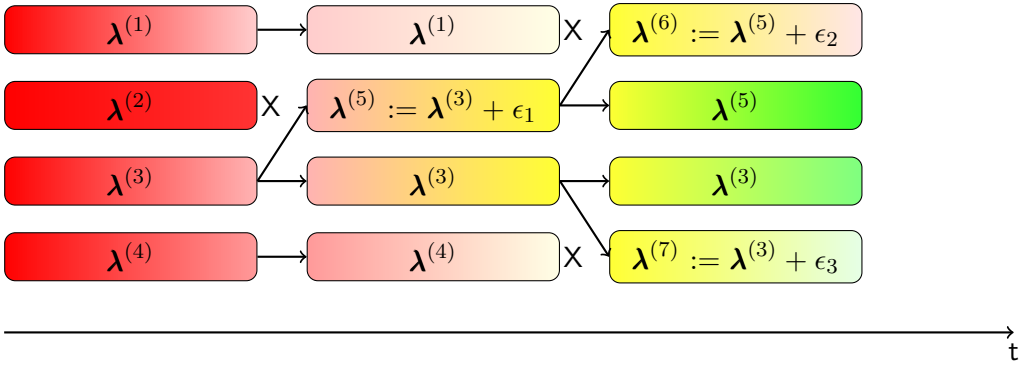

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General workflow of PBT:

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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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⇝ Less parallel compute resources are required(?)

⇝ Scales better to higher dimensional spaces(?)

PBT + BO: Outline

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2. Train population for a bit
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4. Use Bayesian optimization to select new hyperparameter settings
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- Several ideas on how to parallelize BO
  - Randomize the model training or optimization of the acquisition function
  - Thompson sampling to use only a single explanation of the data (in proportion to its likelihood)
  - 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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- BO-Surrogate model predicts the cost improvement over time:

$$c_{\text{PBT}}^{(t)}(\boldsymbol{\lambda}) = \frac{c^{(t)}(\boldsymbol{\lambda}) - c^{(t-1)}(\boldsymbol{\lambda})}{\Delta t}$$

where $c^{(t)}(\boldsymbol{\lambda})$ is the cost for a given hyperparameter setting at time step t.

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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