# AutoML: Neural Architecture Search (NAS) Speedup Techniques

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

# Overview of NAS Speedup Methods

- Multi-fidelity optimization
- Learning curve prediction
- Meta-learning across datasets
- Network morphisms & weight inheritance
- Weight sharing & the one-shot model

# NAS Speedup Technique 1: Multi-fidelity optimization

- Analogous to multi-fidelity optimization in HPO
  - Many evaluations for cheaper fidelities (less epochs, smaller datasets, down-sampled images, shallower networks, etc)
  - Fewer evaluations necessary for more expensive fidelities

# NAS Speedup Technique 1: Multi-fidelity optimization

- Analogous to multi-fidelity optimization in HPO
  - Many evaluations for cheaper fidelities (less epochs, smaller datasets, down-sampled images, shallower networks, etc)
  - Fewer evaluations necessary for more expensive fidelities
- Compatible with any blackbox optimization method
  - Using random search: ASHA [Li and Talwalkar. 2019]
  - Using Bayesian optimization: BOHB [Zela et al. 2018]
  - Using differential evolution: DEHB [Awad et al. under review]
  - Using regularized evolution: progressive dynamic hurdles [So et al. 2019]

### NAS Speedup Technique 1: Multi-fidelity optimization

- Analogous to multi-fidelity optimization in HPO
  - Many evaluations for cheaper fidelities (less epochs, smaller datasets, down-sampled images, shallower networks, etc)
  - Fewer evaluations necessary for more expensive fidelities
- Compatible with any blackbox optimization method
  - Using random search: ASHA [Li and Talwalkar. 2019]
  - Using Bayesian optimization: BOHB [Zela et al. 2018]
  - Using differential evolution: DEHB [Awad et al. under review]
  - Using regularized evolution: progressive dynamic hurdles [So et al. 2019]
- Often used for joint optimization of architecture & hyperparameters
  - Auto-Pytorch [Mendoza et al. 2019; Zimmer et al. 2020]
  - "Auto-RL" [Runge et al. 2019]

# NAS Speedup Technique 2: Learning Curve Prediction

- Analogous to learning curve prediction in HPO
  - Observe initial learning curve and predict performance at the end
  - Can use features of the architecture as input (just like hyperparameters as inputs)

### NAS Speedup Technique 2: Learning Curve Prediction

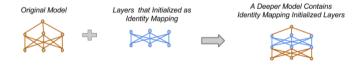
- Analogous to learning curve prediction in HPO
  - Observe initial learning curve and predict performance at the end
  - Can use features of the architecture as input (just like hyperparameters as inputs)
- Often used for joint optimization of architecture & hyperparameters
- Compatible with any blackbox optimization method
  - Using random search and Bayesian optimization: [Domhan et al. 2015]
  - Using reinforcement learning: [Baker et al. 2018]

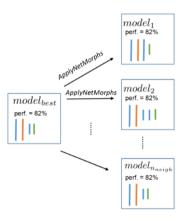
# NAS Speedup Technique 3: Meta-Learning

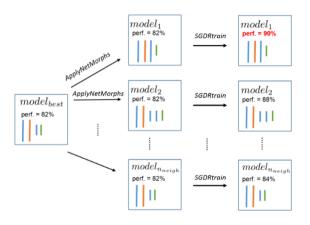
- Lots of work on meta-learning for HPO
- Only little work on meta-learning for NAS
  - Find a set of good architectures to initialize BOHB in Auto-Pytorch [Zimmer et al. 2020]
  - Learn RL agent's policy network on previous datasets [Wong et al. 2018]
  - Learn neural architecture that can be quickly adapted [Lian et al. 2019; Elsken et al. 2019]

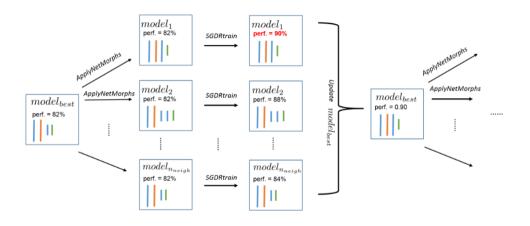
#### NAS Speedup Technique 4: Network Morphisms

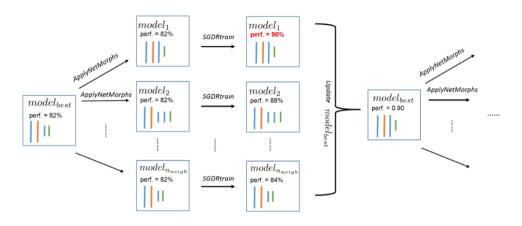
- Network Morphisms [Chen et al. 2016; Wei et al. 2016; Cai et al. 2017]
  - Change the network structure, but not the modelled function
  - I.e., for every input the network yields the same output as before applying the network morphisms operations
  - Examples: "Net2DeeperNet", "Net2WiderNet", etc.









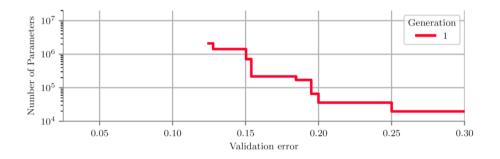


#### Weight inheritance avoids expensive retraining from scratch

[Real et al. 2017; Cai et al. 2018; Elsken et al. 2017; Cortes et al. 2017; Cai et al. 2018; Elsken et al. 2019]

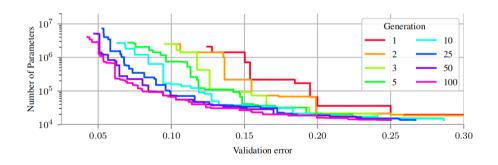
# Network Morphisms for Multi-objective NAS [Elsken et al. 2019]

- To trade off error vs. resource consumption (e.g, #parameters):
  - Maintain a Pareto front of the two objectives
  - ▶ Evolve a population of Pareto-optimal architectures over time



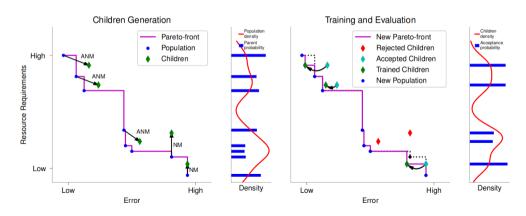
### Network Morphisms for Multi-objective NAS [Elsken et al. 2019]

- To trade off error vs. resource consumption (e.g, #parameters):
  - Maintain a Pareto front of the two objectives
  - ▶ Evolve a population of Pareto-optimal architectures over time



# Network Morphisms for Multi-objective NAS [Elsken et al. 2019]

- LEMONADE: Lamarckian Evolution for Multi-Objective Neural Architecture Design
- Weight inheritance through approximate morphisms (ANMs)
  - ▶ Dropping layers, dropping units within a layer, etc (function not preserved perfectly)



[Pham et al. 2018; Bender et al. 2018]

• All possible architectures are subgraphs of a large supergraph: the one-shot model

[Pham et al. 2018; Bender et al. 2018]

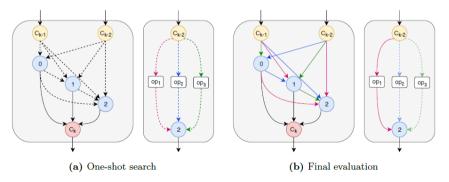
- All possible architectures are subgraphs of a large supergraph: the one-shot model
- Weights are shared between different architectures with common edges in the supergraph

[Pham et al. 2018; Bender et al. 2018]

- All possible architectures are subgraphs of a large supergraph: the one-shot model
- Weights are shared between different architectures with common edges in the supergraph
- Search costs are reduced drastically since one only has to train a single model (the one-shot model).

[Pham et al. 2018; Bender et al. 2018]

- The one-shot model can be seen as a directed acyclic multigraph
  - ⇒ Nodes latent representations.
  - ⇒ Edges (dashed) operations.



• Architecture optimization problem: Find optimal path from the input to the output

#### Questions to Answer for Yourself / Discuss with Friends

- Repetition:
   List five methods to speed up NAS over blackbox approaches
- Repetition:
   Which speedup techniques directly carry over from HPO to NAS?
- Discussion:
   Why do network morphisms and the one-shot model only apply to NAS, and not to HPO?