

# AutoML: Dynamic Configuration & Learning

## Overview

Bernd Bischl   Frank Hutter   Lars Kotthoff  
Marius Lindauer   Joaquin Vanschoren

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
- We discussed how to extend AutoML to a more **grey-box approach**:
  - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g, intermediate results

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
- We discussed how to extend AutoML to a more **grey-box approach**:
  - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g, intermediate results
  - ▶ We might can control the “box” a bit, e.g., early termination

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
- We discussed how to extend AutoML to a more **grey-box approach**:
  - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g, intermediate results
  - ▶ We might can control the “box” a bit, e.g., early termination
  - ▶ E.g., learning curve predictions, multi-fidelity optimization, ...

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
- We discussed how to extend AutoML to a more **grey-box approach**:
  - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g., intermediate results
  - ▶ We might can control the “box” a bit, e.g., early termination
  - ▶ E.g., learning curve predictions, multi-fidelity optimization, ...
  - ↪ often more efficient than black-box approaches (if done right)

# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
  - ▶ Black box: We choose input to the black box and observe outcome
  - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
- We discussed how to extend AutoML to a more **grey-box approach**:
  - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g, intermediate results
  - ▶ We might can control the “box” a bit, e.g., early termination
  - ▶ E.g., learning curve predictions, multi-fidelity optimization, ...
  - ↪ often more efficient than black-box approaches (if done right)
- Ultimately, we would like to treat AutoML as a **white-box problem**
  - ▶ White-box: We can observe and control all details of an algorithm run



# Black vs. Grey vs. White Box

- Often we treat AutoML as a **black-box problem**
    - ▶ Black box: We choose input to the black box and observe outcome
    - ▶ E.g., classical hyperparameter optimizer:  
Input: Hyperparameter configuration → Output: Accuracy
  - We discussed how to extend AutoML to a more **grey-box approach**:
    - ▶ Grey Box: We still choose the input, but we can observe more than the outcome, e.g, intermediate results
    - ▶ We might can control the “box” a bit, e.g., early termination
    - ▶ E.g., learning curve predictions, multi-fidelity optimization, ...
    - ~> often more efficient than black-box approaches (if done right)
  - Ultimately, we would like to treat AutoML as a **white-box problem**
    - ▶ White-box: We can observe and control all details of an algorithm run
- ~> Goal: **Replace algorithm components by learned policies**

# Iterative Optimization Heuristics

## IOHs

Iterative Optimization Heuristics (IOHs) propose a set of solution candidates in each iteration based on previous evaluations.

# Iterative Optimization Heuristics

## IOHs

Iterative Optimization Heuristics (IOHs) propose a set of solution candidates in each iteration based on previous evaluations.

Important Observations:

- Many ML algorithms are **iterative** in nature, in particular for big data, e.g.:
  - ▶ SGD (for linear models or for deep neural networks)
  - ▶ Tree-based algorithms

# Iterative Optimization Heuristics

## IOHs

Iterative Optimization Heuristics (IOHs) propose a set of solution candidates in each iteration based on previous evaluations.

Important Observations:

- Many ML algorithms are **iterative** in nature, in particular for big data, e.g.:
  - ▶ SGD (for linear models or for deep neural networks)
  - ▶ Tree-based algorithms
- Often we have only a **single solution candidate** (e.g., weights of neural network)
  - ▶ If we use a evolutionary strategy as in neural evolution, we have a population of solution candidates

# Iterative Optimization Heuristics

## IOHs

Iterative Optimization Heuristics (IOHs) propose a set of solution candidates in each iteration based on previous evaluations.

Important Observations:

- Many ML algorithms are **iterative** in nature, in particular for big data, e.g.:
  - ▶ SGD (for linear models or for deep neural networks)
  - ▶ Tree-based algorithms
- Often we have only a **single solution candidate** (e.g., weights of neural network)
  - ▶ If we use a evolutionary strategy as in neural evolution, we have a population of solution candidates
- Hopefully, the **quality** of solution candidates **improves** in each iteration
  - ▶ Update of the weights of a neural network

# Iterative Optimization Heuristics

## IOHs

Iterative Optimization Heuristics (IOHs) propose a set of solution candidates in each iteration based on previous evaluations.

Important Observations:

- Many ML algorithms are **iterative** in nature, in particular for big data, e.g.:
  - ▶ SGD (for linear models or for deep neural networks)
  - ▶ Tree-based algorithms
- Often we have only a **single solution candidate** (e.g., weights of neural network)
  - ▶ If we use a evolutionary strategy as in neural evolution, we have a population of solution candidates
- Hopefully, the **quality** of solution candidates **improves** in each iteration
  - ▶ Update of the weights of a neural network
- Main component is the **heuristic for proposal mechanism** of new solution candidates

## Dynamic Adaptation of Hyperparameters

The goal is to dynamically adapt hyperparameters based on some feedback from the algorithm.

# Learning for IOHs

## Dynamic Adaptation of Hyperparameters

The goal is to dynamically adapt hyperparameters based on some feedback from the algorithm.

## Dynamic Algorithm Configuration: DAC

The goal of DAC is to learn a policy from data that adapts the [hyperparameter settings](#) of an IOH.



# Learning for IOHs

## Dynamic Adaptation of Hyperparameters

The goal is to dynamically adapt hyperparameters based on some feedback from the algorithm.

## Dynamic Algorithm Configuration: DAC

The goal of DAC is to learn a policy from data that adapts the [hyperparameter settings](#) of an IOH.

## Learning to Learn: L2L

The goal of L2L is to learn a [proposal mechanism](#) from data.