AutoML:
From Full Automation to A Human-Centric Approach

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Folien

Rise of Literacy

Photo by Anna Hunko on Unsplash

- Only priests were able to read and write
- People believed that they don't need to read and write
- They went to the holy buildings

- Today, everyone can read and write
- No one doubts the benefits of it

- **⇒ Democratization of literacy**

Inspired by Andrew Ng

Rise of AI Literacy?

Photo by Max Duzij on Unsplash

- Only highly educated people can program new AI applications
- Power lies only with the large IT companies

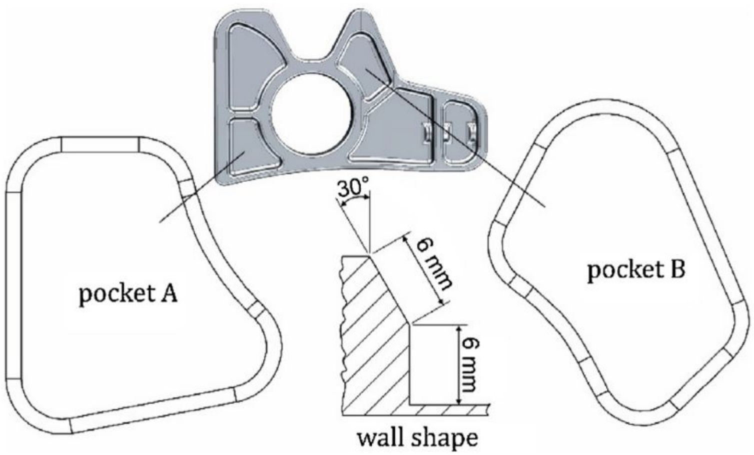
- In an age of limited resources, the need for efficient use gets more important

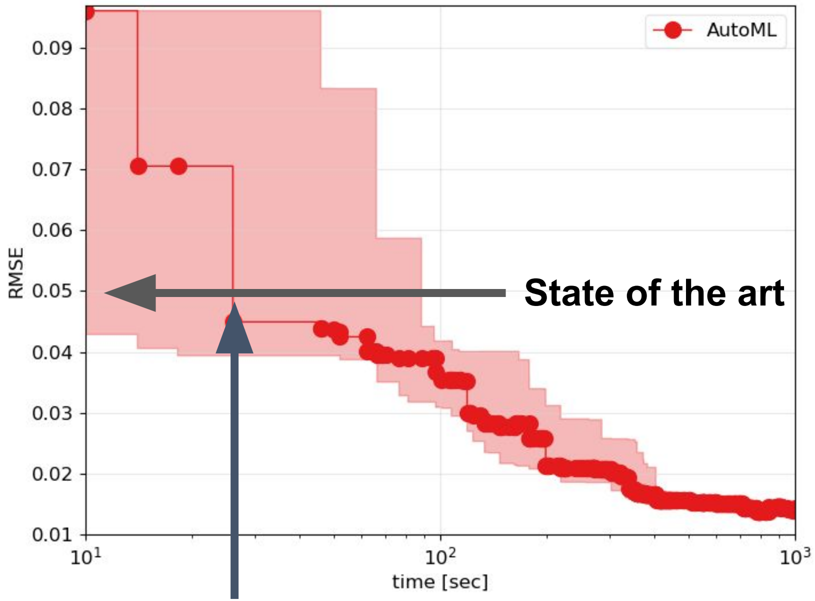
- **AutoML contributes to AI literacy!**

[See also my TEDx Talk]

Shape Error Prediction in Milling Process

[Denkena et al. SSRN'20]

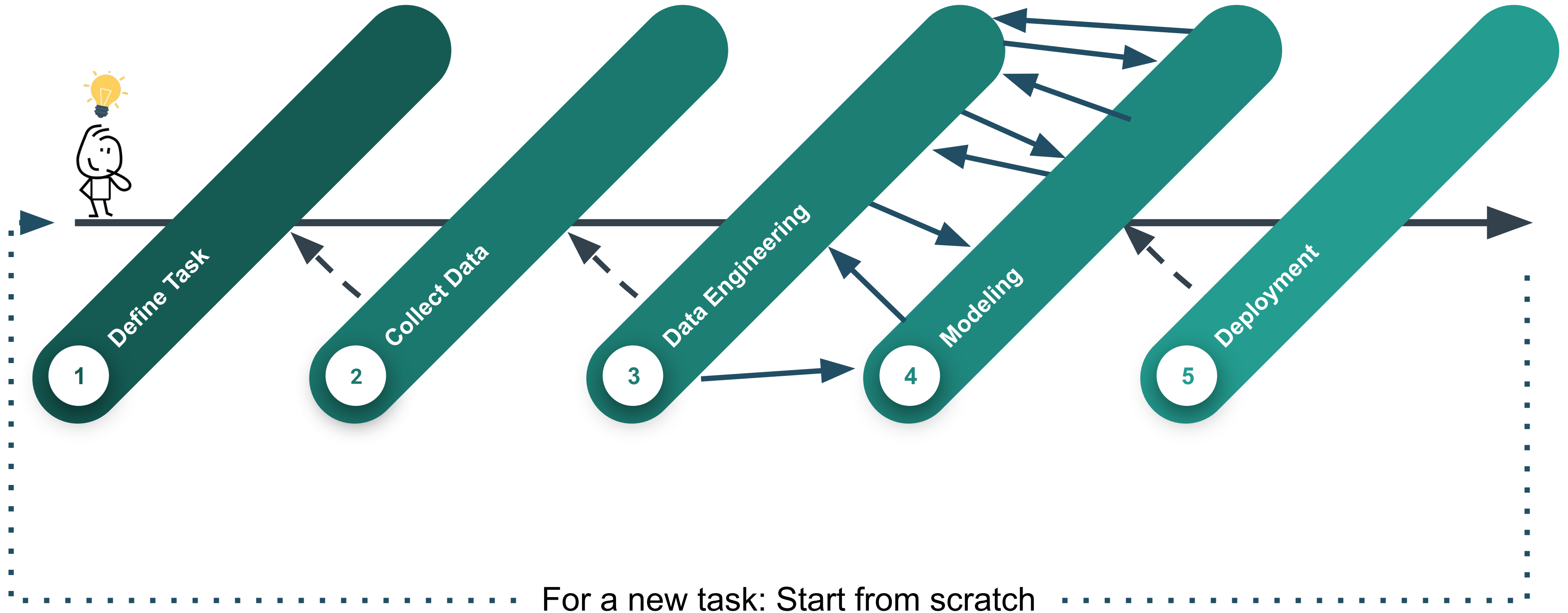




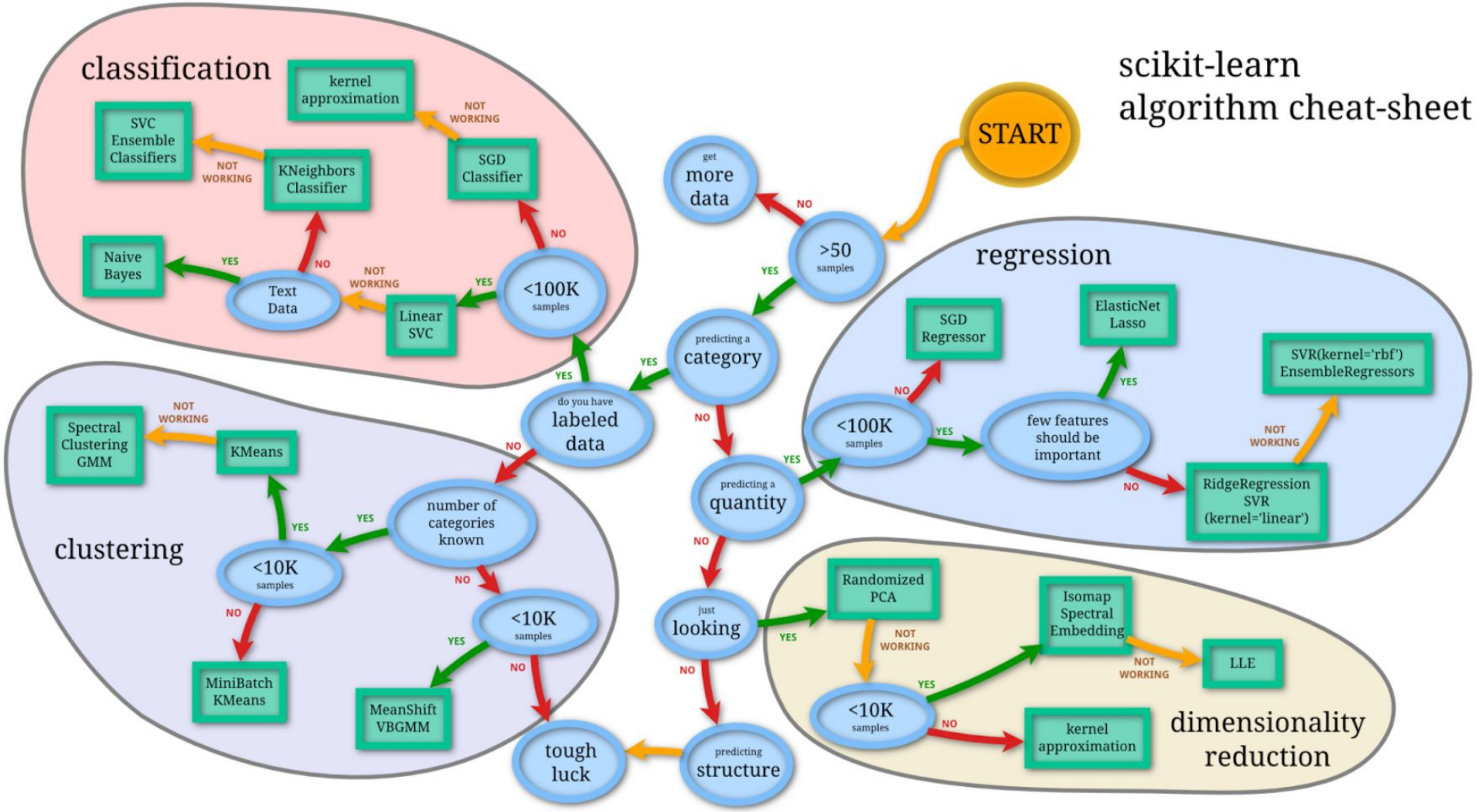
State of the art

Better than state of the art in less than 30sec!

Why does ML development take a lot of time?



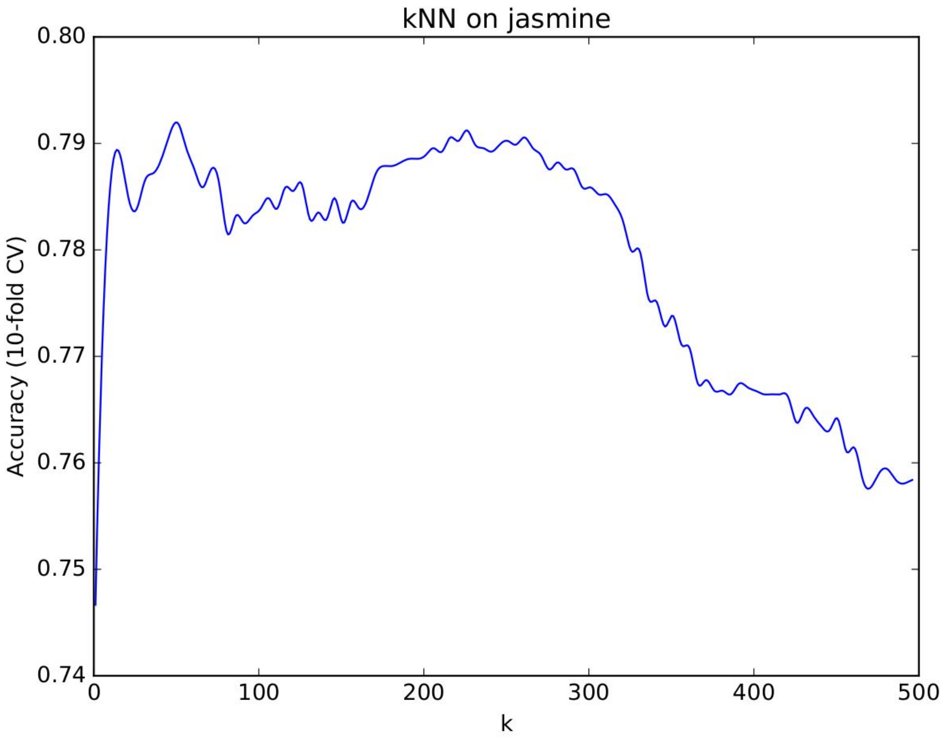
Design-Decisions?



source: https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

Toy Example: kNN

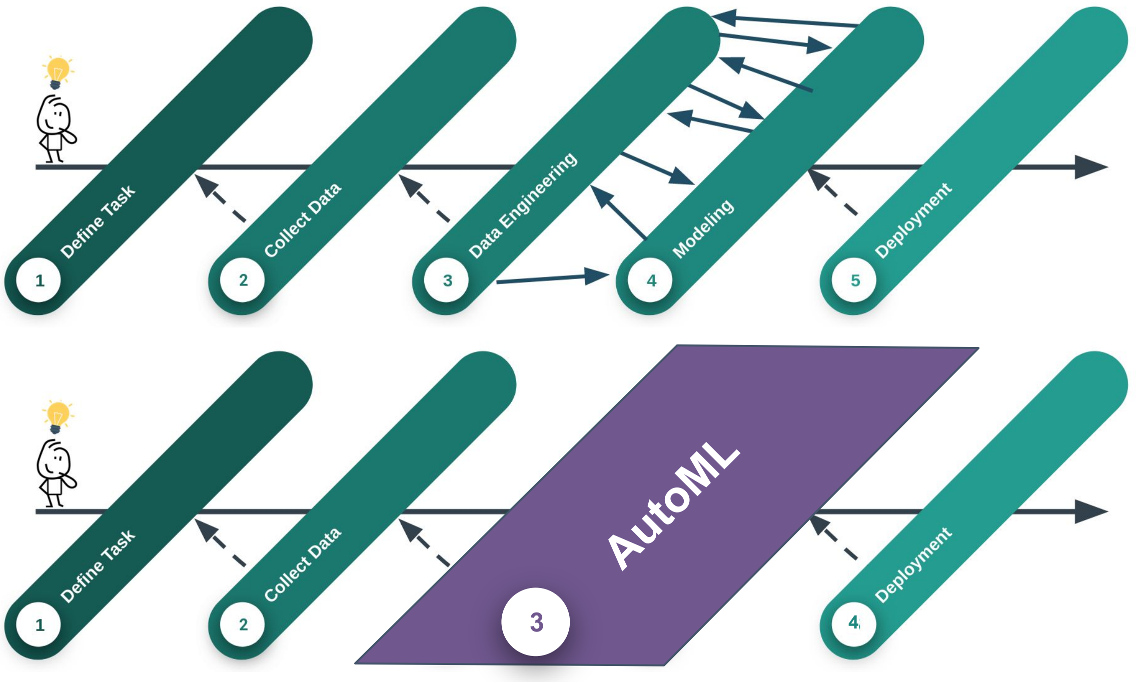
- *k*-nearest neighbors (kNN) is one of the **simplest ML algorithms**
- Size of neighbourhood (*k*) **is very important for its performance**
- The performance function depending on *k* is **quite complex** (not at all convex)



From ML Alchemy to Science

"You can teach an old dog new tricks" [Ruffinelli et al. 2020]
→ Hyperparameter optimization might not be the only required solution, but without it, it will also be hard.

ML vs AutoML



1
Define Task
2
Collect Data
3
Data Engineering
4
Modeling
5
Deployment
1
Define Task
2
Collect Data
3
AutoML
4
Deployment

Topics of AutoML

- **model selection** (e.g., Neural Architecture Search, ensembling)
- **configuration/tuning** (e.g., hyperparameter optimization via evolutionary algorithms, Bayesian optimization)
- **AutoML methodologies** (e.g., reinforcement learning, meta-learning, in-context learning, warmstarting, portfolios, multi-objective optimization, constrained optimization)
- **pipeline automation** (e.g., automated data wrangling, feature engineering, pipeline synthesis, and configuration)
- **automated procedures for diverse data** (e.g., tabular, relational, multimodal, etc.)
- **ensuring quality of results in AutoML** (e.g., fairness, interpretability, trustworthiness, sustainability, robustness, reproducibility)
- supporting **analysis and insight** from automated systems

Advantages

AutoML enables

- 🚀 More **efficient** research and development of ML applications
  - → AutoML has been shown to outperform humans on subproblems
- 🧮 More **systematic** research and development of ML applications
  - → no (human) bias or unsystematic evaluation
- 📋 More **reproducible** research
  - → since it is systematic!
- 🦾 **Broader use** of ML methods
  - → less required ML expert knowledge
  - → not only limited to computer scientists

Challenges

But, it is not that easy, because

🔁 Each dataset potentially requires **different optimal ML-designs**

→ Design decisions have to be made for each dataset again

⌛ Training of a single ML model can be **quite expensive**

→ We can not try many configurations

❓ Mathematical **relation** between design and performance is (often) **unknown**

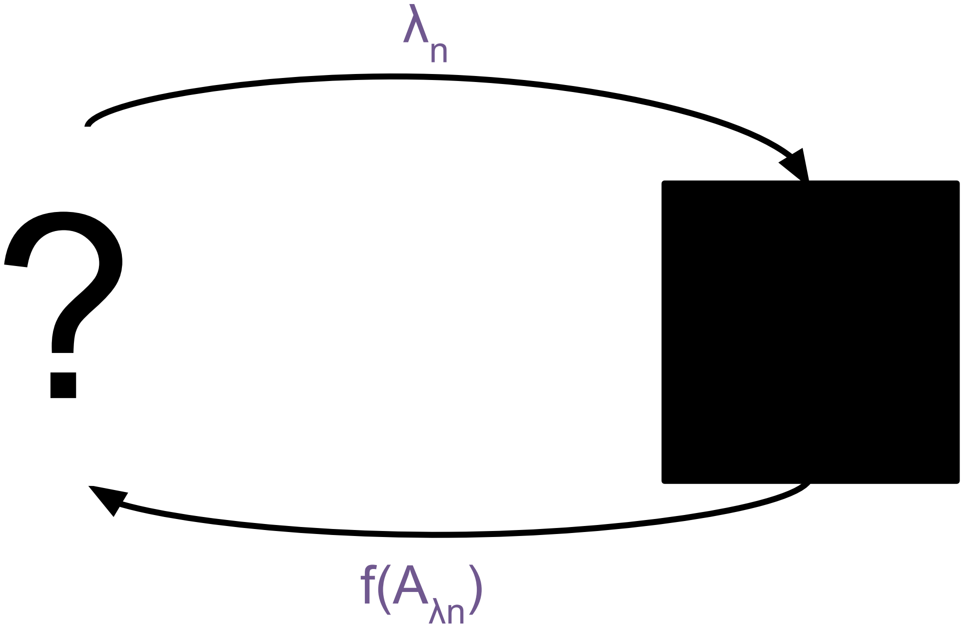
→ Gradient-based optimization not easily possible

🎛️ 🎚️ Optimization in **highly complex spaces**

→ including categorical, continuous and conditional dependencies

Some Basics on Hyperparamter Optimization

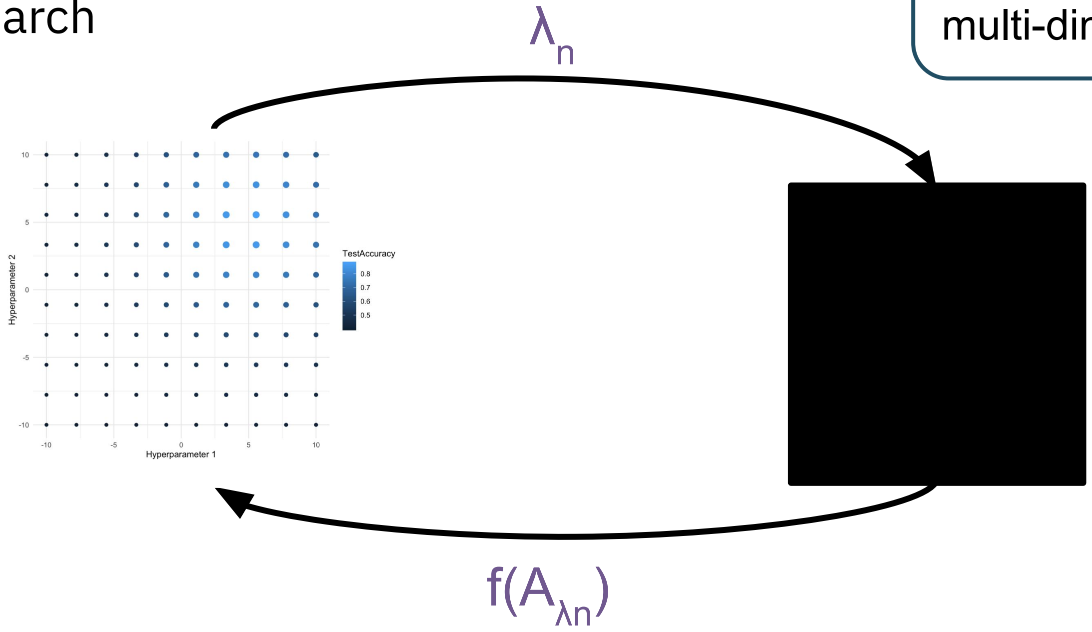
Black-Box Optimization Problem



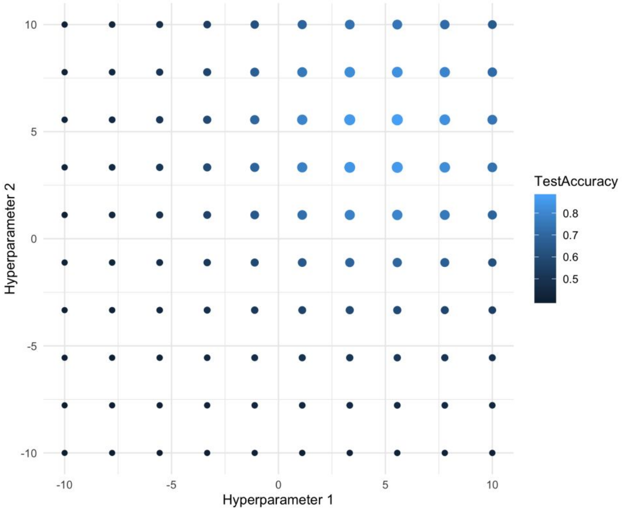
Option 1: Grid Search

a.k.a. exhaustive search;
a.k.a. advanced manual search

Popular technique: Evaluates all combinations on a pre-defined multi-dimensional grid



Option 1: Grid Search II



Advantages

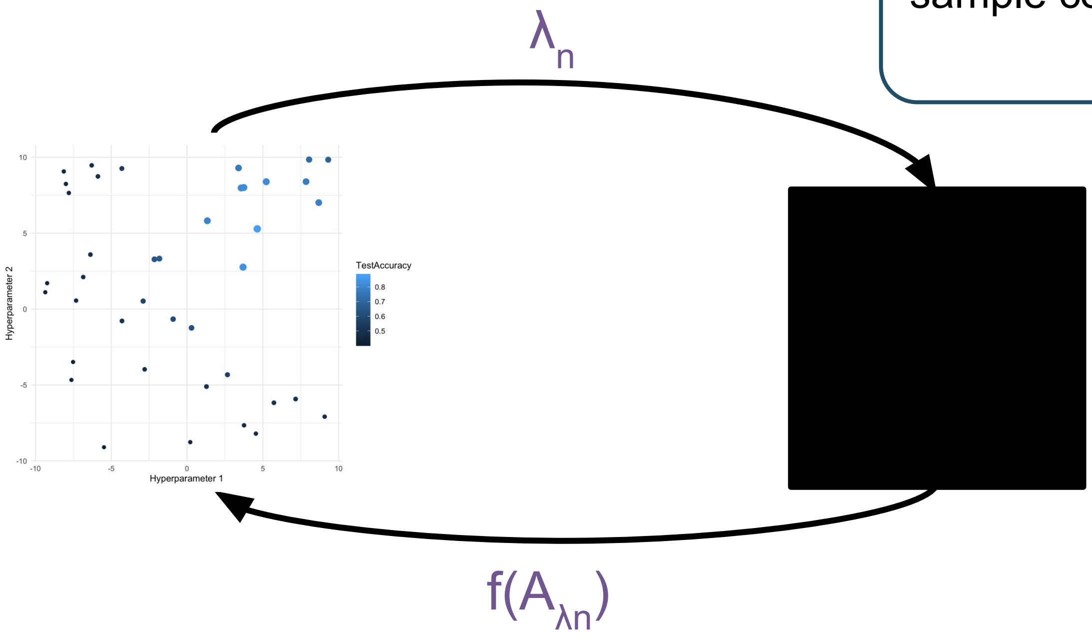
- Very easy to implement
- Very easy to parallelize
- Can handle all types of hyperparameters

Disadvantages

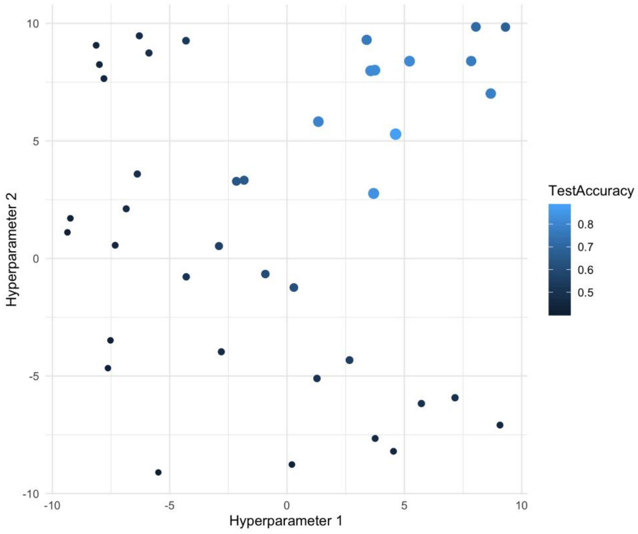
- Scales badly with #dimensions
- Inefficient: Searches irrelevant areas
- Requires to manual define discretization
- All grid points need to be evaluated

Option 2: Random Search

Variation of Grid Search: Uniformly sample configurations at random



Option 2: Random Search II



Advantages

- Very easy to implement
- Very easy to parallelize
- Can handle all types of hyperparameters
- No discretization required
- Anytime algorithm: Can be stopped and continued based on the available budget and performance goal.

Disadvantages

- Scales badly with #dimensions
- Inefficient: Searches irrelevant areas

Grid Search vs. Random Search

With a **budget** of T iterations:

Grid Search evaluates only $T^{\frac{1}{d}}$ unique values per dimension

Random Search evaluates (most likely) T different values per dimension

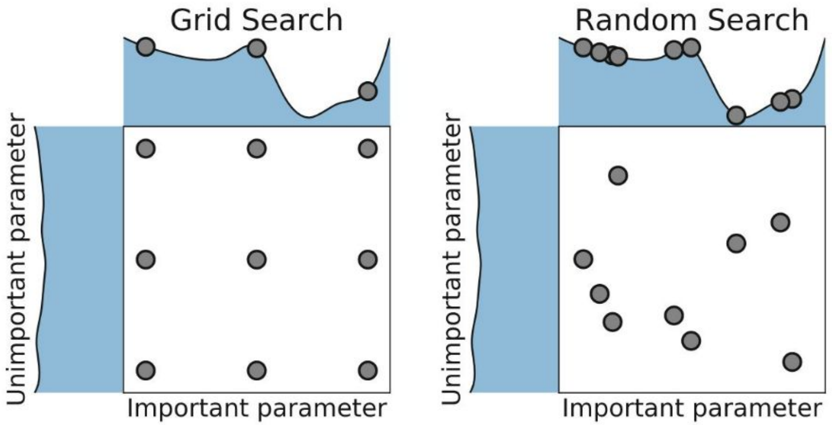
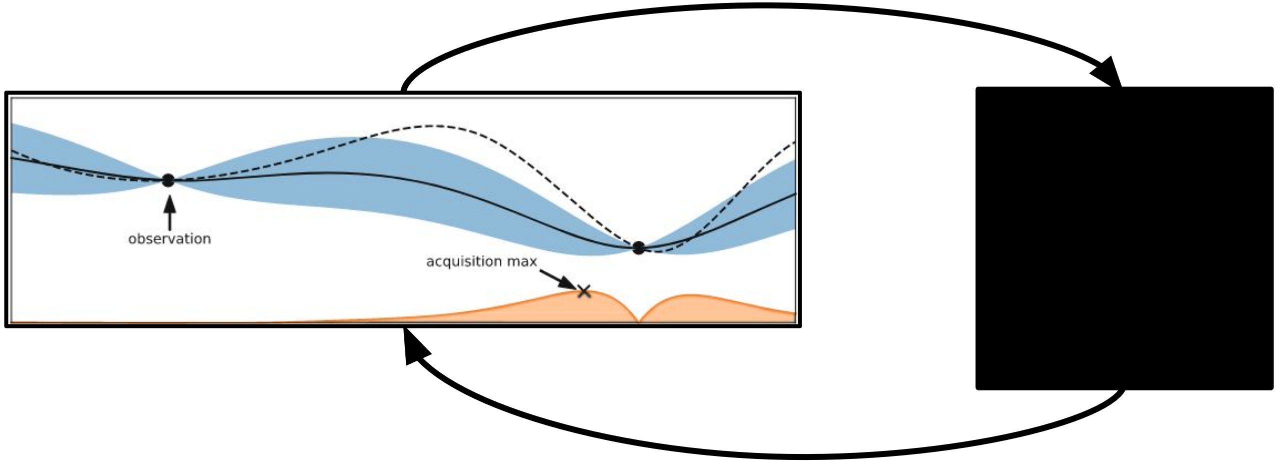


Image source: [Hutter et al. 2019]

→ Grid search can be disadvantageous if some hyperparameters have little of no impact on the performance [Bergstra et al. 2012]

Model-based Optimization

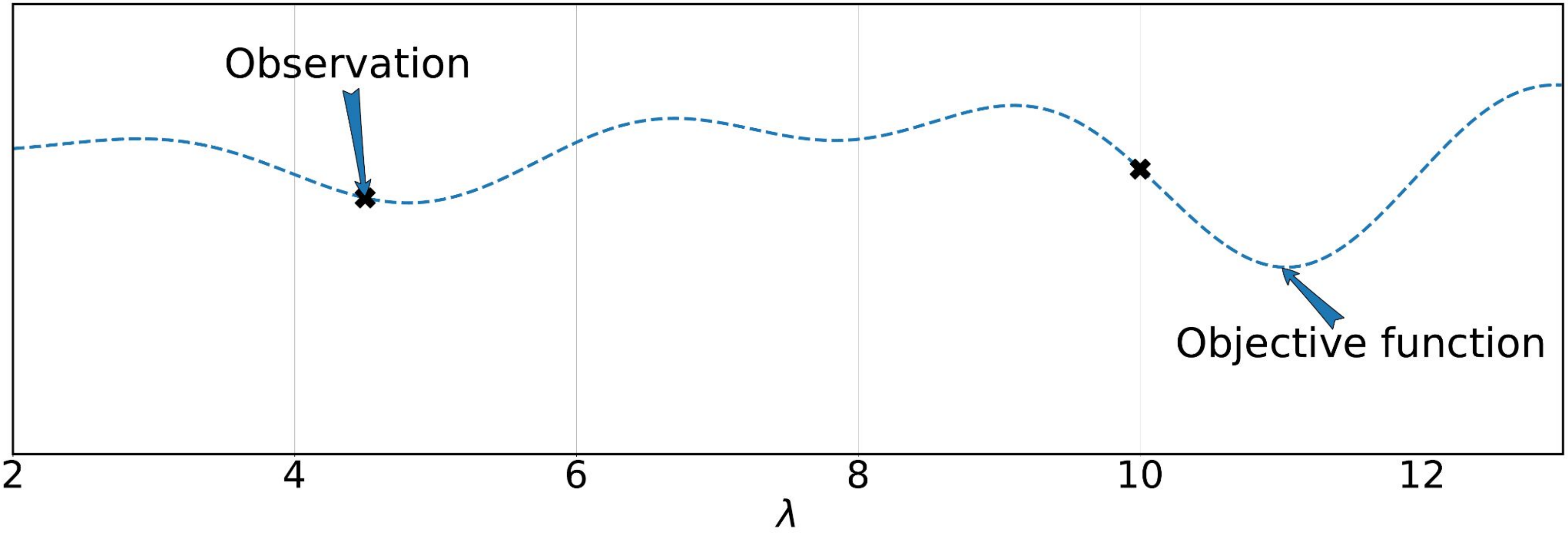
λ_n



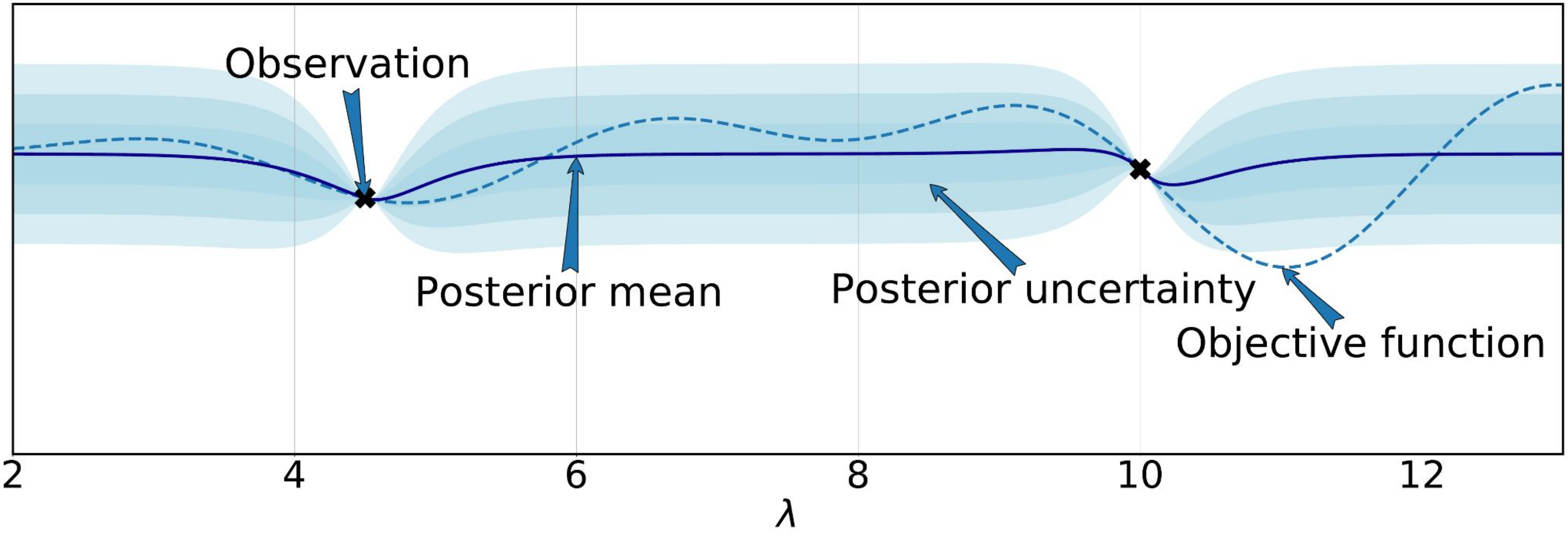
$f(A_{\lambda_n})$

Photo by Wilhelm Gunkel on Unsplash
Image by Feurer, Hutter: Hyperparameter Optimization
In: Automated Machine Learning

Bayesian Optimization in a Nutshell



Bayesian Optimization in a Nutshell



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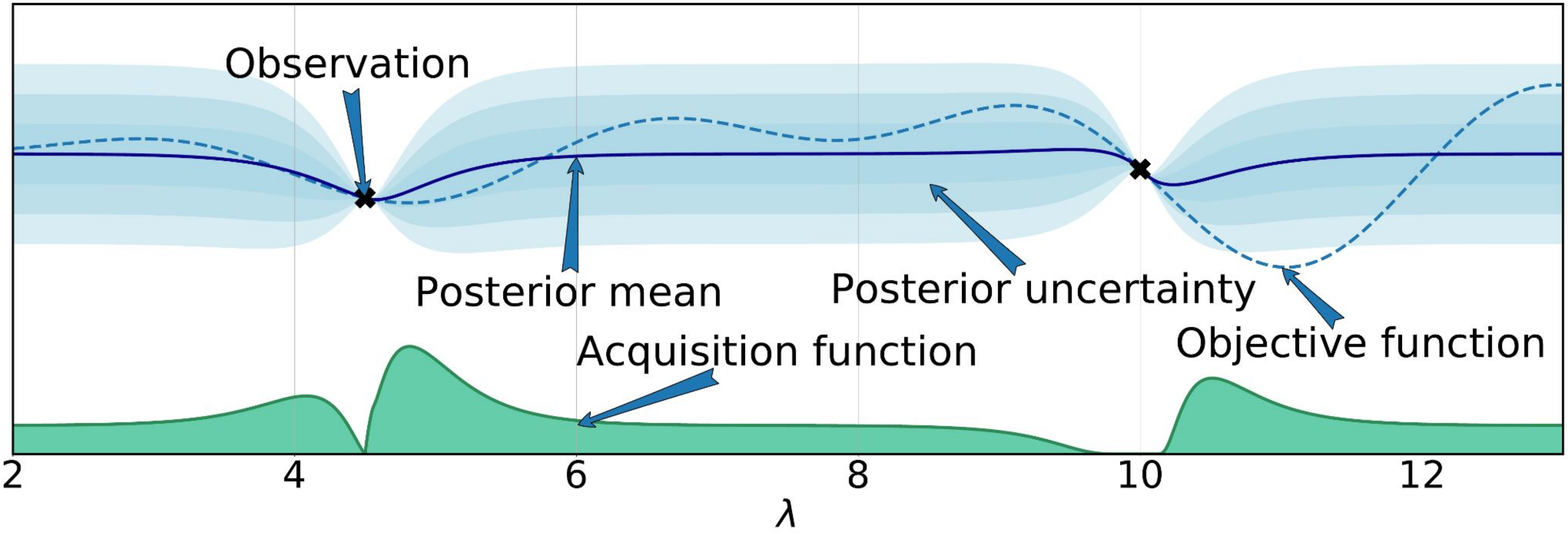
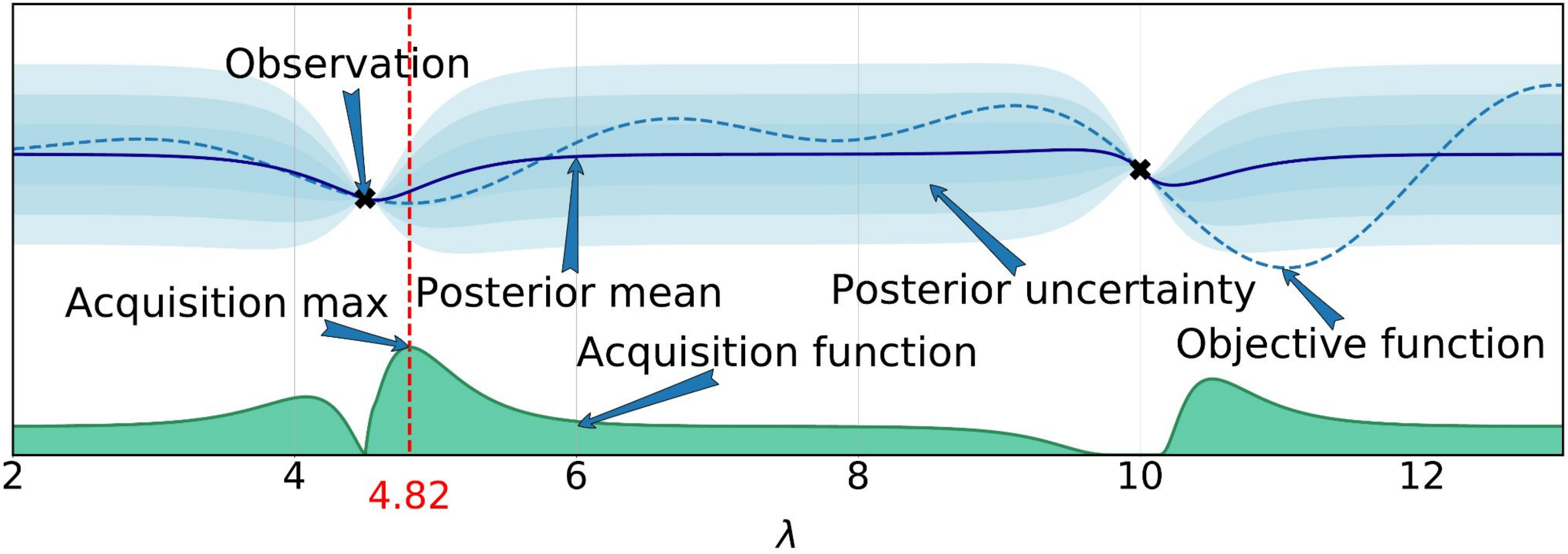


Bayesian Optimization in a Nutshell



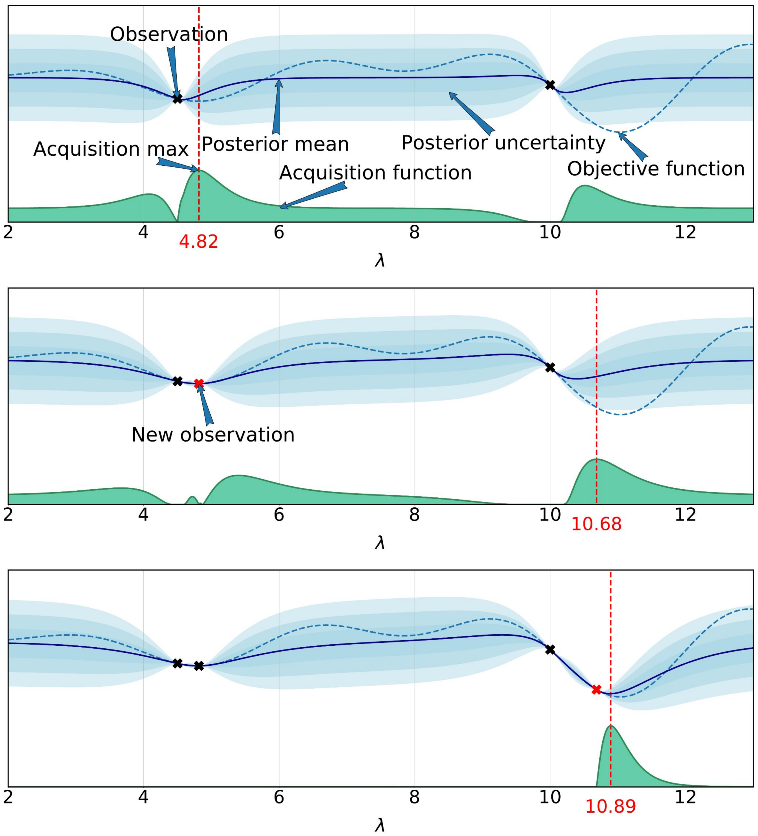
Bayesian Optimization in a Nutshell

General approach

- Fit a probabilistic model to the collected function samples $\langle \boldsymbol{\lambda}, c(\boldsymbol{\lambda}) \rangle$
- Use the model to guide optimization, trading off exploration *vs* exploitation

Popular approach in the statistics literature since Mockus et al. [1978]

- Efficient in #function evaluations
- Works when objective is nonconvex, noisy, has unknown derivatives, etc.
- Recent convergence results
  [Srinivas et al. 2009; Bull et al. 2011; de Freitas et al. 2012; Kawaguchi et al. 2015]



Bayesian Optimization: Pseudocode

BO loop

Require: Search space $\boldsymbol{\Lambda}$, cost function c, acquisition function u, predictive model $\hat{c}$, maximal number of function evaluations T

Result : Best configuration $\hat{\boldsymbol{\lambda}}$ (according to $\mathcal{D}$ or $\hat{c}$)

Initialize data $\mathcal{D}^{(0)}$ with initial observations

for $t = 1$ **to** T **do**

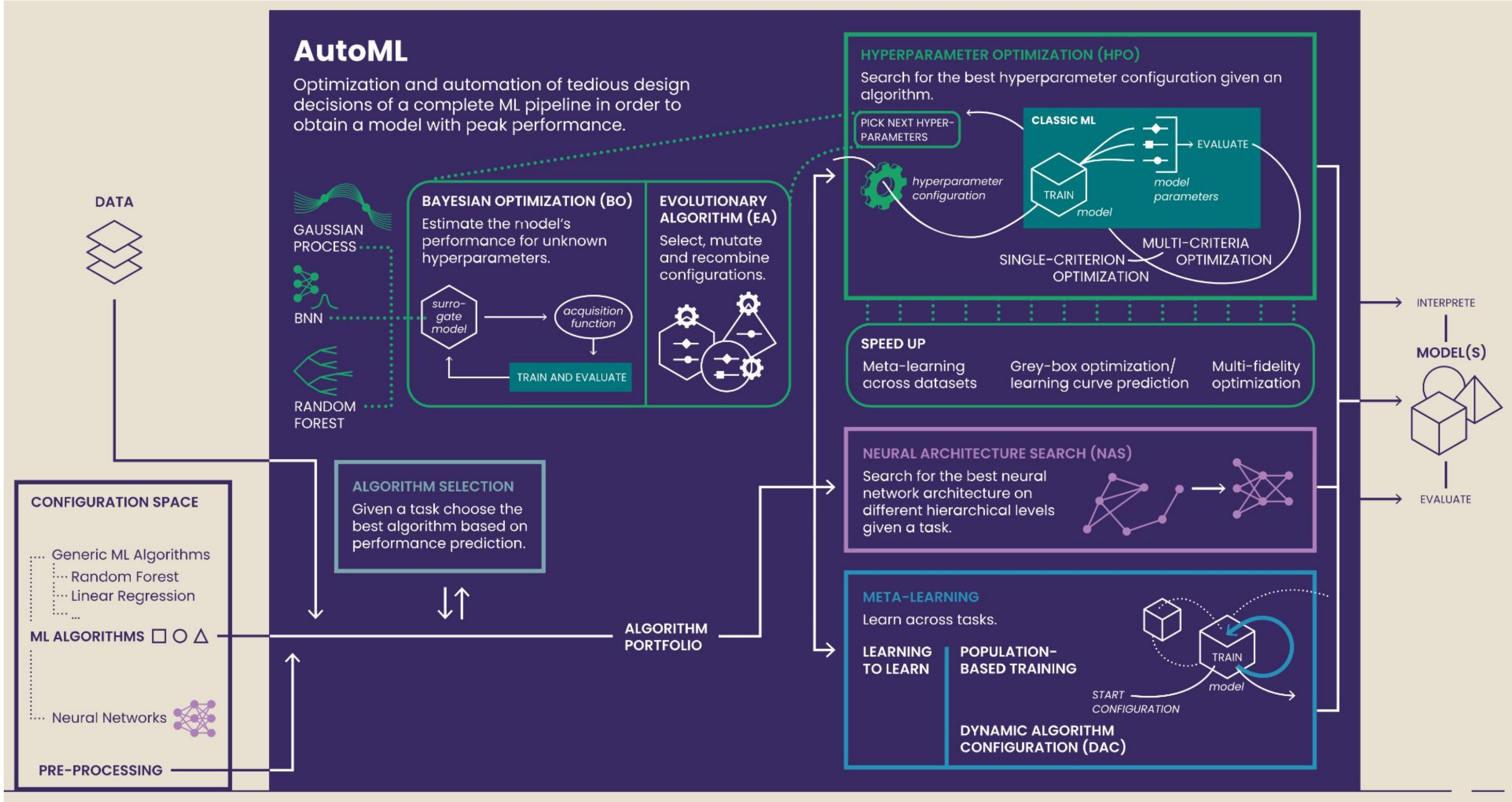
  Fit predictive model $\hat{c}^{(t)}$ on $\mathcal{D}^{(t-1)}$

  Select next query point: $\boldsymbol{\lambda}^{(t)} \in \arg\max_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} u(\boldsymbol{\lambda}; \mathcal{D}^{(t-1)}, \hat{c}^{(t)})$

  Query $c(\boldsymbol{\lambda}^{(t)})$

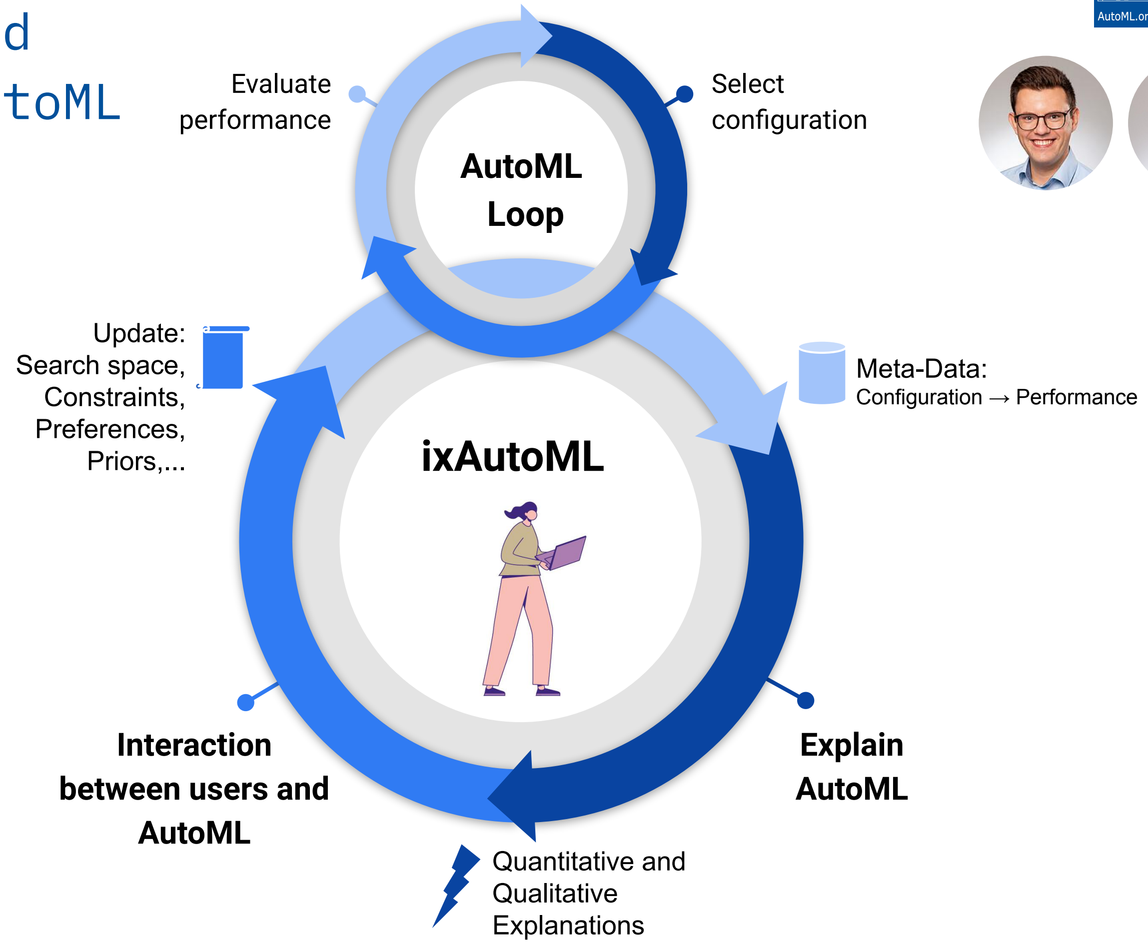
  Update data: $\mathcal{D}^{(t)} \leftarrow \mathcal{D}^{(t-1)} \cup \{\langle \boldsymbol{\lambda}^{(t)}, c(\boldsymbol{\lambda}^{(t)}) \rangle\}$

Is there more to AutoML?



Human-Centered AutoML

ixAutoML: interactive and explainable AutoML

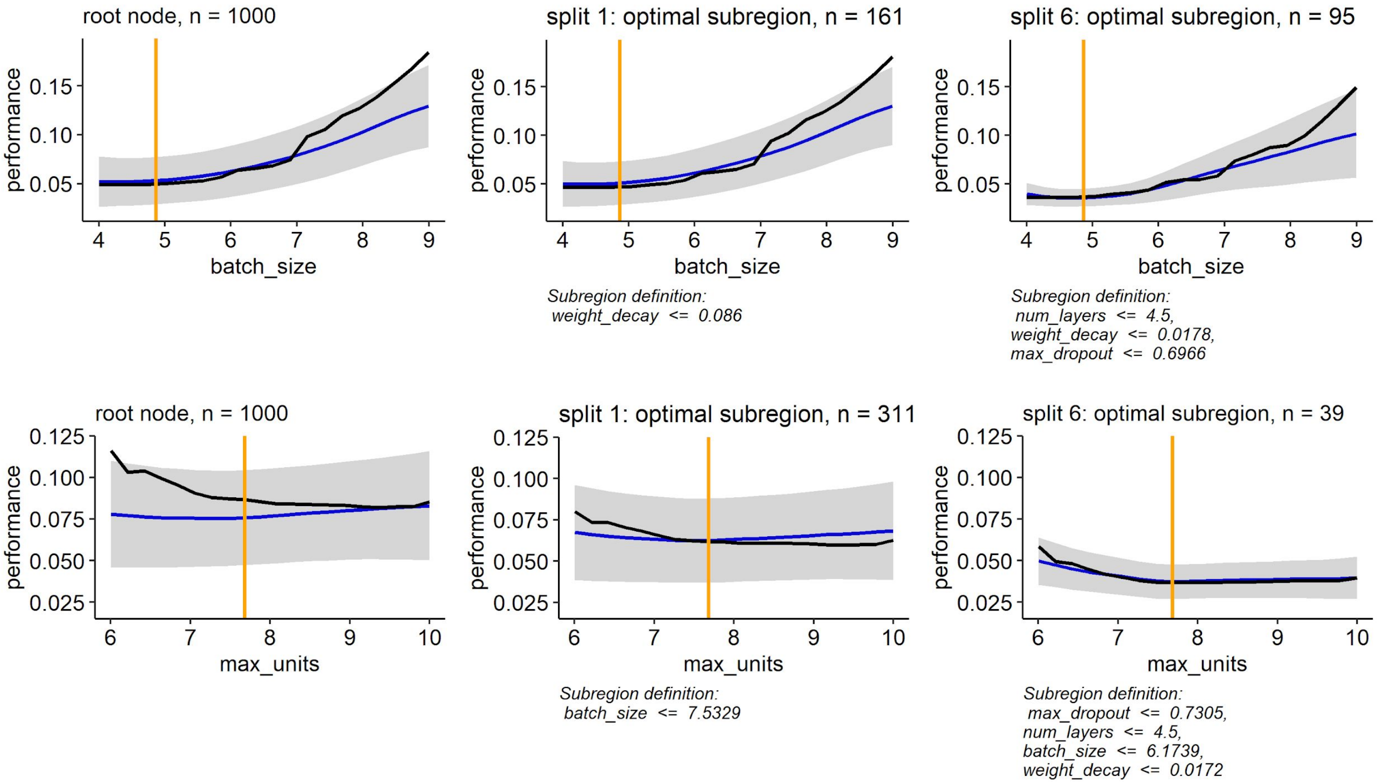


Explaining I: Partial Dependence Plots

Explaining Hyperparameter Effects via PDPs

[Moosbauer et al. NeurIPS’22]

Ground truth
PDP
incumbent



Partial Dependence Plots

[Moosbauer et al. NeurIPS'22]

For, a subset S of the hyperparameters, the partial dependence function is:

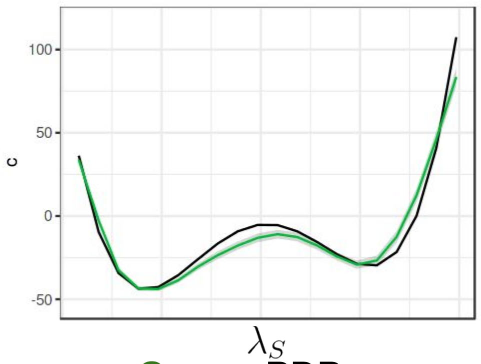
$$c_S(\lambda_S) := \mathbb{E}_{\lambda_C}\left[c(\lambda)\right] = \int_{\Lambda_C} c(\lambda_S, \lambda_C) d\mathbb{P}(\lambda_C)$$

and can be approximated by Monte-Carlo integration
on a surrogate model:

$$\hat{c}_S\left(\lambda_S\right) = \frac{1}{n}\sum_{i=1}^{n} \hat{m}\left(\lambda_S, \lambda_C^{(i)}\right)$$

where $\left(\lambda_C^{(i)}\right)_{i=1,\dots,n} \sim \mathbb{P}(\lambda_C)$ and λ_S for a set of grid points.

→ Average of ICE curves.



Green: PDP
Black: Ground truth

Partial Dependence Plots with Uncertainties

[Moosbauer et al. NeurIPS'22]

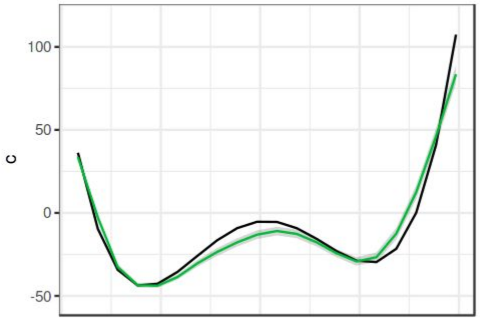
$$\hat{s}^2_S(\lambda_S) = \mathbb{V}_{\hat{c}}\left[\hat{c}_S\left(\lambda_S\right)\right] = \mathbb{V}_{\hat{c}}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{c}\left(\lambda_S, \lambda_C^{(i)}\right)\right] = \frac{1}{n^2}1^\top \hat{K}\left(\lambda_S\right)\ 1.$$

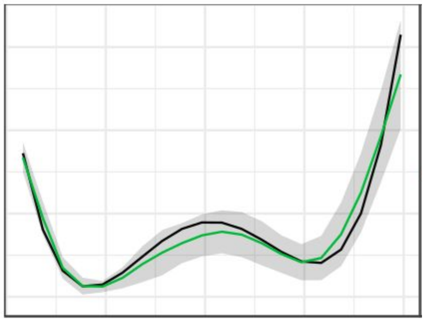
→ requires a kernel correctly specifying the covariance structure (e.g., GPs).

Approximation:

$$\hat{s}^2_S\left(\lambda_S\right) \approx \frac{1}{n}\sum_{i=1}^{n}\hat{K}\left(\lambda_S\right)_{i,i}$$

→ Model-agnostic (local) approximation

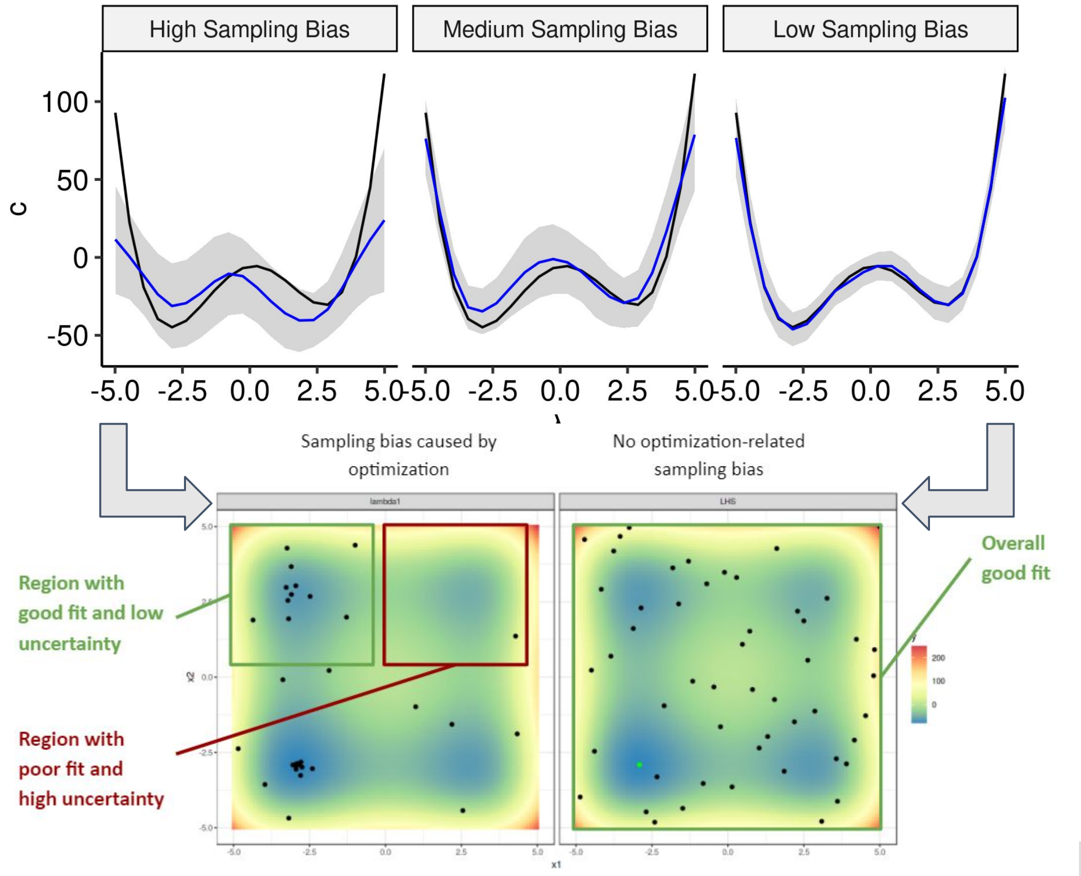




Ground truth
PDP
Uncertainty

Impact of Sampling Bias in Explaining AutoML

[Moosbauer et al. NeurIPS'22]



Explaining II: Symbolic Regression

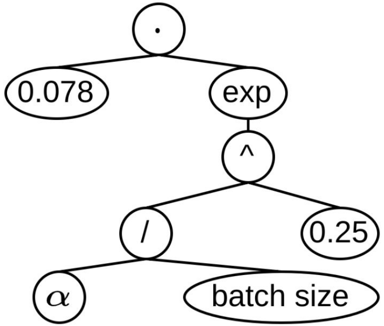
Symbolic Explanations for AutoML

[Segel et al. AutoML'23]

- Hyperparameter optimization (HPO) methods can find well-performing configurations efficiently
- Their **lack of transparency** can lead to missing trust of the users [Hasebrock et al. 2023]

Symbolic Explanations to the Rescue!

$$s(\alpha, \text{batch size}))$$
$$= 0.078 \cdot \exp\left((\alpha/\text{batch size})^{\frac{1}{4}}\right)$$

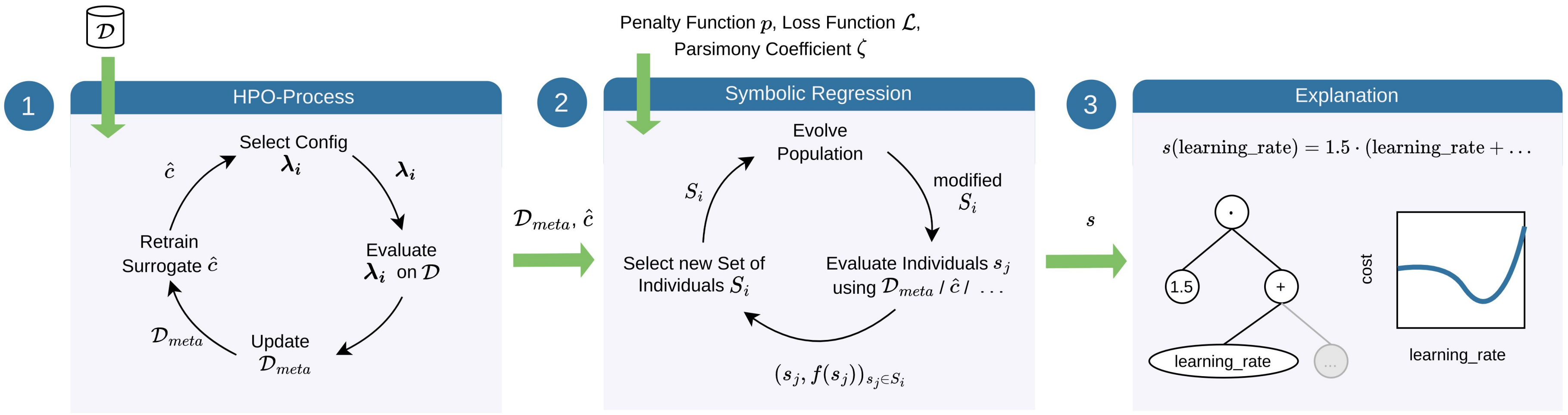


Symbolic Explanations for AutoML

[Segel et al. AutoML'23]

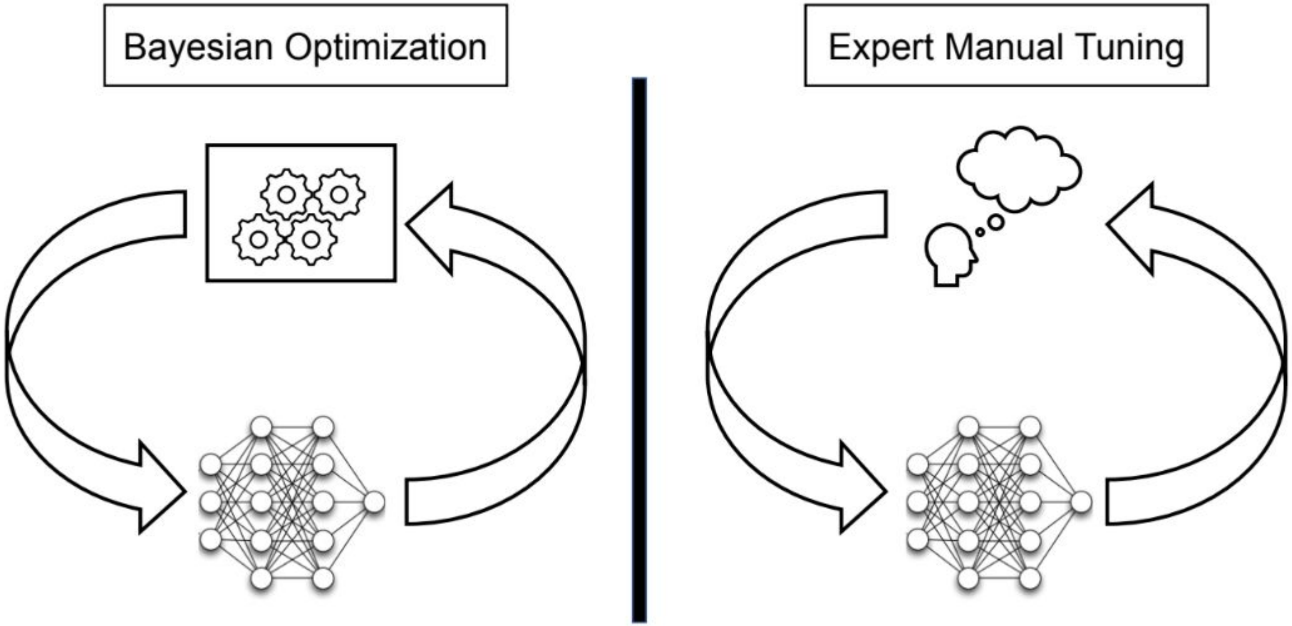
How to get more insights into hyperparameter effects?

- Employ **symbolic regression** to learn an **interpretable formula** that captures the relationship between hyperparameter configurations and model performance

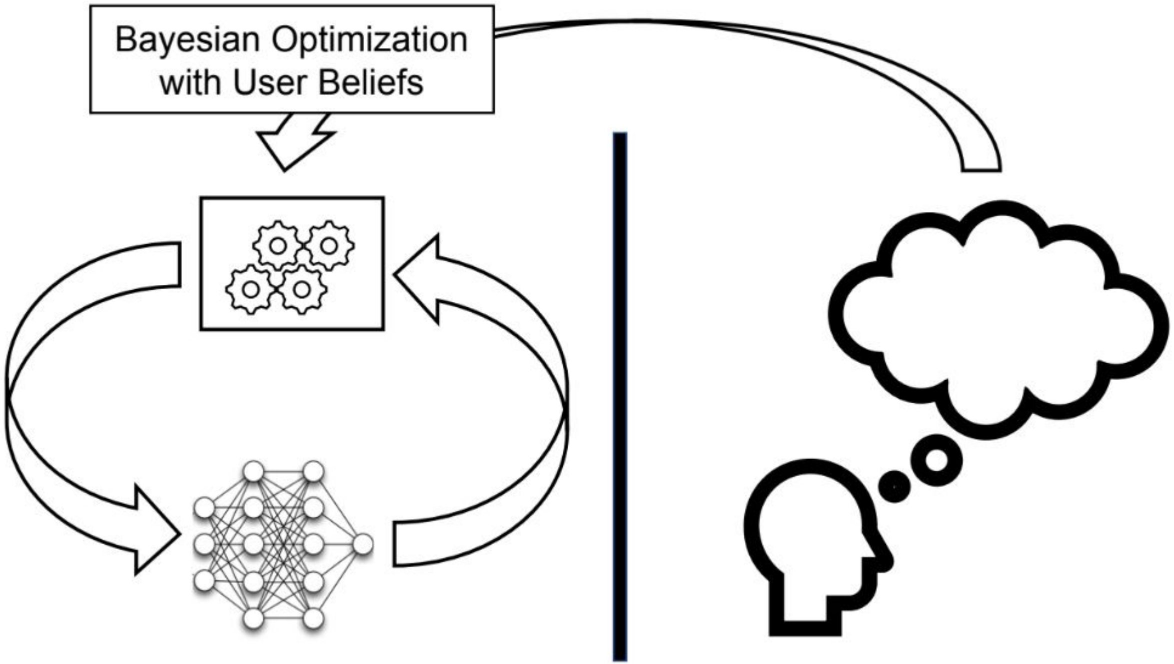


Interaction I: Expert-Priors

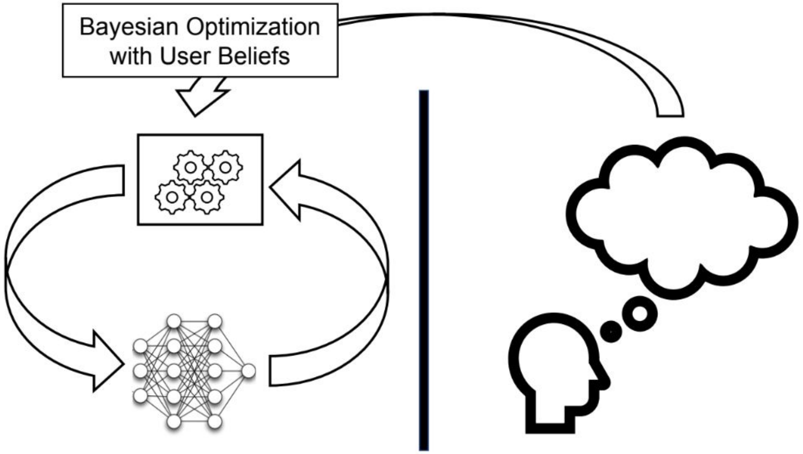
Bayesian Optimization vs Manual Tuning for HPO



Bayesian Optimization with Expert Knowledge



piBO [Hvarfner et al. ICLR'22]



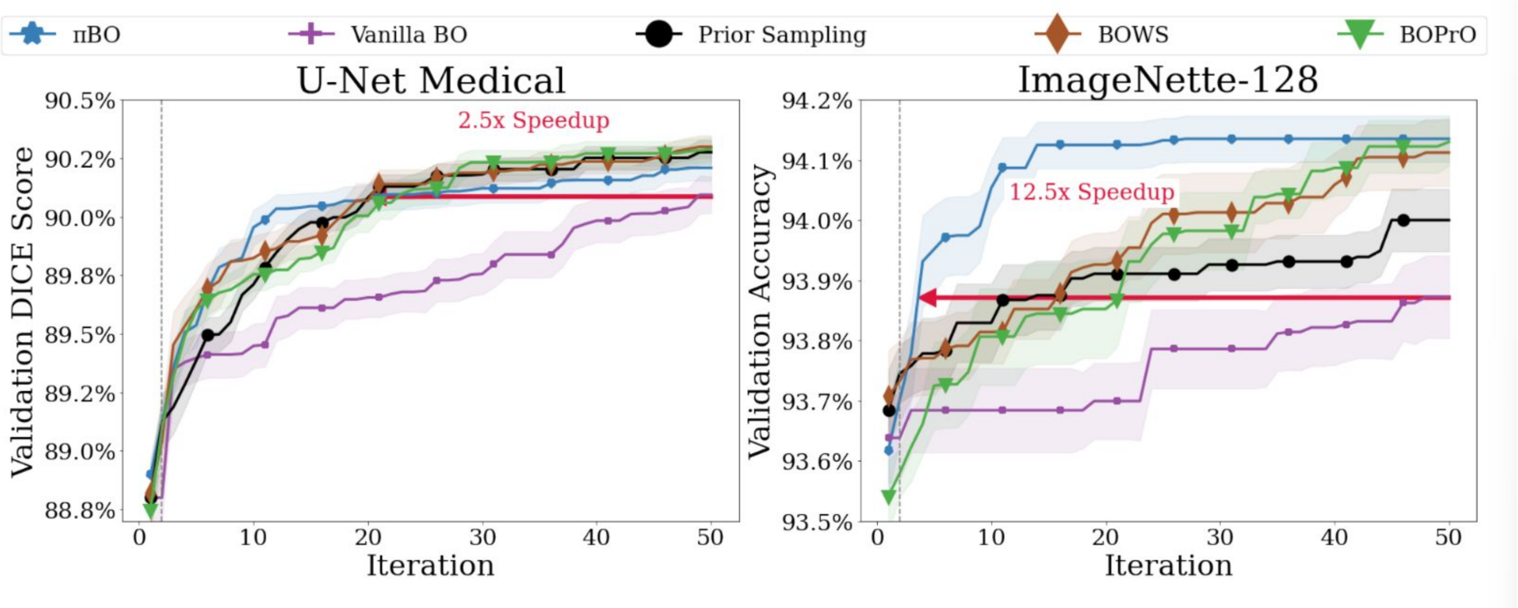
$$\boldsymbol{x}_n \in \underset{\boldsymbol{x} \in \mathcal{X}}{\arg\max}\, \alpha(\boldsymbol{x}, \mathcal{D}_n)\pi(\boldsymbol{x})^{\beta/n}$$

Acquisition Function

User Prior

Speed of forgetting user prior

piBO [Hvarfner et al. ICLR'22]



- ➔ Uses expert knowledge to speed up Bayesian Optimization
- ➔ Robust also against wrong believes
- ➔ Substantially speeds up AutoML
- ➔ Follow up with PriorBand [Mallik et al. NeurIPS'23]

Interaction II: Preferences for Multi-Objective AutoML

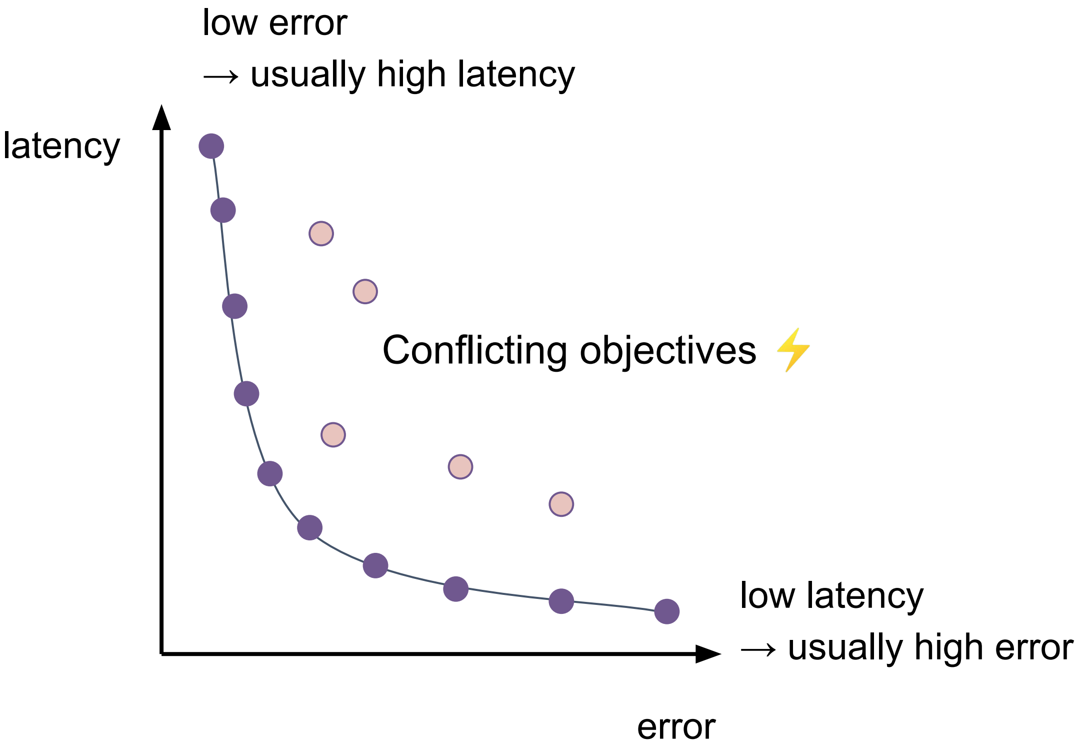
Multi-Objective AutoML

In practice, we often care about more than a single objective, e.g.

- error,
- inference time,
- unfairness,
- energy consumption,
- model complexity,
- and many more

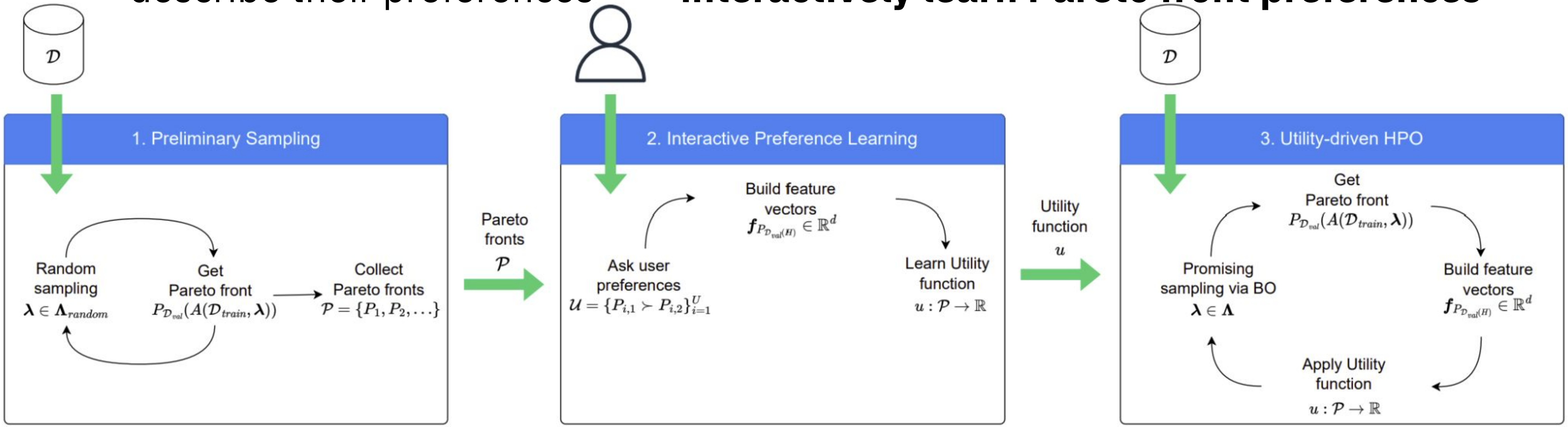
~~Goal: Find a Neural Network with high accuracy and low latency~~

Goal: Find the Pareto Set of Neural Networks that balance accuracy and latency.



Interactive HPO in Multi-Objective Problems via Preference Learning [Giovanelli et al. AAAI'24]

- Multi-objective (Auto)ML gets more and more important
  - e.g., hardware-aware NAS, fairness-aware AutoML or energy-efficient AutoML
- **Practical challenge**: Different multi-objective indicators lead to different approximated Pareto fronts and users cannot always mathematically describe their preferences ⇒ **interactively learn Pareto front preferences**



Evaluation of Preference-Learned Indicators

[Giovanelli et al. AAAI'24]



- Benchmark:
  - LCBench
  - Accuracy vs. Energy-Consumption
- Let's assume : User randomly chose a multi-objective (MO) indicator, but was actually hoping for the behavior of another MO indicator
- ⇒ learned preferences are better than randomly choosing a MO indicator

PB\IB	$HV \uparrow$	$SP \downarrow$	$MS \uparrow$	$R2 \downarrow$
$HV \uparrow$	0.76 (±0.17) \ **0.77 (±0.17)**	**0.76 (±0.17)** \ 0.52 (±0.24)	**0.76 (±0.17)** \ 0.52 (±0.21)	0.76 (±0.17) \ **0.77 (±0.16)**
$SP \downarrow$	**0.01 (±0.01)** \ 0.03 (±0.02)	**0.01 (±0.01)** \ **0.01 (±0.0)**	**0.01 (±0.01)** \ 0.04 (±0.03)	**0.01 (±0.01)** \ 0.04 (±0.02)
$MS \uparrow$	**0.61 (±0.09)** \ 0.19 (±0.08)	**0.61 (±0.09)** \ 0.19 (±0.12)	0.61 (±0.09) \ **0.65 (±0.06)**	**0.61 (±0.09)** \ 0.23 (±0.11)
$R2 \downarrow$	0.23 (±0.16) \ **0.22 (±0.16)**	**0.23 (±0.16)** \ 0.47 (±0.23)	**0.23 (±0.16)** \ 0.45 (±0.21)	0.23 (±0.16) \ **0.21 (±0.16)**

AutoML in Constrained Applications

AutoML in Heavily Constrained Applications

[Neutatz et al. VLDBJ’23]


Default AutoML Configuration

Validation Strategy:	Holdout 66/33
Ensembling:	yes
Incremental Training:	yes
Validation split reshuffle:	no
ML Hyperparameter space:	
SVM:	Yes
SVM_tol:	Yes
SVM_C:	Yes
Extra Trees:	Yes
KNN:	Yes
Multilayer Perceptron:	Yes
Any Feature Preprocessor:	Yes
302 hyperparameters	Yes

Adapt AutoML parameters to ML task and deactivate undesired ML hyperparameters

Dynamic AutoML Configuration

Validation Strategy:	Holdout 46/54
Ensembling:	no
Incremental Training:	yes
Validation split reshuffle:	yes
ML Hyperparameter space:	
SVM:	Yes
SVM_tol:	Yes
SVM_C:	No
Extra Trees:	Yes
KNN:	No
Multilayer Perceptron:	No
Any Feature Preprocessor:	No
302 hyperparameters	Yes/No

Searches for the optimal ML pipeline in the defined search space. A pipeline is defined by the selected ML hyperparameters.

ML Pipeline

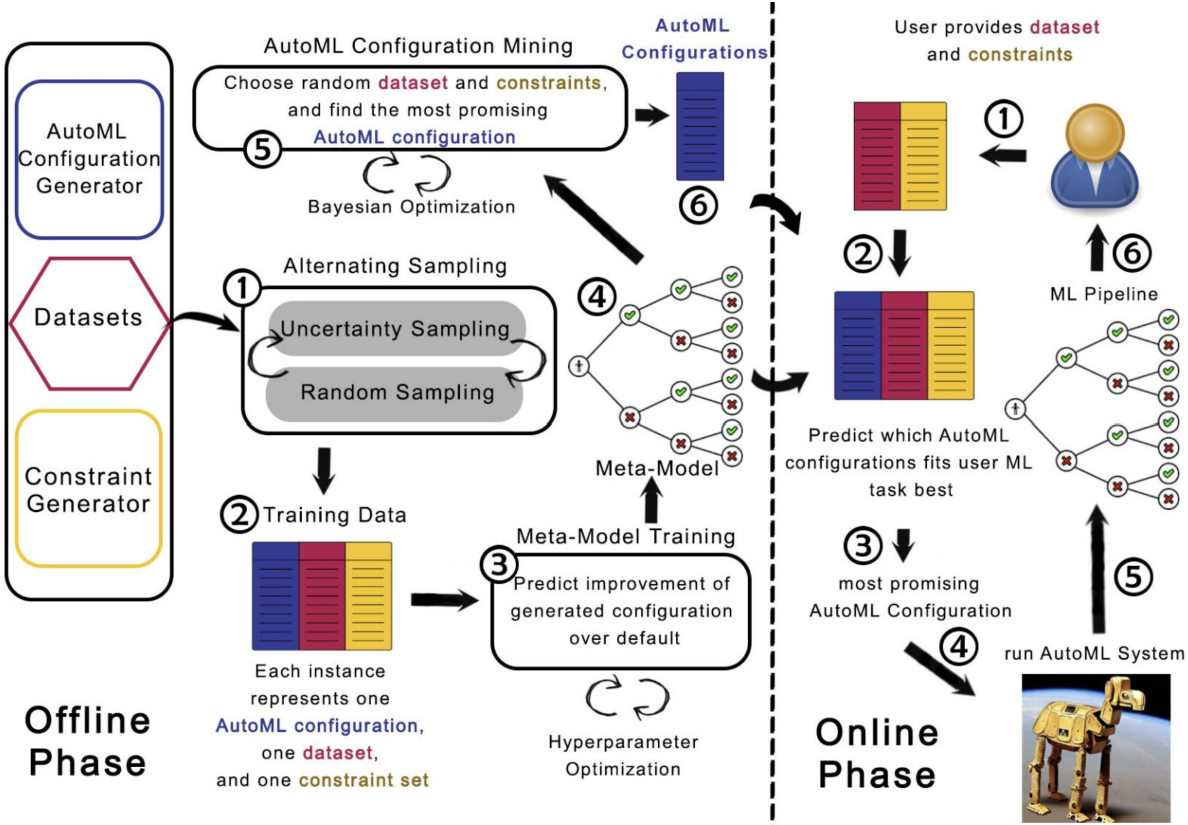
For SVM, the **model parameters** are the weights w:

$$\left[\frac{1}{n}\sum_{i=1}^{n}\max\left(0, 1 - y_i(\mathbf{w}^T\mathbf{x}_i - b)\right)\right] + \lambda\|\mathbf{w}\|^2.$$

ML Hyperparameters:	
SVM:	Yes
SVM_tol:	1e-5
SVM_C:	1.0 (default)
Extra Trees:	No
KNN:	No
Multilayer Perceptron:	No
Any Feature Preprocessor:	No
302 hyperparameters	...

AutoML in Heavily Constrained Applications

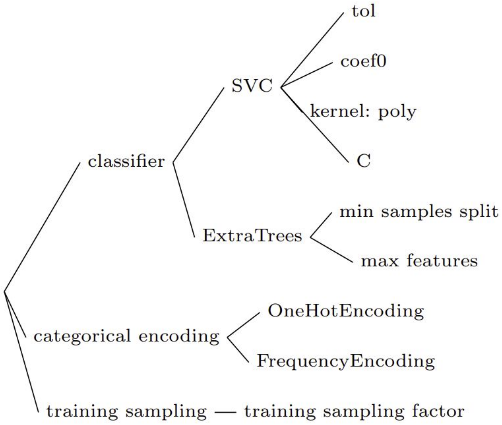
[Neutatz et al. VLDBJ'23]



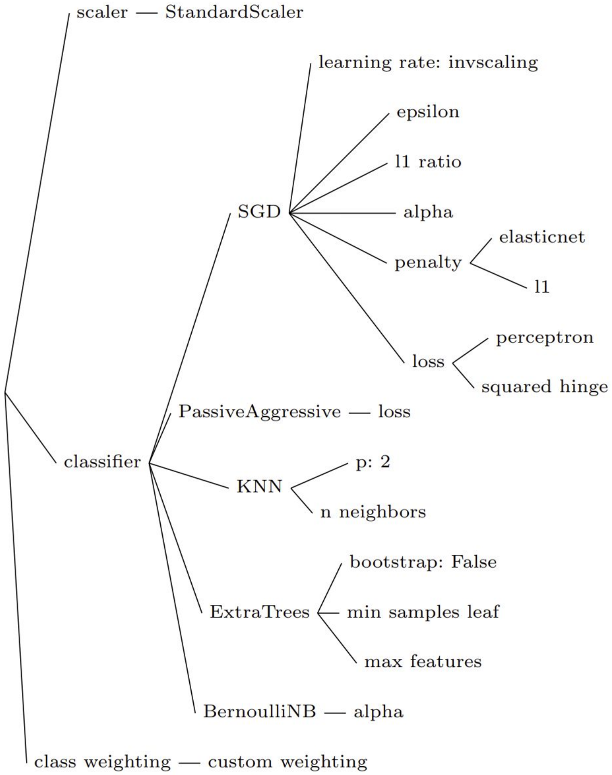
Possible application constraints:

- AutoML budget
- Inference time
- Memory consumption
- Energy consumption
- Fairness thresholds
- ...

Can it learn to select different configuration spaces? [Neutatz et al. 2023]



(a) Christine (1min search time)



(b) Robert (5min search time)

Take-Aways for Meta-Learning AutoML Conf.


- **Assumption**: If we invest more time into the development of AutoML packages (incl. meta-learning), we save a lot of compute resources for using it
- **Positive** take-away:
  Yes, we can meta-learn how to configure AutoML systems and achieve new state-of-the-art performance
- **Negative** take-away:
  We cannot easily do it for large AutoML budgets (beyond 10min) without enormous compute resources
- **Future challenge**: How to configure AutoML on expensive tasks;
  "Expensive" can mean:
  - very expensive ML models (e.g., LLMs)
  - very complex configuration spaces with thousands of ML trainings

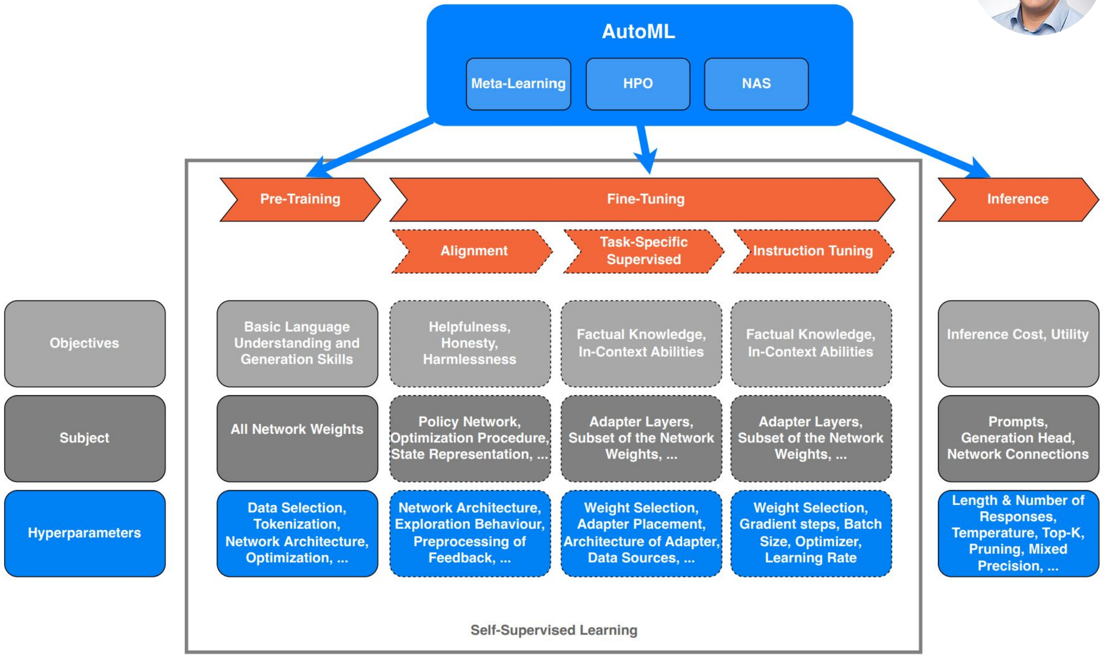
AutoML ⟺ LLMs

AutoML ➡ LLMs [Tornede et al. 2023]

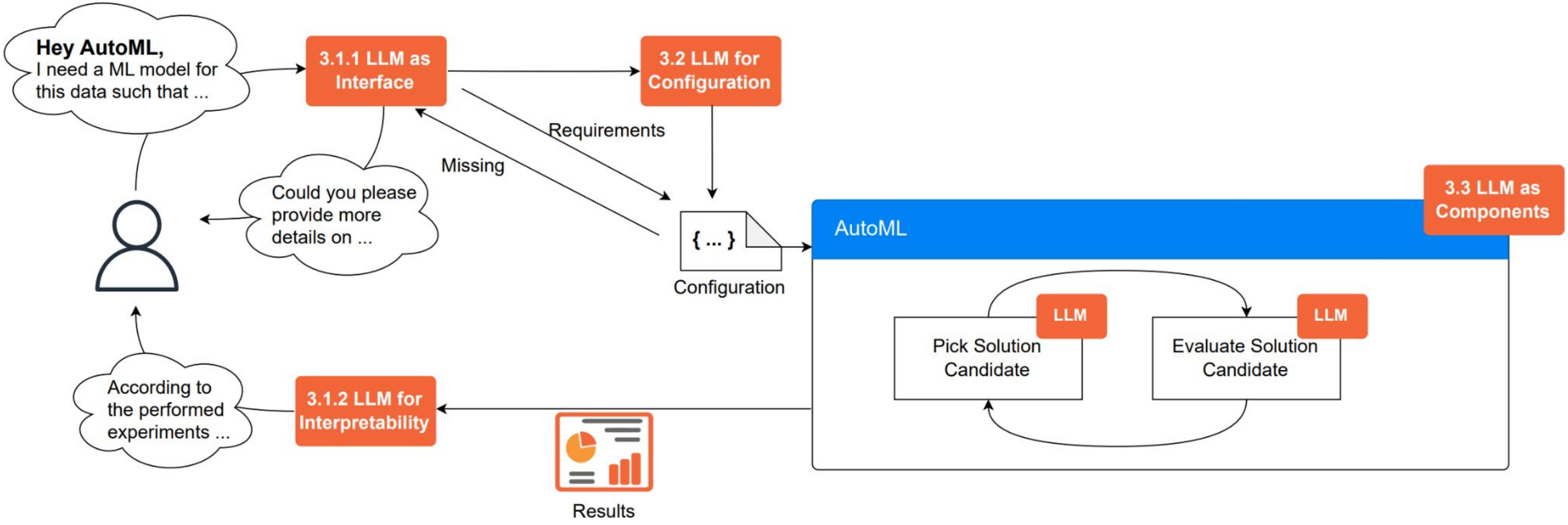
Leibniz Universität Hannover

Challenges

1. Cost of Pre-Training Base Models
2. Multitude of Different Stages
3. Multitude of Performance Indicators
4. Combination of Different Learning Paradigms
5. Determining Neural Architectures for LLMs



AutoML ⟵ LLMs [Tornede et al. 2023]



Green AutoML

Green AutoML



Energy-efficient AutoML

Data compression,
Zero-cost AutoML,
multi-fidelity,
intelligent stopping, …

Searching for Energy-Efficient Models

Model size constraint,
Energy-aware objective functions,
Energy efficient architectures,
Model compression, …

AutoML for Sustainability

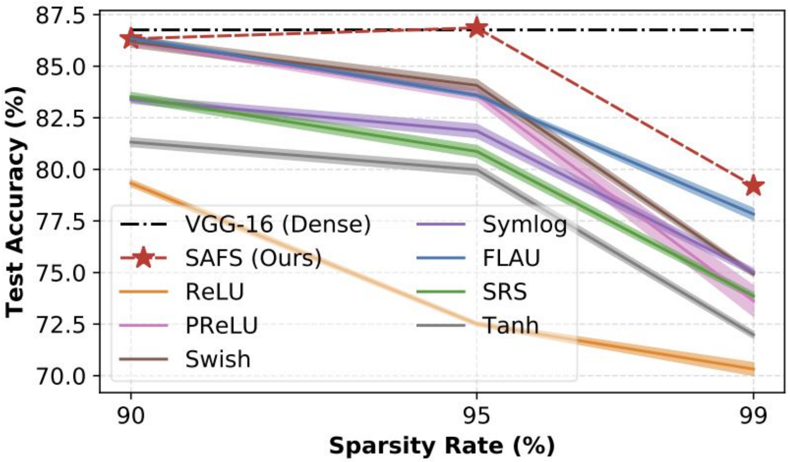
Plastic Litter Detection,
Green Assisted Driving,
Predictive Maintenance, …

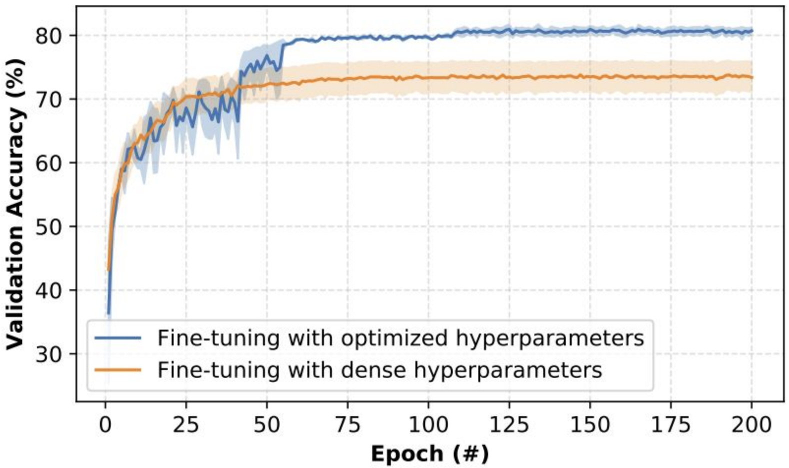
Create Attention

Tracking emissions,
awareness among students,
researchers, industry partners, …

Learning Activation Functions for Sparse Neural Networks [Loni et al. AutoML'23]

- Sparsifying networks can help to save a lot of compute power
- **Insights**:
  1. Using the same activation function class as for the dense network is suboptimal for pruning
  2. Hyperparameters have to adapted accordingly

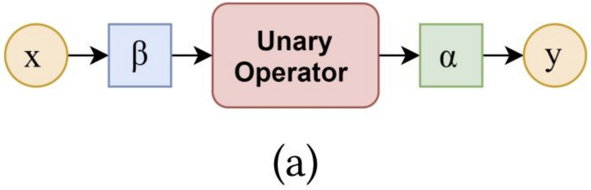




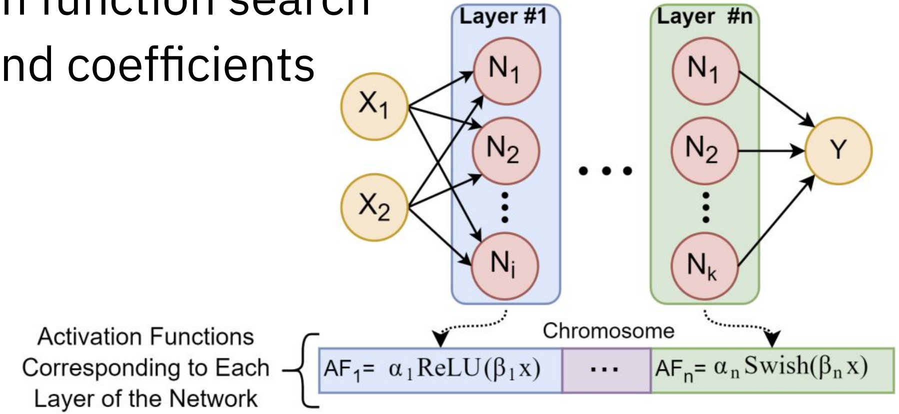
Learning Activation Functions for Sparse Neural Networks [Loni et al. AutoML'23]

Take-Aways:

- Search for activation functions for the pruning process
- Activation functions should even differ for different layers
  - Symlog and Acon in early layers
  - Swish in middle layers
- Stage 1: Use EA (LAHC) for activation function search
- Stage 2: Apply SGD-based HPO to find coefficients



(a)

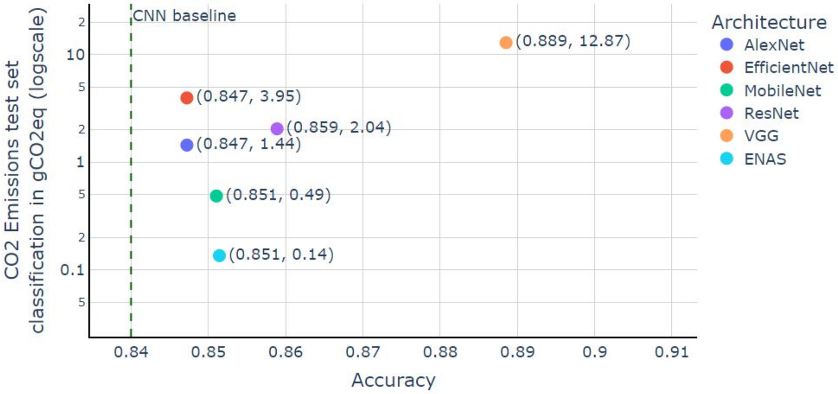


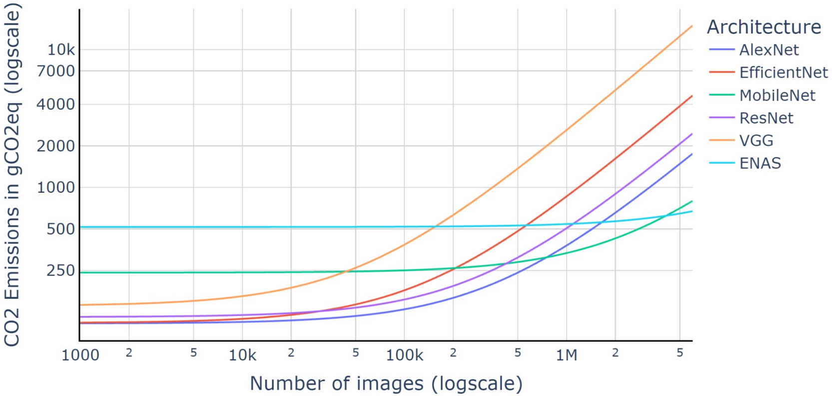
Green AutoML for Plastic Litter Detection

[Theodorakopoulos et al. CCAI’23]

Insights:

1. Architecture of DNNs with better accuracy
2. Architecture with lower CO_2 emissions
3. CO_2 emissions of AutoML training is compensated at inference





Packages from my Group

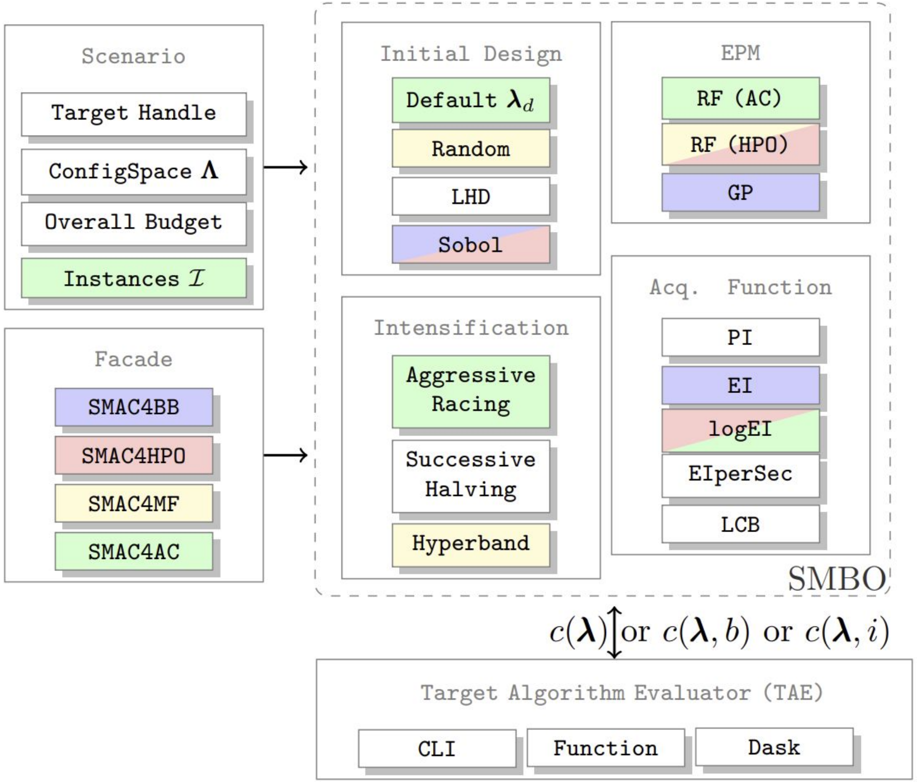
automl / SMAC3 Public

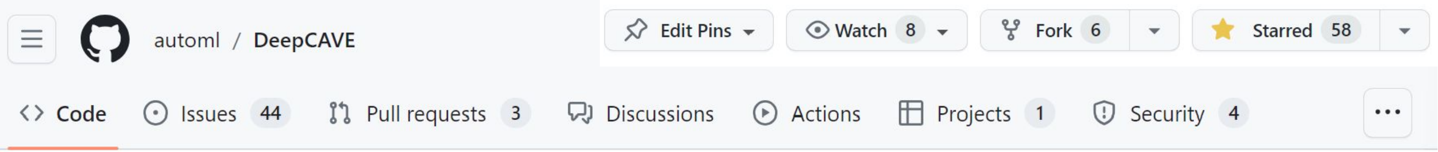
Notifications | Fork 206 | Star 920

Code | Issues 74 | Pull requests 10 | Actions | Projects 1 | Security | ...

> 67k downloads last month!

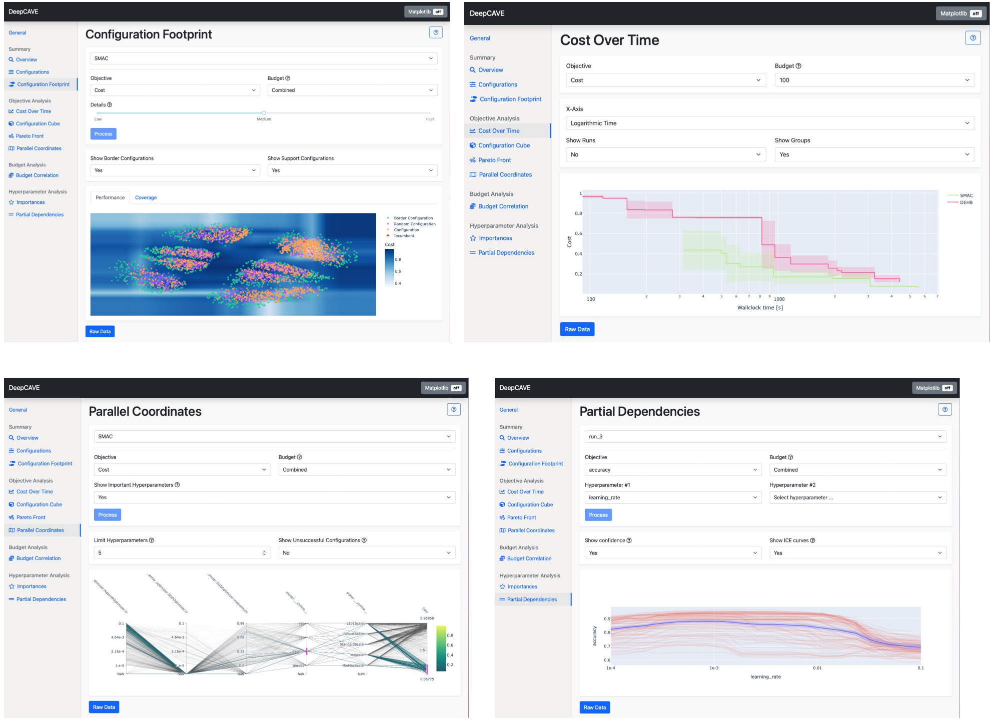
- Covers all kind of hyperparameter optimization use cases
- State-of-the-art techniques and performance
  - Bayesian Optimization
  - Multi-fidelity optimization
  - Multi-objective optimization
  - Algorithm configuration
- Highly configurable and modular
- Parallelizable





DeepCAVE [Sass et al. 2022]

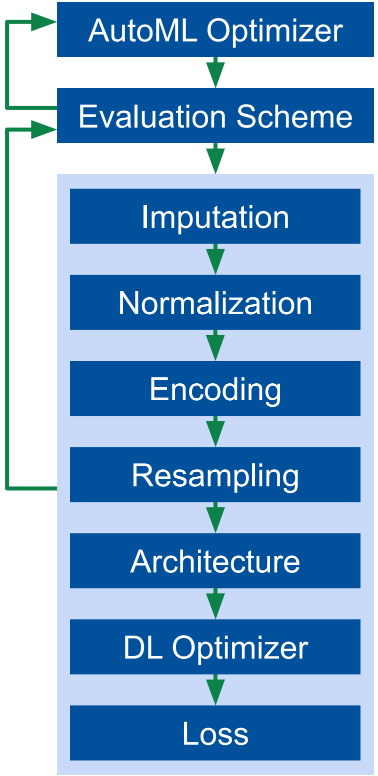
- **Interactive Dashboard** to self-analyze optimization runs/processes.
- **Analyzing while optimizing**
- **Exploration of multiple areas** like performance, hyperparameter and budget analysis.
- **Modularized plugin** structure with access to selected runs/groups to provide maximal flexibility.
- **Asynchronous execution** of expensive plugins and caching of their results.
- **API mode** gives you full access to the code



automl / Auto-PyTorch Public

Notifications | Fork 266 | Star 2.2k

Code | Issues 50 | Pull requests 20 | Actions | Projects 3 | Wiki | Security | ...



1. Automatic deep learning covering the entire DL pipeline
2. Joint hyperparameter and neural architecture search

➜ Auto-PyTorch Tabular
[Zimmer et al. IEEE TPAMI’21]

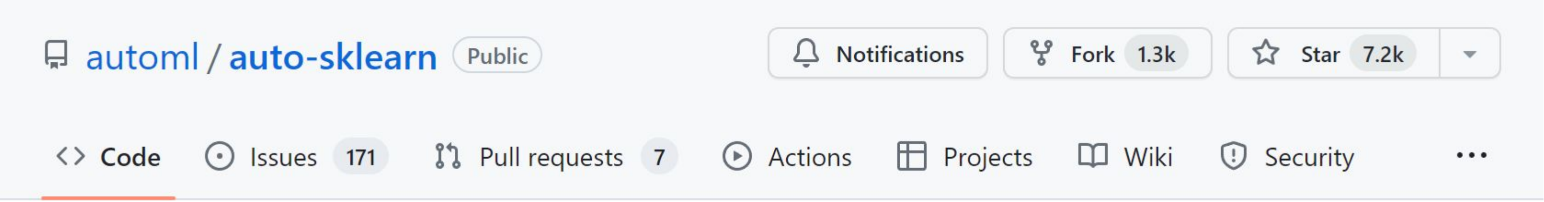
➜ State-of-the-art on tabular data with regularization cocktails
[Kadra et al. NeurIPS’21]

➜ Auto-PyTorch for Time Series Forecasting
[Deng et al. ECML’22]

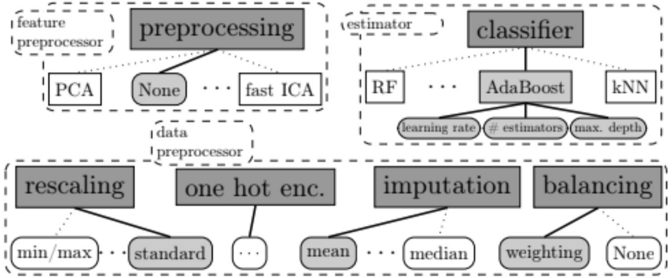
```
# initialise Auto-PyTorch api
api = TabularClassificationTask()

# Search for an ensemble of machine learning algorithms
api.search(
    X_train=X_train,
    y_train=y_train,
    X_test=X_test,
    y_test=y_test,
    optimize_metric='accuracy',
    total_walltime_limit=300,
    func_eval_time_limit_secs=50
)

# Calculate test accuracy
y_pred = api.predict(X_test)
```



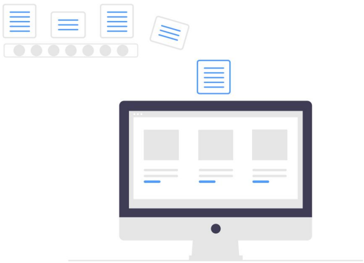
Takes care of finding well-performing ML-pipeline



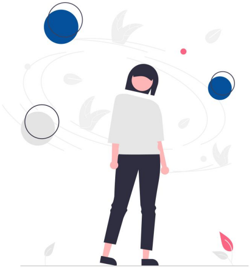
Easy-to-use

```
import autosklearn.classification as cls
automl = cls.AutoSklearnClassifier()
automl.fit(X_train, y_train)
y_hat = automl.predict(X_test)
```

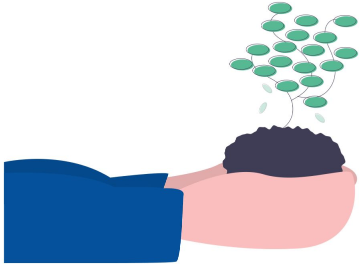
Our Research Foci



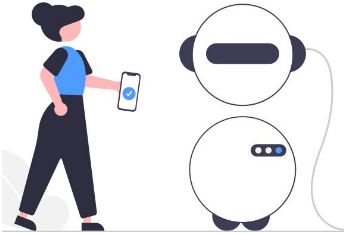
Core AutoML



Human-centered AutoML

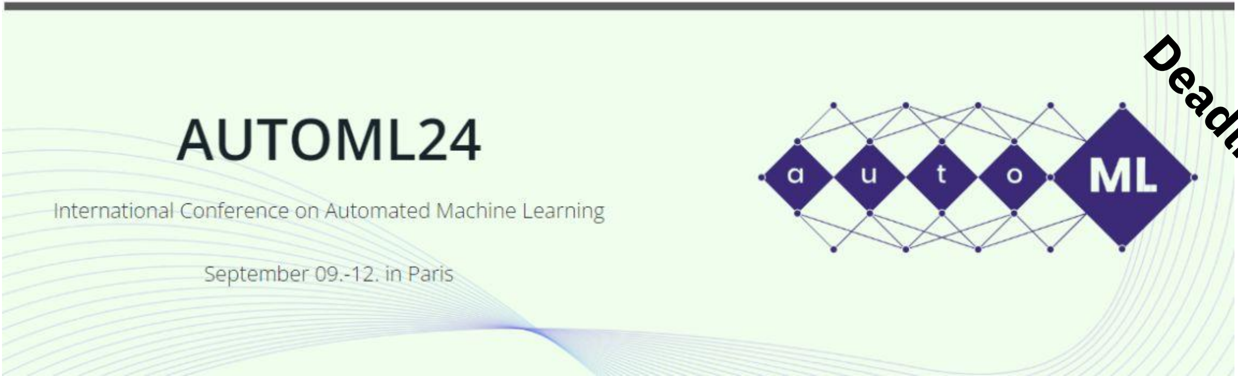


Green AutoML



AutoRL

AutoML Weeks 2024



Submission Deadline Feb 29th

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Niedersachsen