Automated Machine Learning: A Partical Introduction

KonKIS’24 - Conference of the German AI Service Centers

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

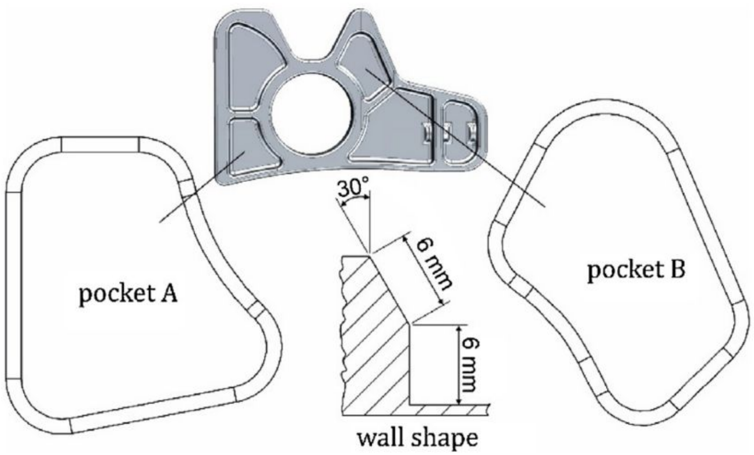
- In an age of limited resources, the need for efficient use gets more important

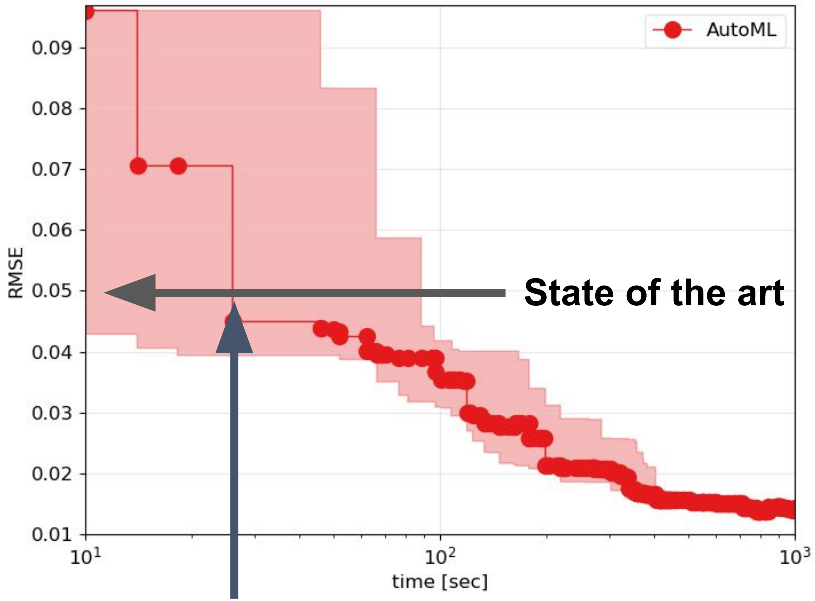
- **AutoML contributes to AI literacy!**

[See also my TEDx Talk]

Shape Error Prediction in Milling Process

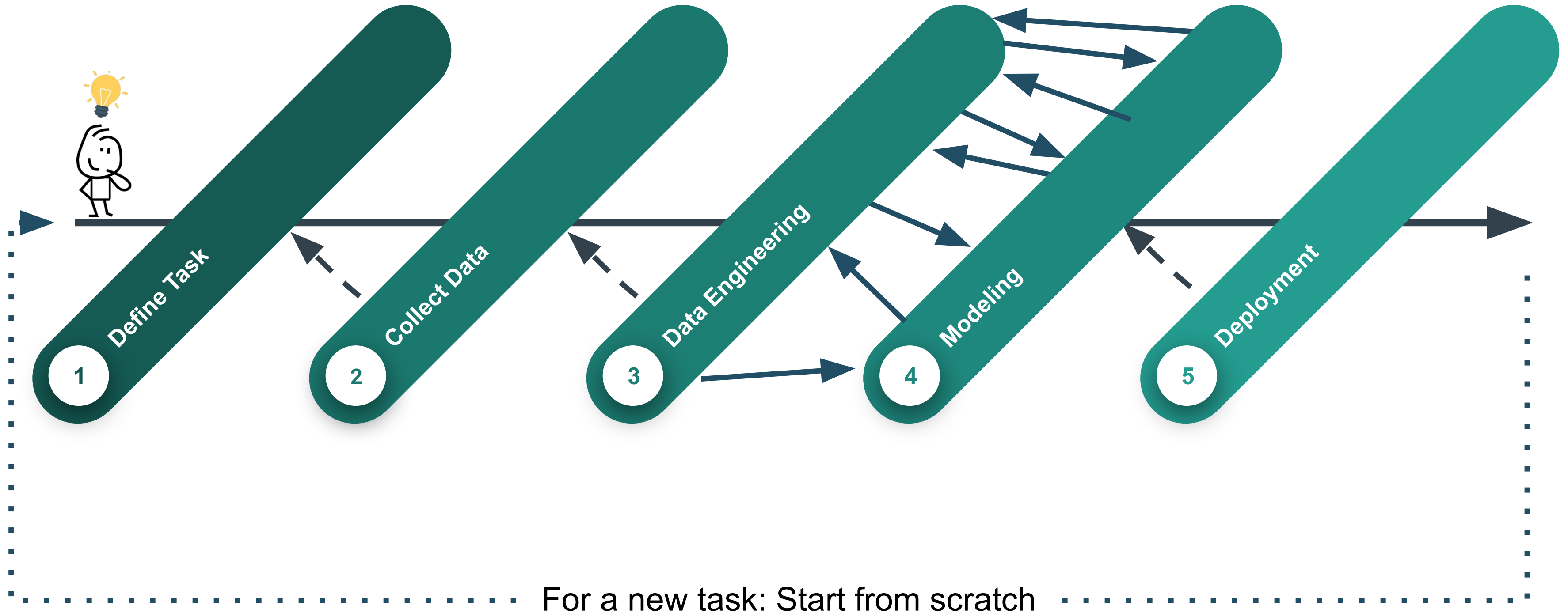
[Denkena et al. SSRN'20]



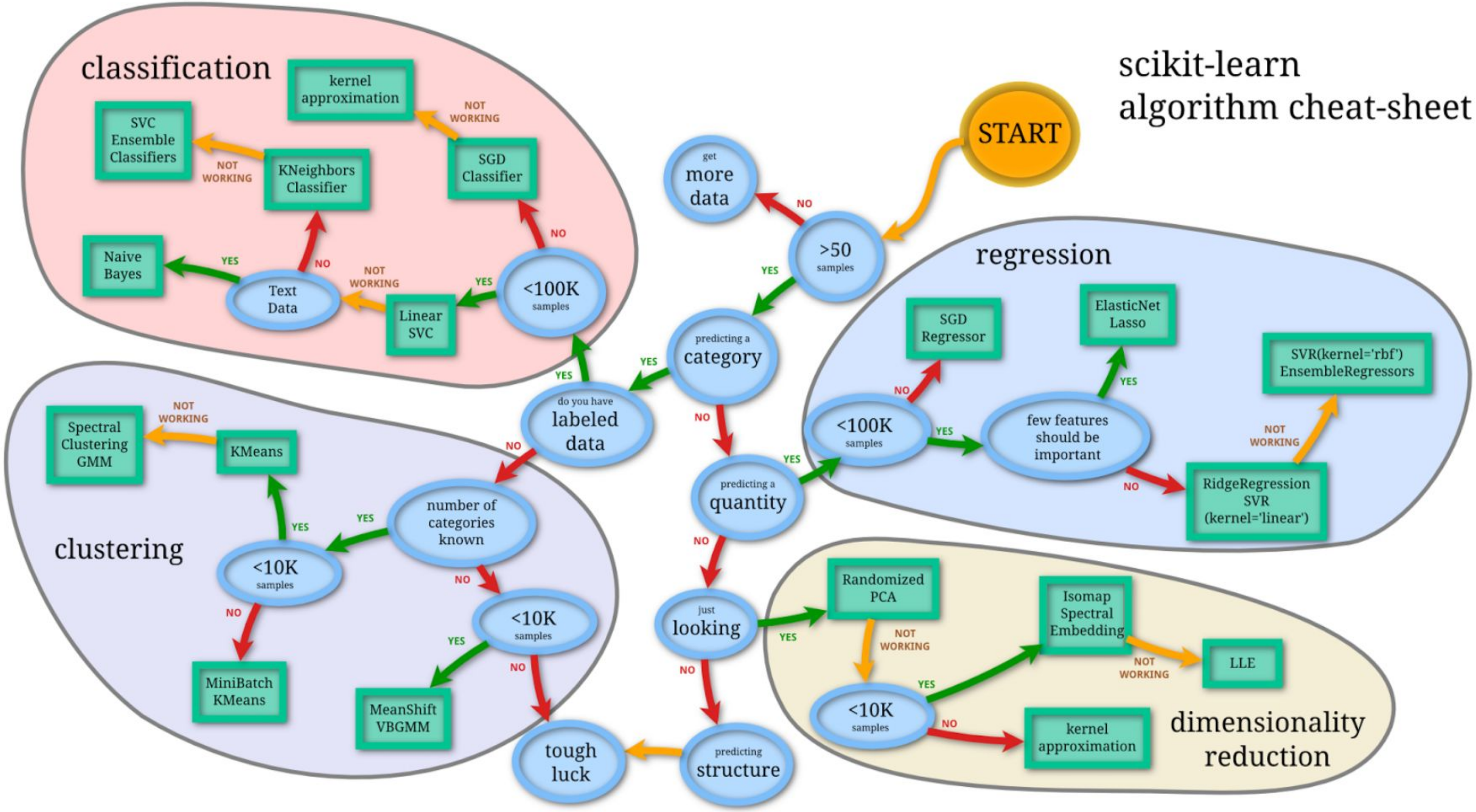


Better than state of the art in less than 30sec!

Why does ML development take a lot of time?



Design-Decisions? That's not how it works!



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

Hyperparameters are everywhere

SGD

CLASS torch.optim.SGD(*params, lr=0.001, momentum=0, dampening=0, weight_decay=0, nesterov=False, *, maximize=False, foreach=None, differentiable=False, fused=None*) [SOURCE]

Parameters

- **params** (*iterable*) – iterable of parameters to optimize or dicts defining parameter groups
- **lr** (*float, optional*) – learning rate (default: 1e-3)
- **momentum** (*float, optional*) – momentum factor (default: 0)
- **weight_decay** (*float, optional*) – weight decay (L2 penalty) (default: 0)
- **dampening** (*float, optional*) – dampening for momentum (default: 0)
- **nesterov** (*bool, optional*) – enables Nesterov momentum (default: False)

Hyperparameters are everywhere

stable

Search docs

- Installation Guide
- Building From Source
- Get Started with XGBoost
- XGBoost Tutorials
- Frequently Asked Questions
- XGBoost User Forum
- GPU Support
- XGBoost Parameters
- Prediction
- Tree Methods

Python Package

Scikit-Learn API

Scikit-Learn Wrapper interface for XGBoost.

class `xgboost.XGBRegressor`(**, objective='reg:squarederror', **kwargs*)

Bases: `XGBModel`, `RegressorMixin`

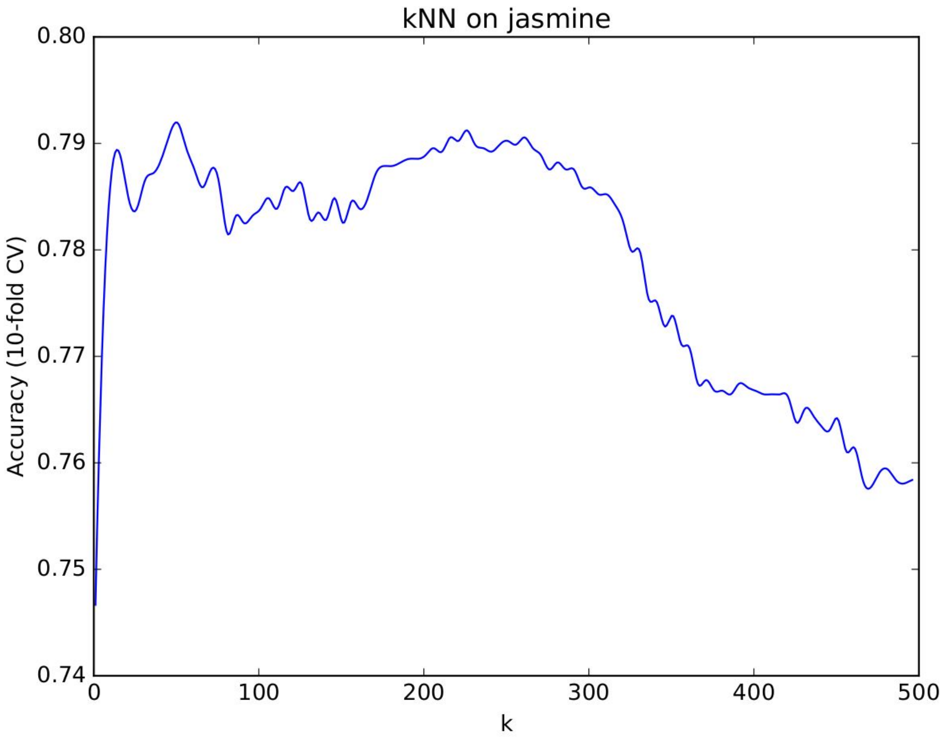
Implementation of the scikit-learn API for XGBoost regression. See Using the Scikit-Learn Estimator Interface for more information.

Parameters:

- **n_estimators** (*Optional[int]*) – Number of gradient boosted trees. Equivalent to number of boosting rounds.
- **max_depth** (*Optional[int]*) – Maximum tree depth for base learners.
- **max_leaves** (*Optional[int]*) – Maximum number of leaves; 0 indicates no limit.
- **max_bin** (*Optional[int]*) – If using histogram-based algorithm, maximum number of bins per feature
- **grow_policy** (*Optional[str]*) – Tree growing policy.
  - depthwise: Favors splitting at nodes closest to the node,
  - lossguide: Favors splitting at nodes with highest loss change.
- **learning_rate** (*Optional[float]*) – Boosting learning rate (xgb's "eta")

Simplest Example Ever: kNN

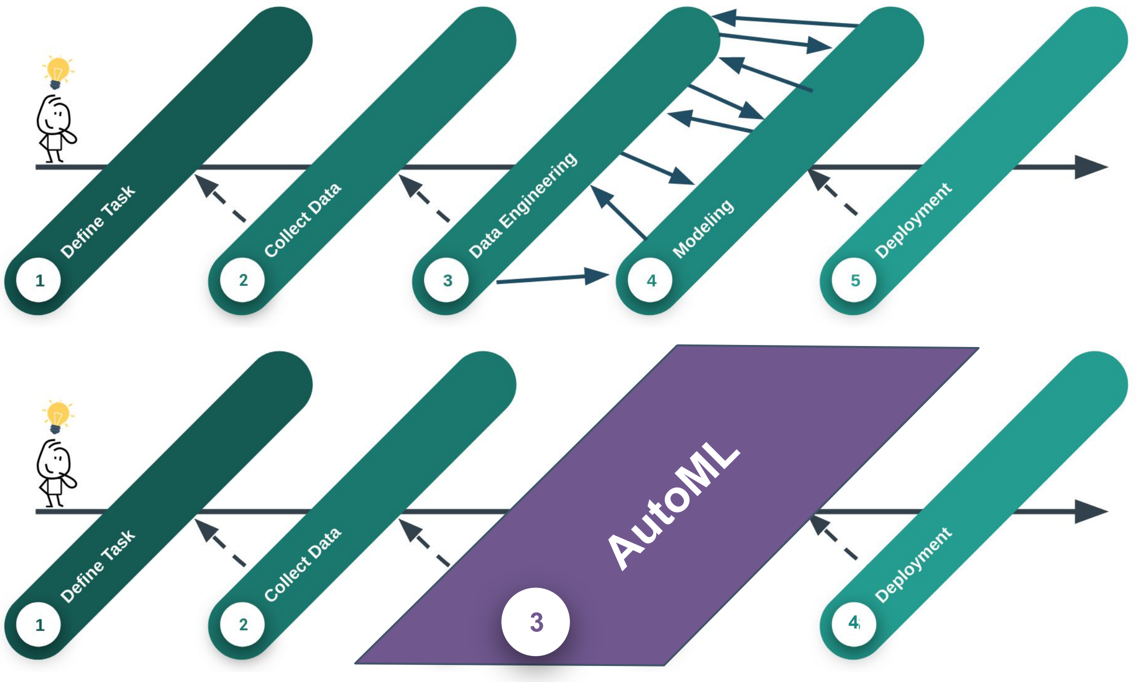
- *k*-nearest neighbors (kNN) is one of the **simplest ML algorithms**
- Size of neighbourhood (*k*) **is very important for its performance**
- The performance function depending on *k* is **quite complex** (not at all convex)
- BUT: We cannot get these curves in practice!



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

AutoML Packages

A brief History of AutoML Packages

- **2004**: Ensemble Selection from a set of models
- **2012**: AutoWeka: Efficient in a hierarchy of models and hyperparameters
- **2015**: Auto-Sklearn: Warmstarting of AutoML and ensembling
- **2016**: TPOT: Tree-based Pipeline Optimization for AutoML
- **2019**: AutoKeras: AutoML for Deep Learning
- **2020**: AutoGluon: Stacked Ensemble for diverse Models
- **2021**: AutoPyTorch: Multi-Fidelity for AutoDL powered by SMAC3
- **2022**: TabPFN: In-Context Learning of Tabular ML

Credits to Matthias Feurer for this list automl / SMAC3 Public

SMAC

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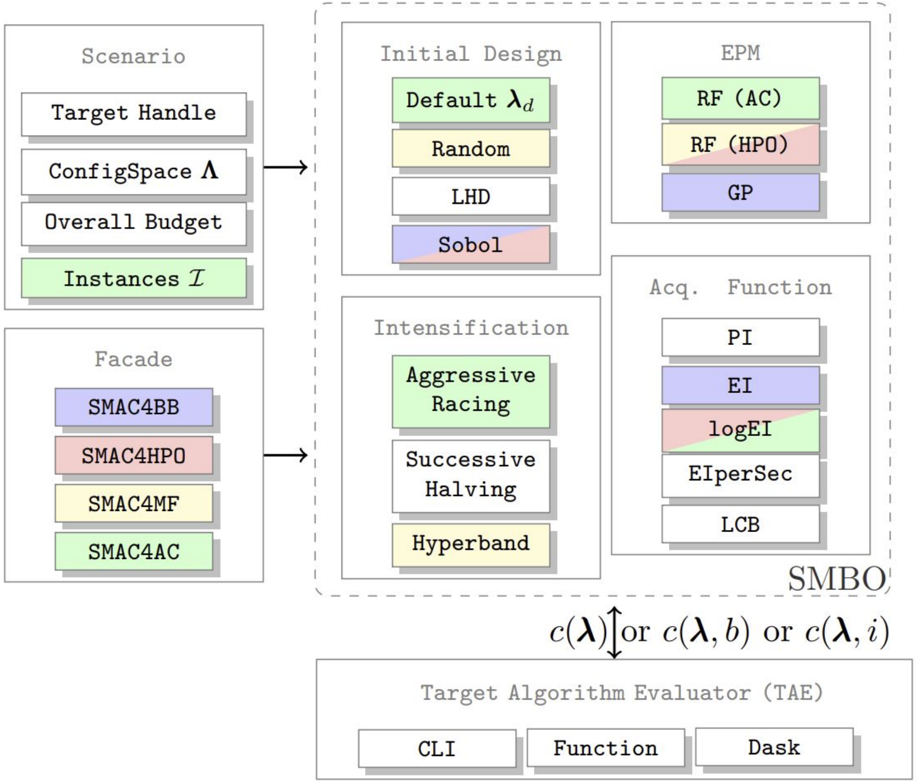
- **Use case**: there exits a code base for DS/ML that needs further improvements
- Covers all kind of hyperparameter optimization use cases
- State-of-the-art techniques and performance
    - Bayesian Optimization
    - Multi-fidelity optimization
    - Multi-objective optimization
- Highly configurable and modular
- Parallelizable



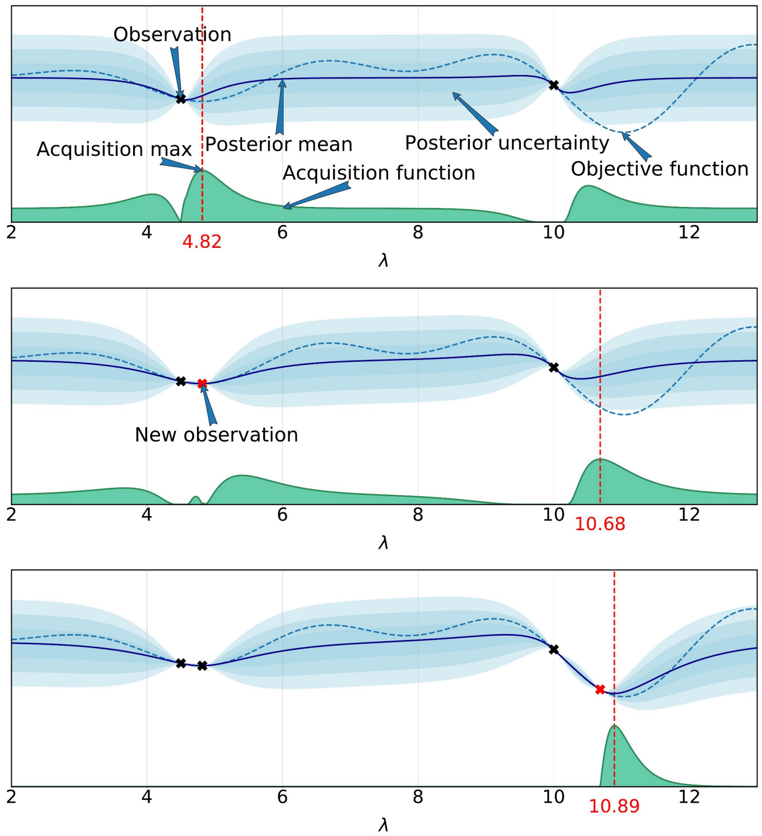
Bayesian Optimization in a Nutshell

General approach:

1. Fit a probabilistic model to predict the performance of unknown Hyperparametrer configurations
2. Trade-off exploration and exploitation for choosing the next configuration to be evaluated

Comments:

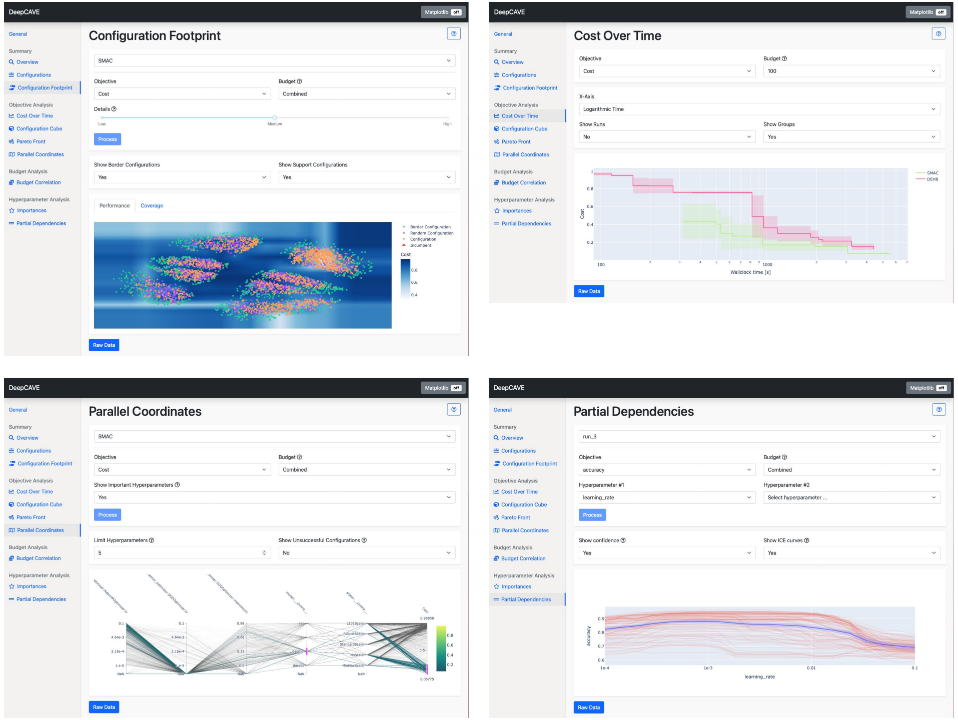
- very efficient in number of evaluations; **<u>much more efficient than grid search and random search</u>**
    - random search is competitive if you have thousands of CPUs/GPUs
- There are convergence results for Bayesian Optimization

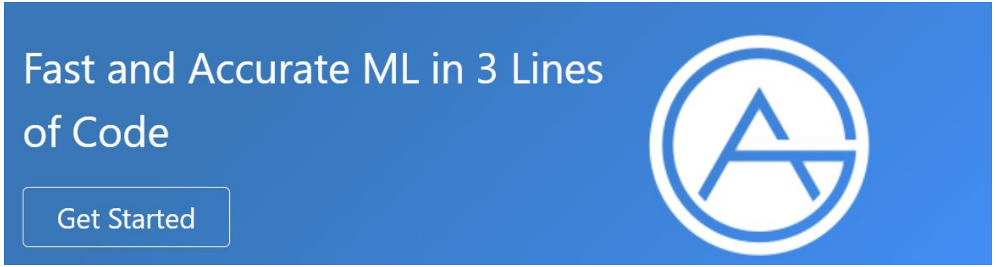


DeepCAVE

DeepCAVE [Sass et al. 2022]

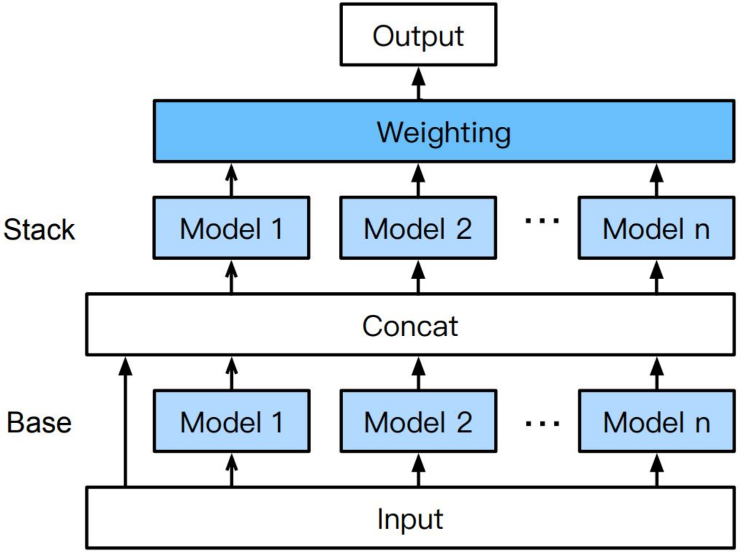
- **Interactive Dashboard** to analyze optimization runs/processes.
- **Exploration of multiple areas** like performance, hyperparameter and budget analysis.
- **Modularized plugin** structure with access to selected runs/groups to provide maximal flexibility.
- **Asynchronous execution** of expensive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





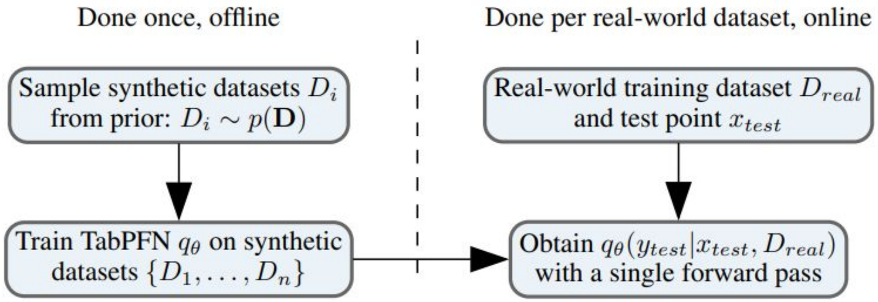
AutoGluon [Erickson et al. 2020]

- **Use case**: Push-Button to obtain a very good model
- Multi-level Stacking instead of Hyperparameter Optimization
  - under restricted time budgets, time is better invested in thoroughly evaluating good defaults settings
  - Inference time can be large
- Hand-defined list of hyperparameter configurations
- Default machine learning model at AWS



TabPFN [Hollmann et al. 2022]

- **Use case**: Training is a bottleneck and training data has a reasonable size
- Based on meta-learned transformers
  - offline training is done of synthetic datasets
- **No training for new data required!**
  - New training data are part of the context input
- No hyperparameter optimization needed
- Very efficient because of missing training
  - but can be limited in data complexity
  - inference time depends on training data (i.e. context) size



(a) Prior-fitting and inference

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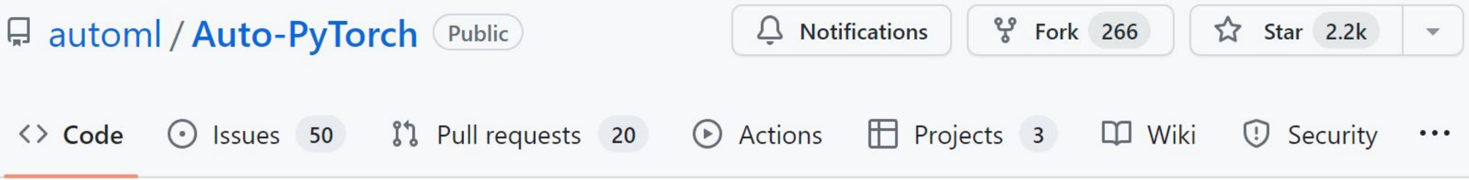
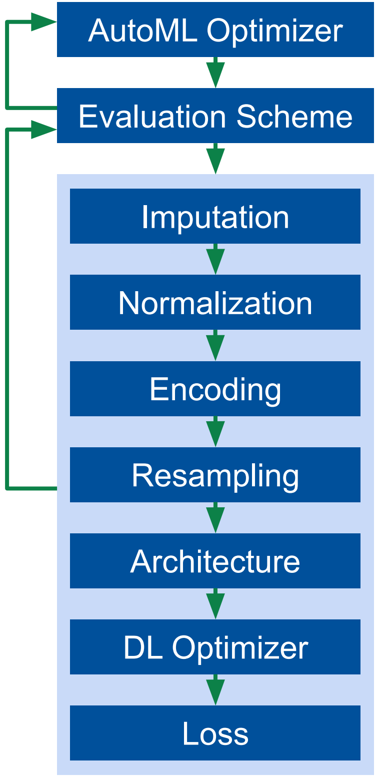
Niedersachsen

Appendix





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]

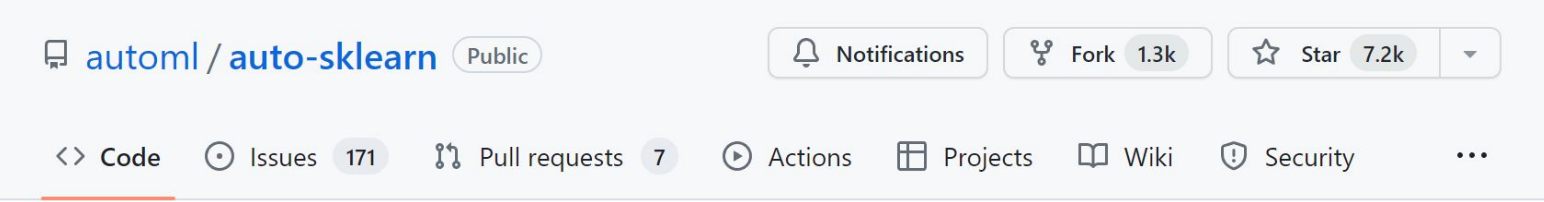
➜ State-of-the-art on tabular data with regularization cocktails [Kadra et al. NeurIPS'21]

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

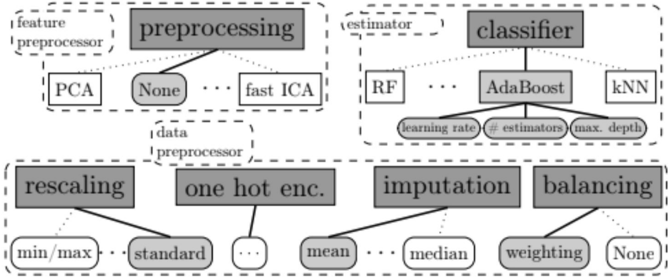
```
# initialise Auto-PyTorch api
api = TabularClassificationTask()

# 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

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