Universiteit Leiden

Automated Machine Learning for Science

Jan N. van Rijn

Leiden University

AWASES Workshop

[1] Based on Baratchi et al., 2024

Scope

Scope

Predictive AI vs Generative AI

Scope

Predictive AI vs Generative AI

Single Purpose AI vs Multi-Purpose AI

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Single Purpose AI vs Multi-Purpose AI

Training of AI vs Inference using existing models

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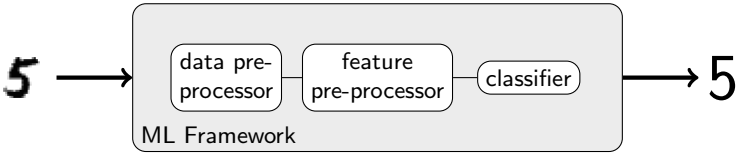
Predictive AI vs Generative AI

Single Purpose AI vs Multi-Purpose AI

Training of AI vs Inference using existing models

AutoML can be applied to all, but today we focus **mostly** on the training of Single Purpose Predictive AI

The Machine Learning Pipeline



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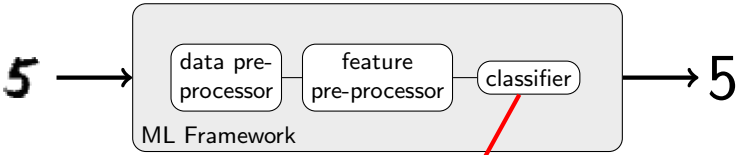
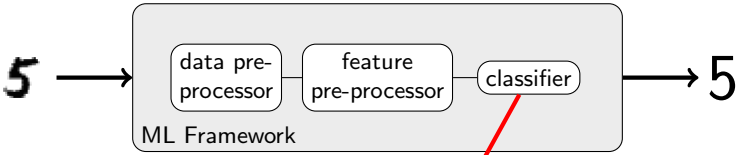


classifier	$\#\lambda$
Adaboost	4
Bernoulli Naive Bayes	2
Decision Tree	4
Extra Trees	5
Gradient Boosting	6
k-NN	3
LDA	4
...	

The Machine Learning Pipeline



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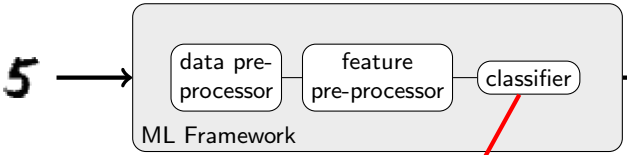

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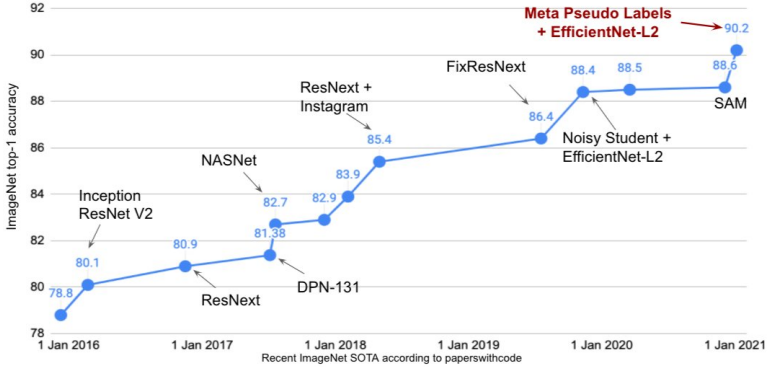
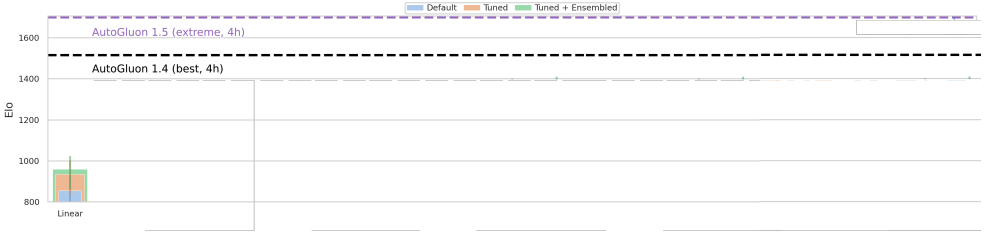
ImageNet – Progress of the State of the Art



[https://x.com/quocleix/status/1349443438698143744/photo/1]

The right choices matter



[Figure: TabArena Leaderboard on Hugging Face (per May 21).]

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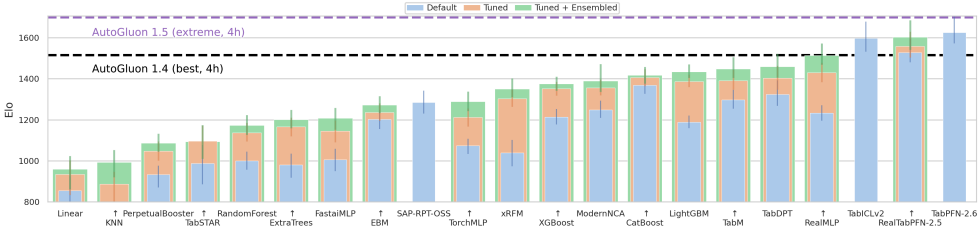
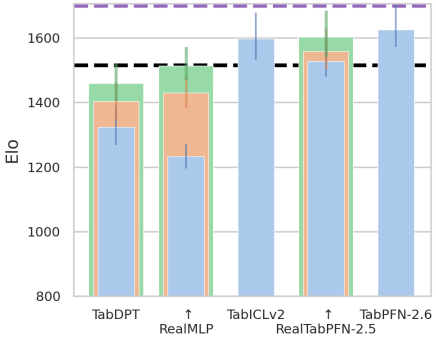


[Figure: TabArena Leaderboard on Hugging Face (per May 21).]

Various AutoML solutions

[Figure by: Satyam Kumar (2020), Medium.com blogpost.]

What about TabPFN?



[Grinsztajn, ..., Hutter, TabPFN-3: Technical Report, May 2026]]

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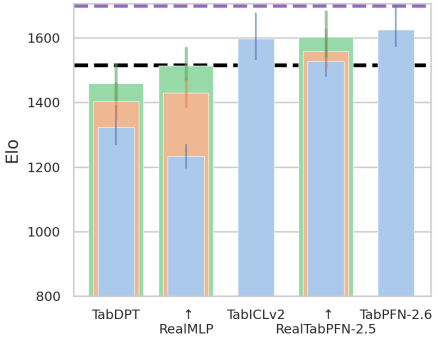

- Foundation model for tabular data

[Grinsztajn, ..., Hutter, TabPFN-3: Technical Report, May 2026]]

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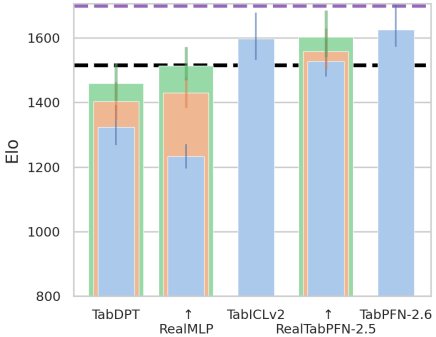

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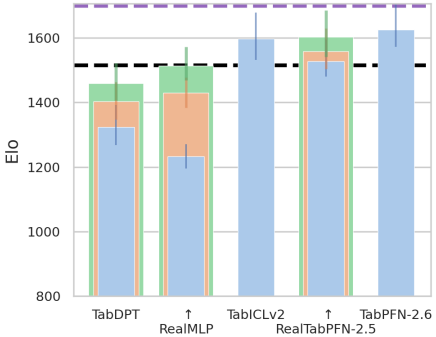

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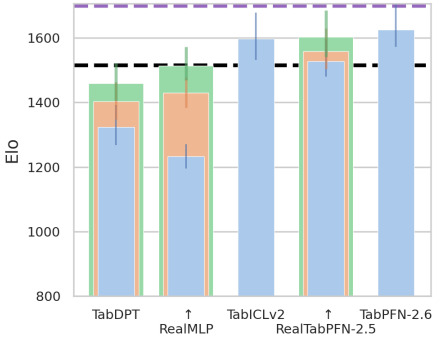

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- In-context learning: Similar idea as LLM-inference

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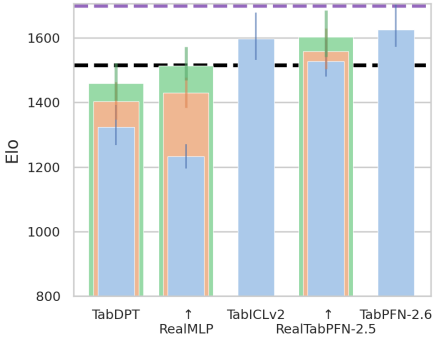
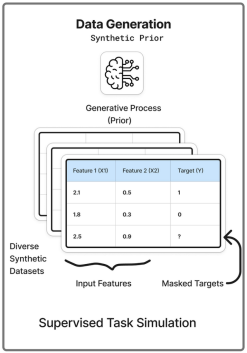


- Foundation model for tabular data
- Based on transformer architecture
- Pre-trained on massive amounts of data, only inference needed at runtime
- In-context learning: Similar idea as LLM-inference
- Initially limited to small(er) datasets, but solved in latest version

[Grinsztajn, ..., Hutter, TabPFN-3: Technical Report, May 2026]]

TabPFN architecture



[TowardsDataScience.com]

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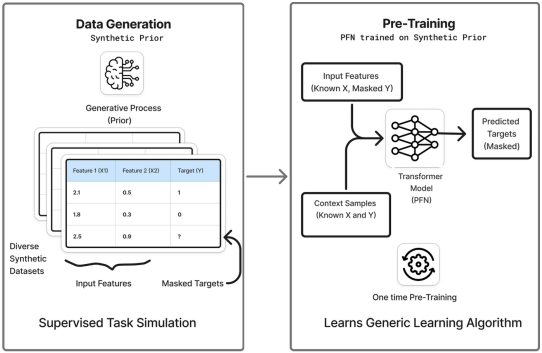

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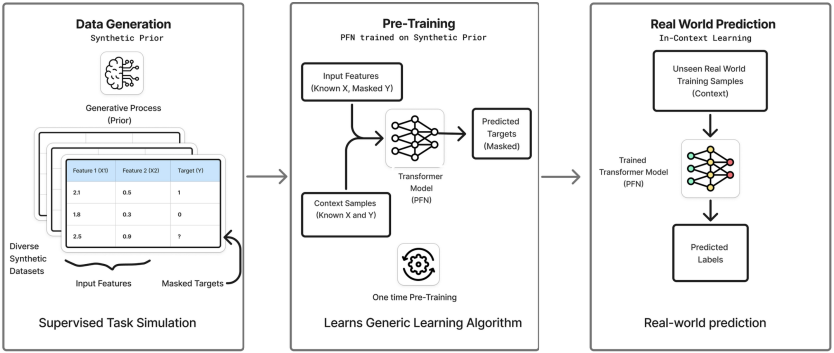

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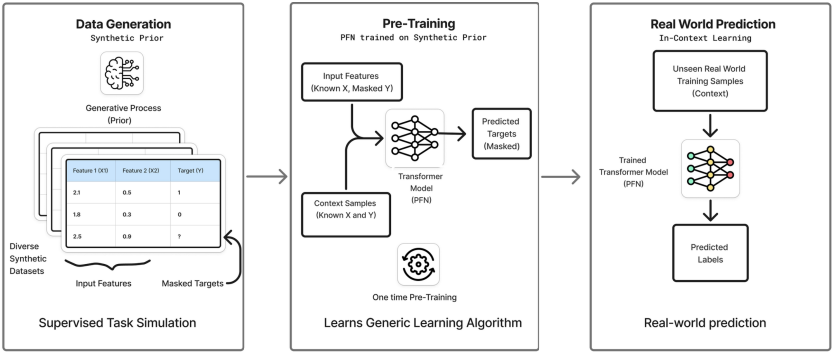

In-context learning: Similar idea as LLM-inference

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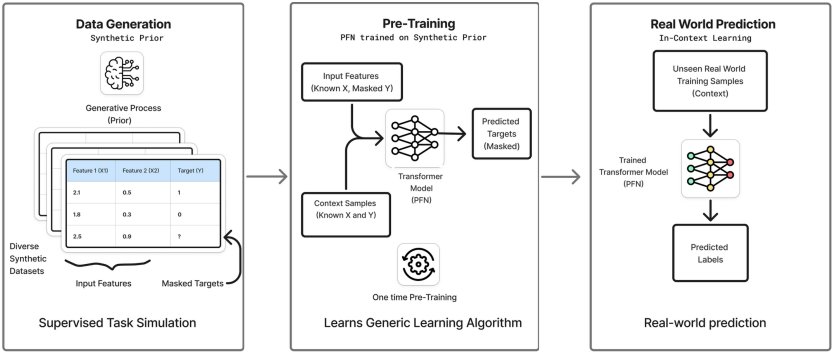

In-context learning: Similar idea as LLM-inference

Disadvantages: Robustness, Sustainability, Black-box

[TowardsDataScience.com]

Automated Machine Learning: Past, Present and Future

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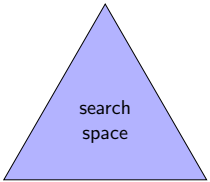
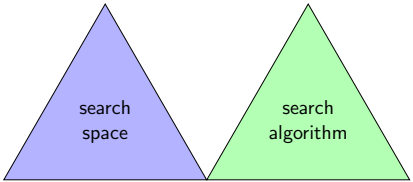
search space

- hyperparameters to explore
- ranges
- which are important?
- how to sample?



Automated Machine Learning: Past, Present and Future



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search algorithm

- random/grid search
- Bayesian optimisation
- hyperband

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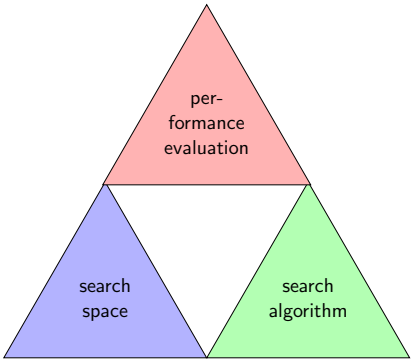

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evaluation mechanism

- train/validation/test set
- optimisation criteria
- multi-armed bandits
- learning curves

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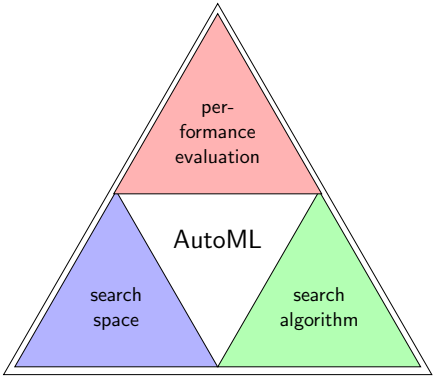

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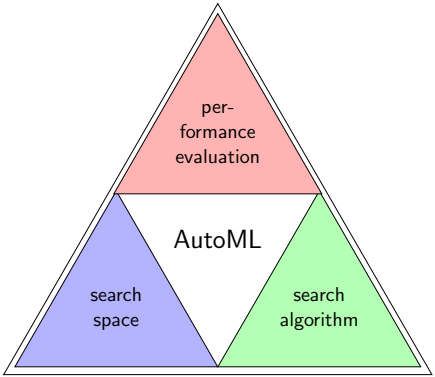
AutoML

- Auto-sklearn
- Auto-pytorch
- Auto-sklearn (2.0)

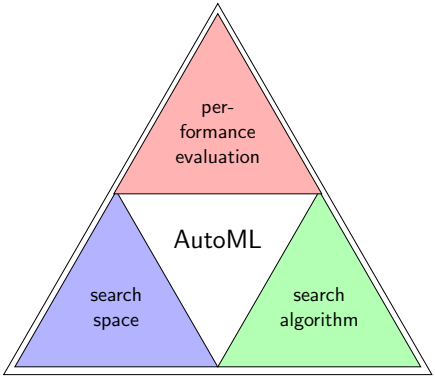
Components of AutoML



Hyperparameter optimisation problem:

$$\lambda^* \in \arg\min_{\lambda \in \Lambda} c(A_\lambda, D_{train}, D_{valid})$$

Components of AutoML



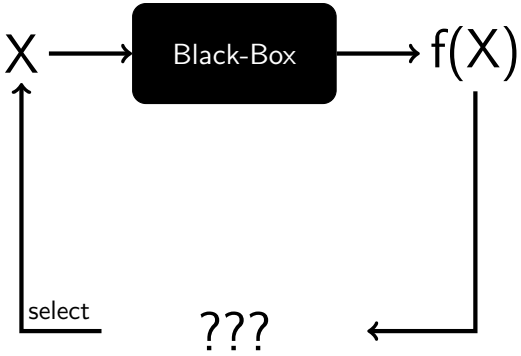
Hyperparameter optimisation problem:

$$\lambda^* \in \underset{\lambda \in \Lambda}{\arg\min}\ c(A_\lambda, D_{train}, D_{valid})$$

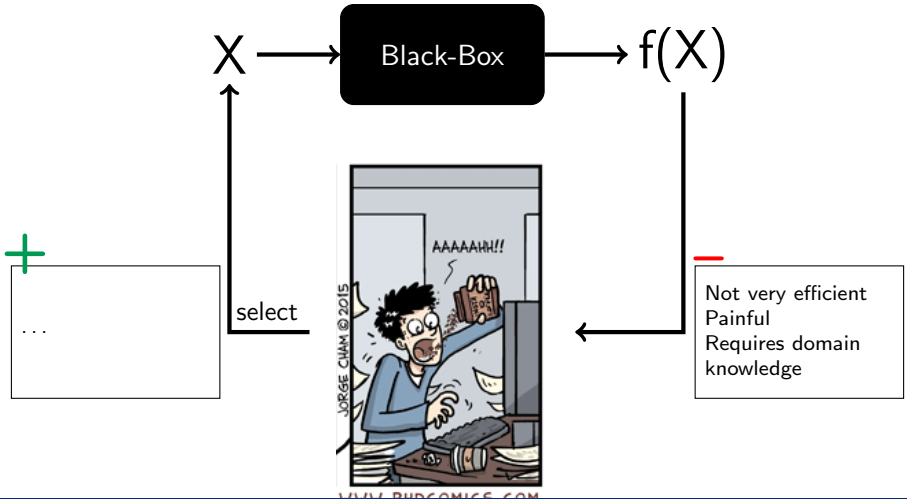
Search Algorithm

Black-Box Optimisation

The Loop



The Human in the Loop

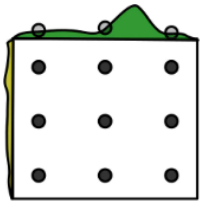


Grid Search

X → Black-Box → f(X)

\+ Very simple approach
Can be used to study the problem

select



− Does not scale to high dimensions
Grid needs to be defined

Random Search

\+

Even more simple
Easily parallelizable
Eventually converges to optimum

\−

Not data efficient
Computationally expensive

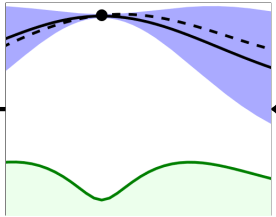
Bayesian Optimisation

X → Black-Box → f(X)

\+

Data efficient
State of the art

select



−

Not easy to paral-
lelise

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Search Space

sklearn.neural_network.MLPClassifier

class sklearn.neural_network.MLPClassifier(*hidden_layer_sizes=(100,)*, *activation='relu'*, ***, *solver='adam'*, *alpha=0.0001*, *batch_size='auto'*, *learning_rate='constant'*, *learning_rate_init=0.001*, *power_t=0.5*, *max_iter=200*, *shuffle=True*, *random_state=None*, *tol=0.0001*, *verbose=False*, *warm_start=False*, *momentum=0.9*, *nesterovs_momentum=True*, *early_stopping=False*, *validation_fraction=0.1*, *beta_1=0.9*, *beta_2=0.999*, *epsilon=1e-08*, *n_iter_no_change=10*, *max_fun=15000*) [source]

Multi-layer Perceptron classifier.

This model optimizes the log-loss function using LBFGS or stochastic gradient descent.

New in version 0.18.

Parameters:

hidden_layer_sizes : *tuple, length = n_layers - 2, default=(100,)*
The ith element represents the number of neurons in the ith hidden layer.

activation : *{'identity', 'logistic', 'tanh', 'relu'}, default='relu'*
Activation function for the hidden layer.

- 'identity', no-op activation, useful to implement linear bottleneck, returns f(x) = x
- 'logistic', the logistic sigmoid function, returns f(x) = 1 / (1 + exp(-x)).
- 'tanh', the hyperbolic tan function, returns f(x) = tanh(x).
- 'relu', the rectified linear unit function, returns f(x) = max(0, x)

solver : *{'lbfgs', 'sgd', 'adam'}, default='adam'*
The solver for weight optimization.

- 'lbfgs' is an optimizer in the family of quasi-Newton methods.
- 'sgd' refers to stochastic gradient descent.
- 'adam' refers to a stochastic gradient-based optimizer proposed by Kingma, Diederik, and Jimmy Ba

Note: The default solver 'adam' works pretty well on relatively large datasets (with thousands of training samples or more) in terms of both training time and validation score. For small datasets, however, 'lbfgs' can

Configuration Space

- Categorical
  - e.g., activation function
- Numerical
  - continuous, e.g., learning rate, learning rate init
  - integer, e.g., hidden layers size, batch size
- Conditional Hyperparameters
  - e.g., beta_1, beta_2 (for controlling Adam)
- Other important aspects:
  - Range
  - Sampling strategy (uniform, log-scale)
  - Some hyperparameters should not be optimised (random seed, ensemble size, . . .)

*Scikit-learn implementation does not cover interesting features that are covered by Tensorflow and pyTorch

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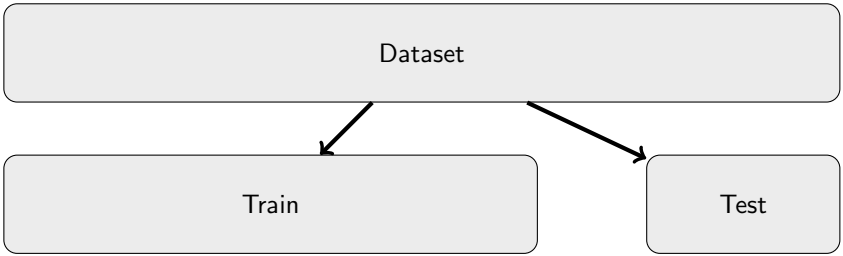
Evaluation Mechanism

Test set

- (automated) machine learning is all about generalisation
- Tested using a test set, that can only be inspected once!
- Repeatedly inspecting the test set:
  - violation of assumptions
  - leads to overly optimistic performance estimations

Validation set Vs. Test set



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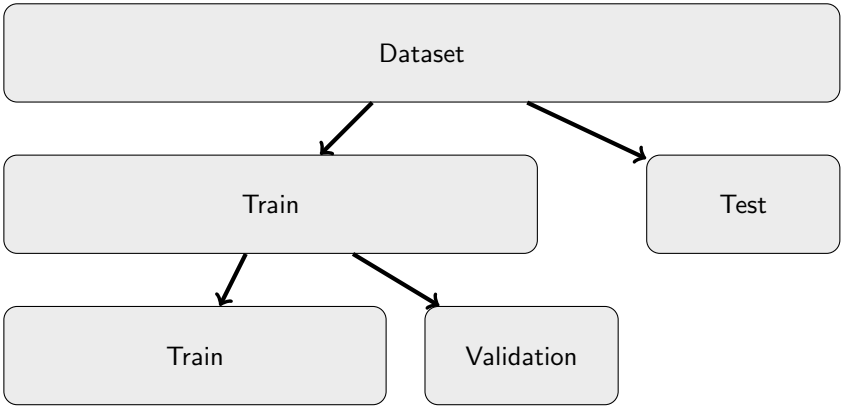
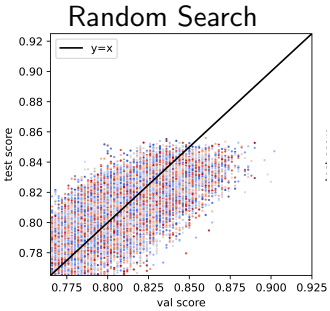


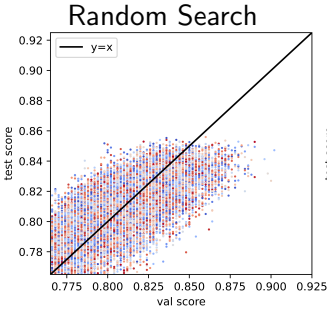
Overfitting



Colour indicates the iteration in the random search process

Figure by Schröder et al. (2024), MSc thesis.

Overfitting



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Effects of overfitting can be mitigated by

- using a large validation set (at the cost of train data)
- having multiple classes
- multiple validation folds (e.g., use multiple folds at inner level)
- shuffling validation and test splits

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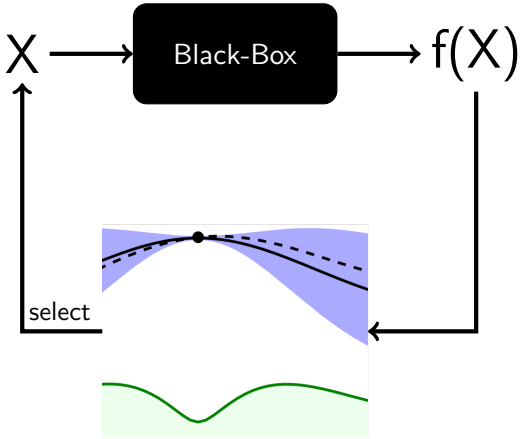
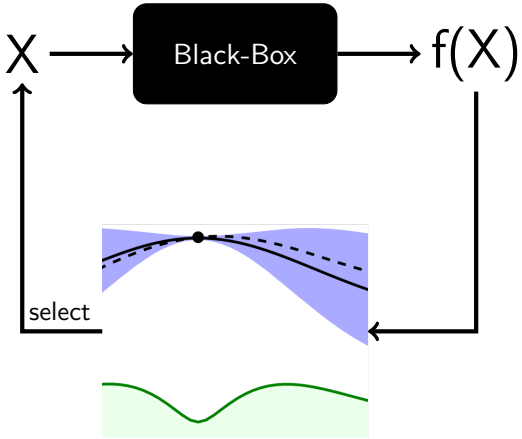
Explainable AutoML

Rashomon set and AutoML



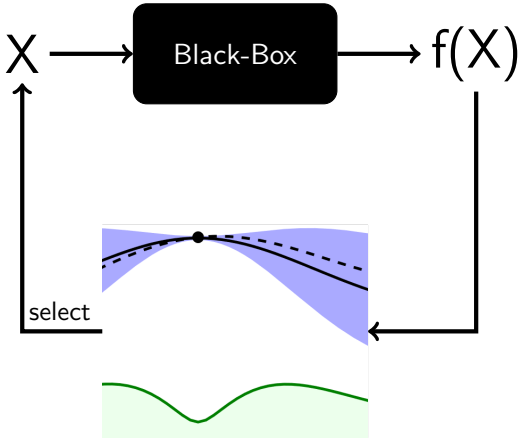
Rashomon set and AutoML



- Rashomon set is already used in practice (e.g., AutoGluon)

[Cavus et al., Quantifying Model Uncertainty with AutoML and Rashomon Partial Dependence Profiles: Enabling Trustworthy and Human-centered XAI, 2026]

Rashomon set and AutoML



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- Goal: more insight into the black box using the Rashomon set

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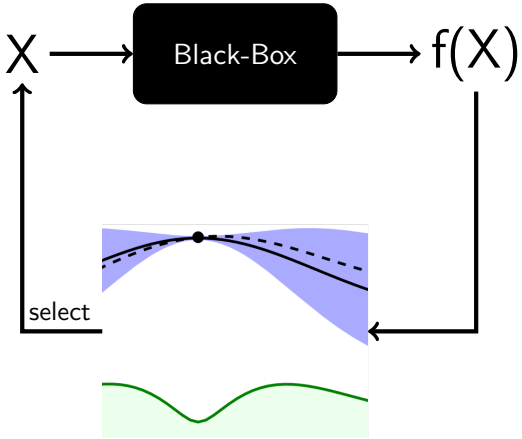

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- Partial Dependency Plots: AutoML for regression

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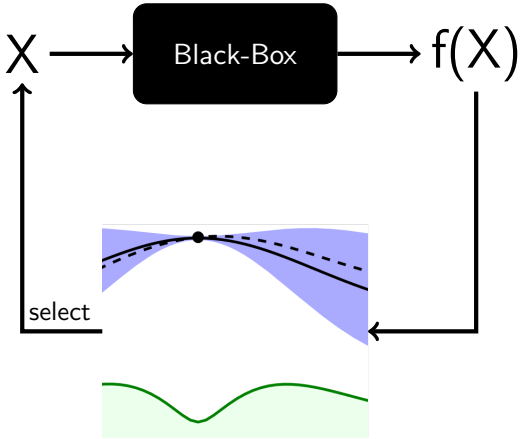
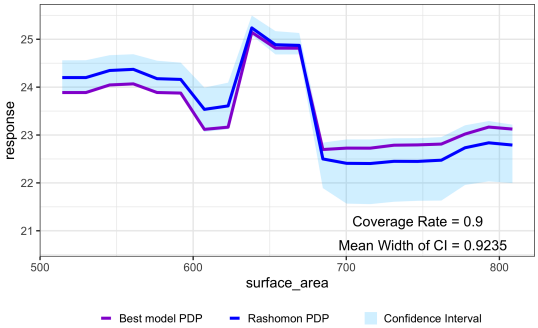
Rashomon set and AutoML



- Rashomon set is already used in practice (e.g., AutoGluon)
- Goal: more insight into the black box using the Rashomon set
- Partial Dependency Plots: AutoML for regression
- Discrepancy in explanation is not necessarily bad

[Cavus et al., Quantifying Model Uncertainty with AutoML and Rashomon Partial Dependence Profiles: Enabling Trustworthy and Human-centered XAI, 2026]

Partial Dependency Plot



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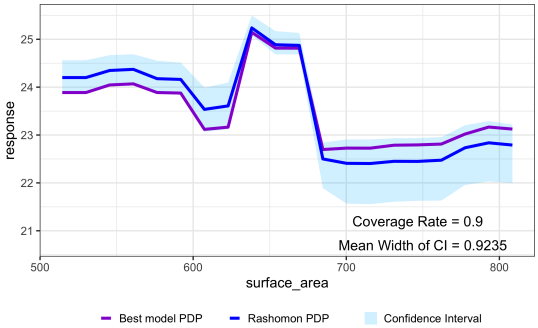
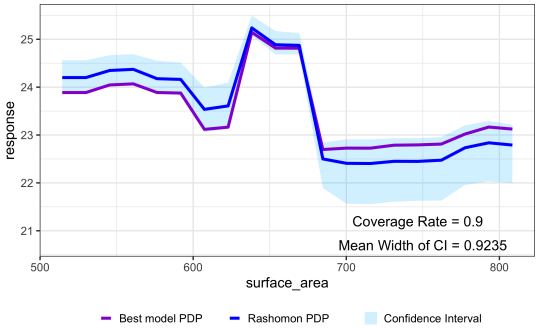


- Shows for each input variable the expected output

[Cavus et al., Quantifying Model Uncertainty with AutoML and Rashomon Partial Dependence Profiles: Enabling Trustworthy and Human-centered XAI, 2026]

Partial Dependency Plot



- Shows for each input variable the expected output
- Metric: Mean with of Confidence Interval

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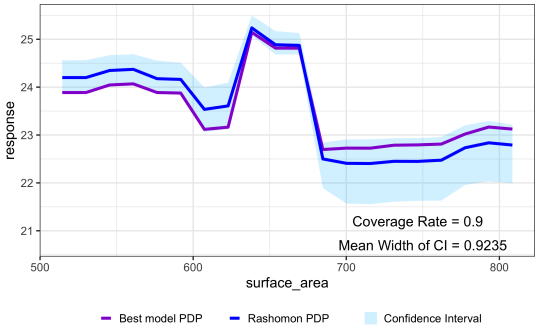

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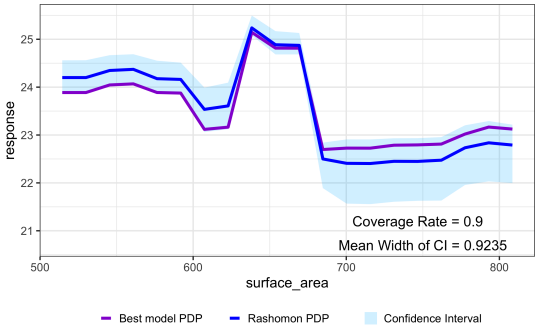

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- No ground-truth available for real-world datasets

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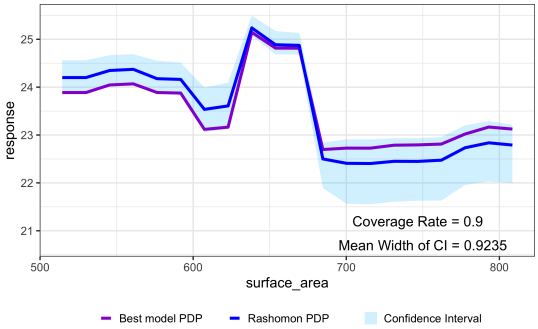

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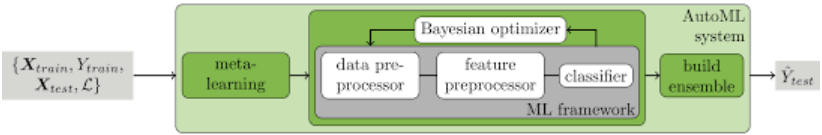
- https://github.com/mcavs/ - AutoML integration on the way

[Cavus et al., Quantifying Model Uncertainty with AutoML and Rashomon Partial Dependence Profiles: Enabling Trustworthy and Human-centered XAI, 2026]

AutoML

Auto-sklearn



- Defines a distance function between tasks
- Initialises Bayesian optimisation with configurations that worked well on similar tasks
- Additionally: builds ensembles of several well-working solutions
- See also: Auto-WEKA, Auto-sklearn 2.0

Figure and content based on original version. [Feurer et al. (2015), Efficient and Robust Automated Machine Learning.]

A Simple Example

The first step is to prepare your data. Here we use the MNIST dataset as an example

```
(x_train, y_train), (x_test, y_test) = mnist.load_data()
print(x_train.shape)  # (60000, 28, 28)
print(y_train.shape)  # (60000,)
print(y_train[:3])  # array([7, 2, 1], dtype=uint8)
```

The second step is to run the ImageClassifier. It is recommended have more trials for more complicated datasets. This is just a quick demo of MNIST, so we set max_trials to 1. For the same reason, we set epochs to 10. You can also leave the epochs unspecified for an adaptive number of epochs.

```
# Initialize the image classifier.
clf = ak.ImageClassifier(overwrite=True, max_trials=1)
# Feed the image classifier with training data.
clf.fit(x_train, y_train, epochs=10)


# Predict with the best model.
predicted_y = clf.predict(x_test)
print(predicted_y)


# Evaluate the best model with testing data.
print(clf.evaluate(x_test, y_test))
```

AutoML libraries

[Figure by: Satyam Kumar (2020), Medium.com blogpost.]

AutoML libraries

[Figure by: Satyam Kumar (2020), Medium.com blogpost.]

Some distinguishing features:

- Bayesian optimisation
- Genetic algorithms
- Multi-armed bandits
- Ensembles
- Meta-learning
- Stacking
- Multi-layer stacking
- ...

AutoML libraries

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Which AutoML tool to select?

Conclusions

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- Explainable AI methods available for traditional AutoML

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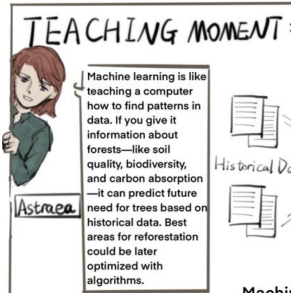
AutoML Comic



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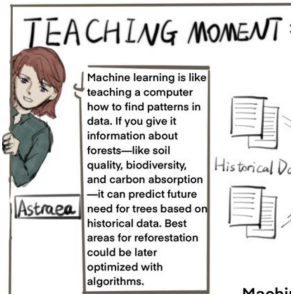
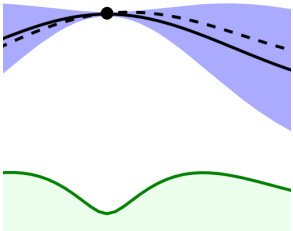


AutoML intro



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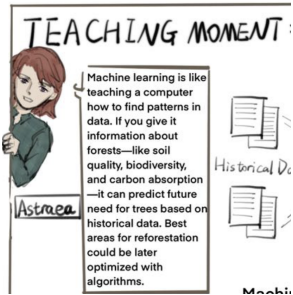
AutoML Comic



AutoML intro