# Speeding-up Hyperparameter Optimization with transfer and meta learning

## Metaheuristics Summer School.

David Salinas. July 2024.

# Goals

- Understand benefit of transfer learning to speed-up HPO
- Understand the key challenges to apply transfer learning to HPO
- Get an idea of the main techniques being used in state-of-the-art methods
- Know how to apply transfer learning to your problem

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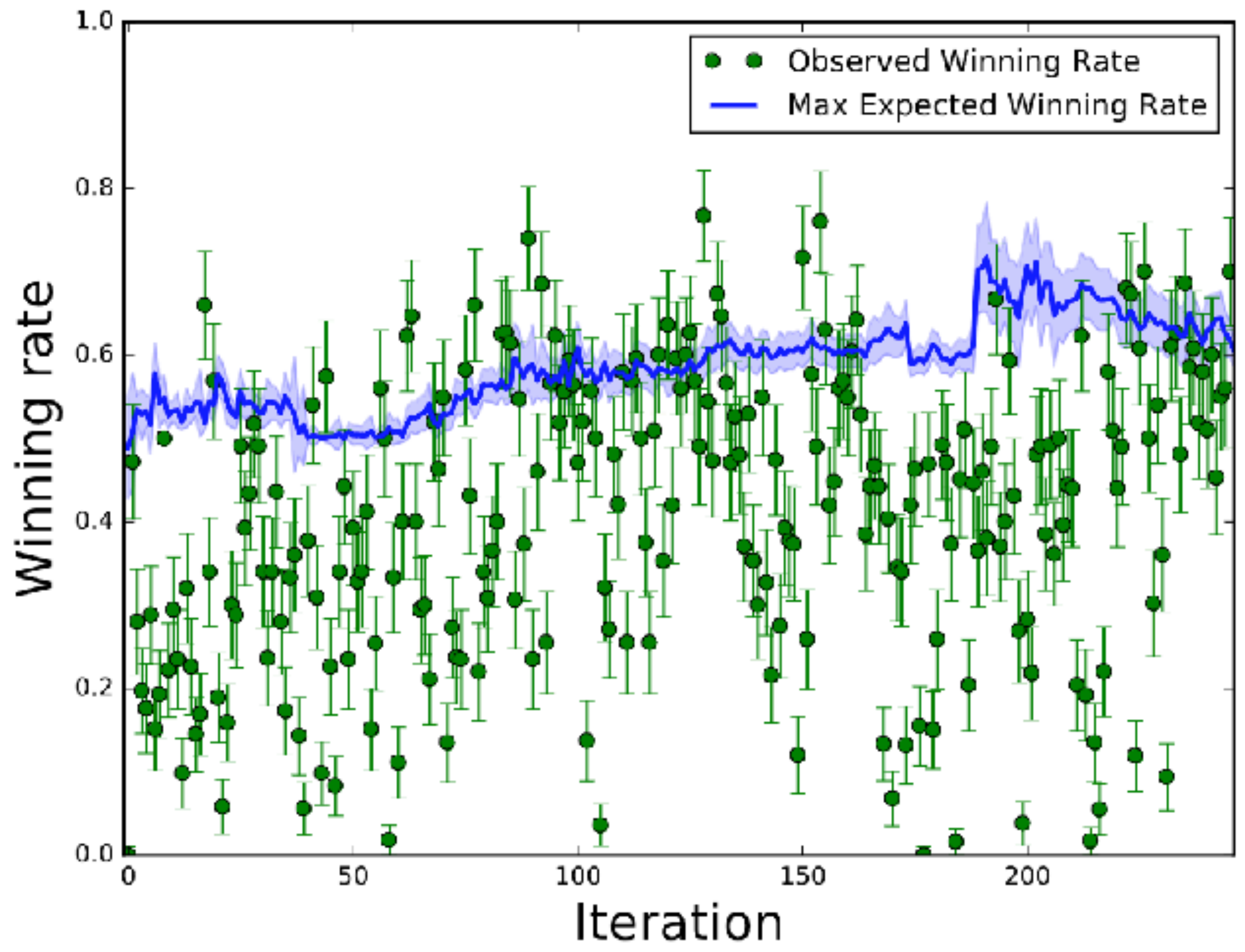


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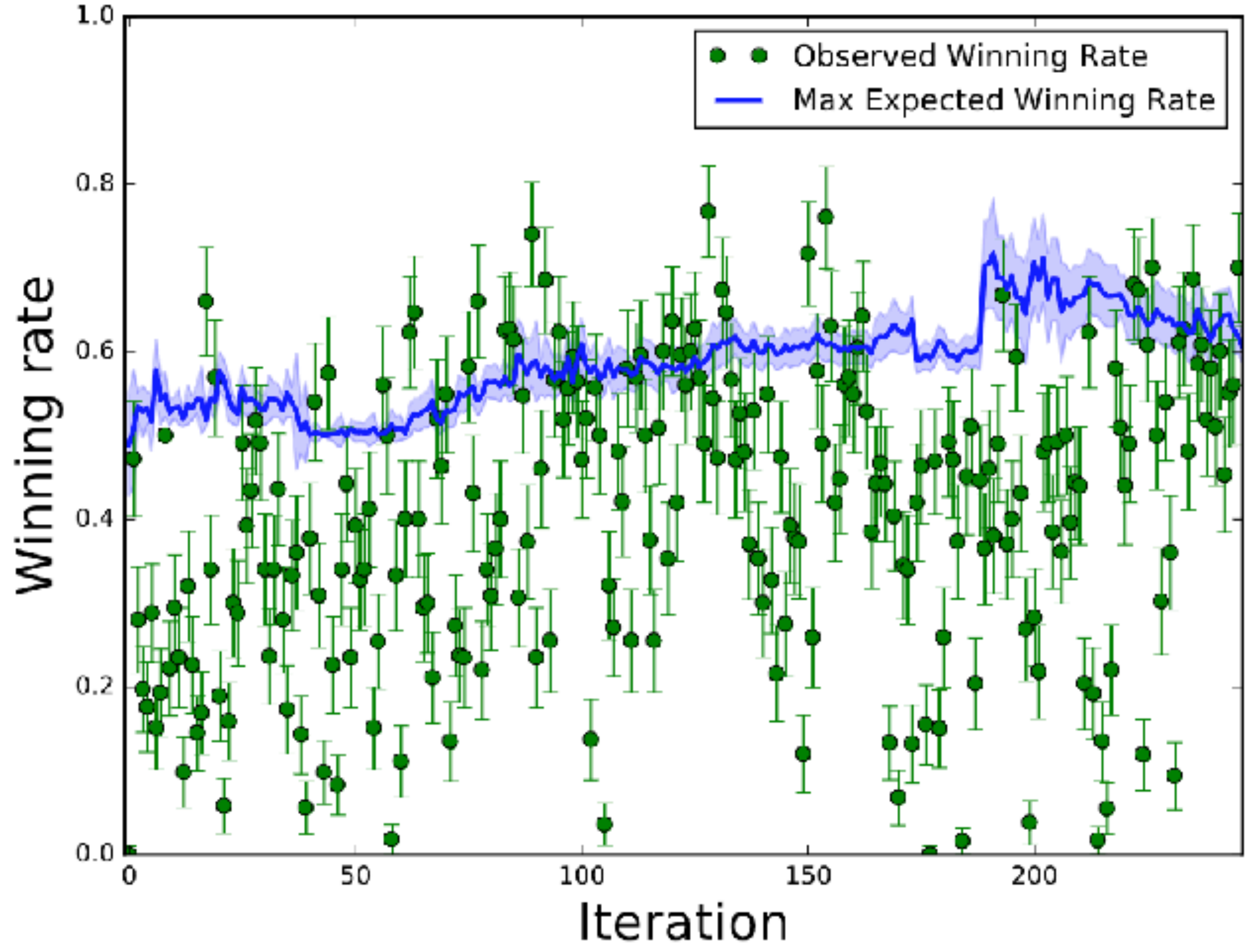


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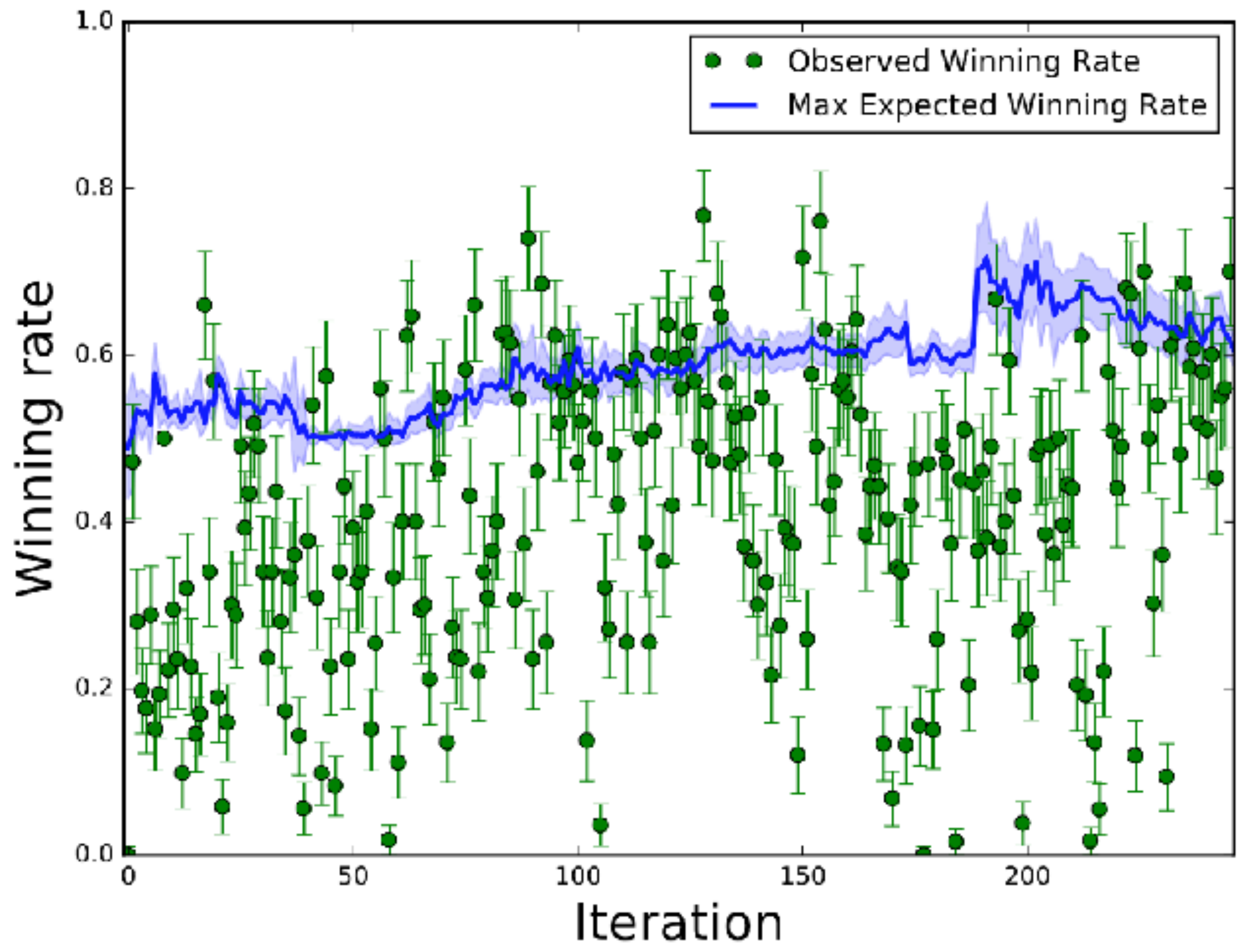


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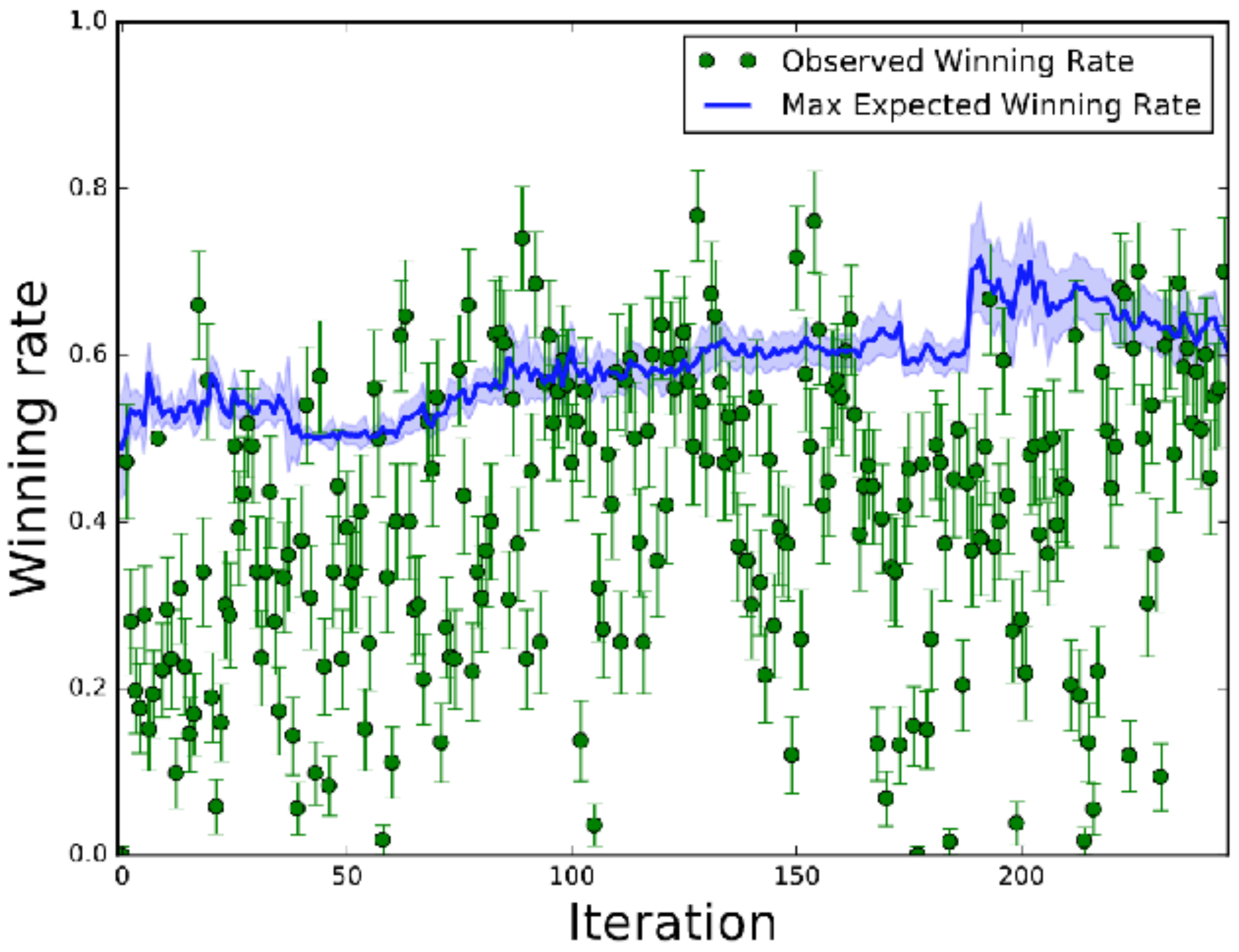


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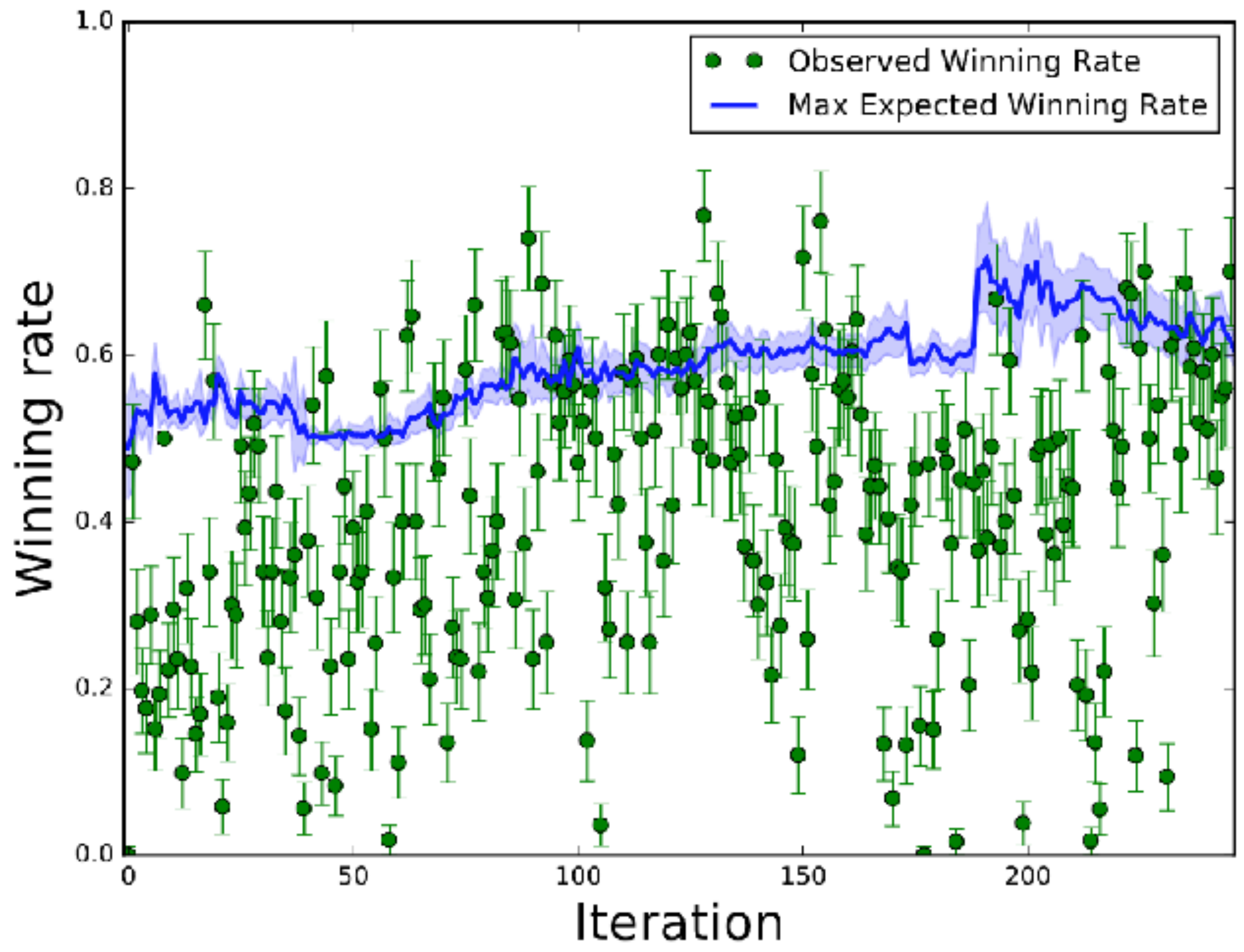


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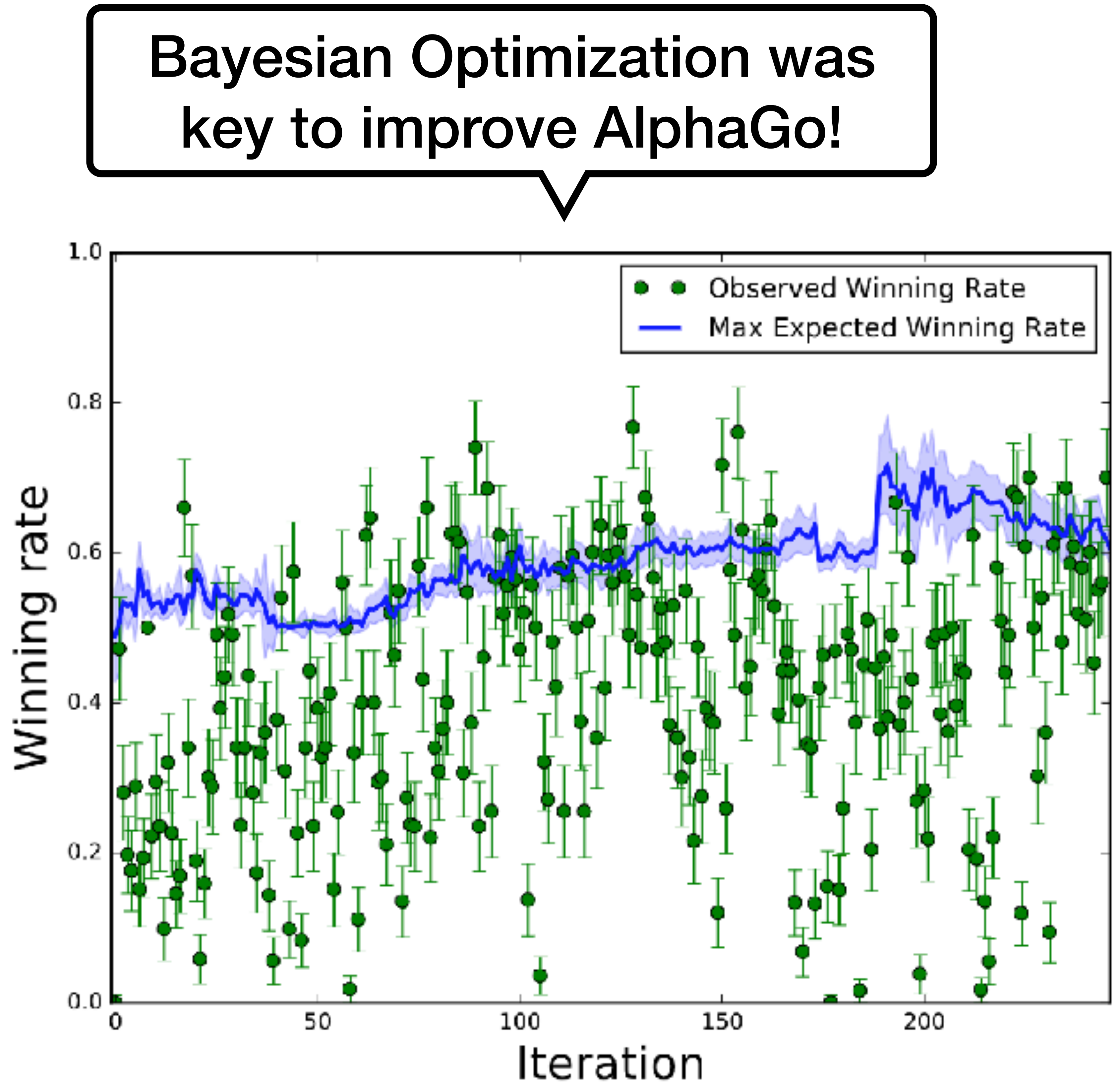


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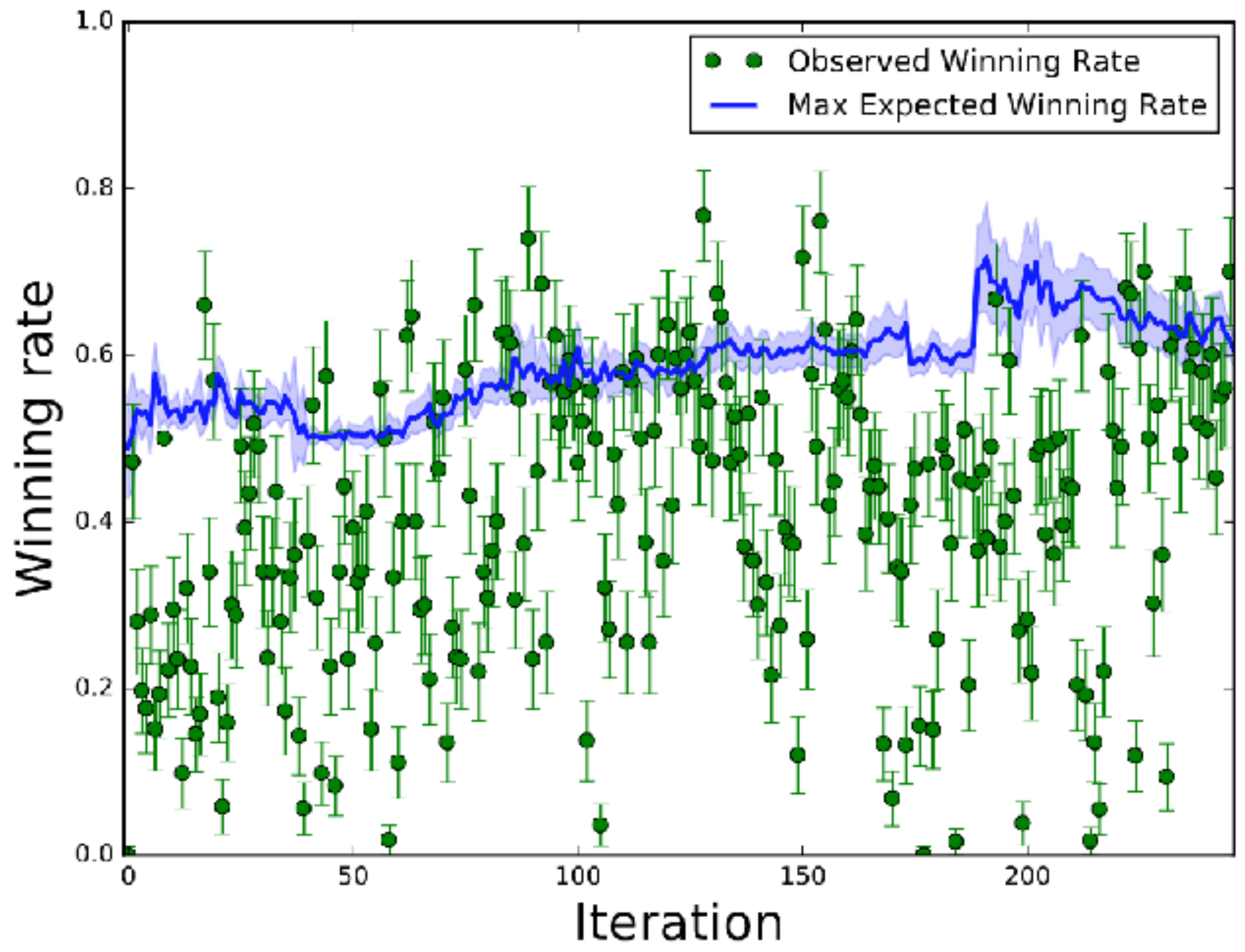


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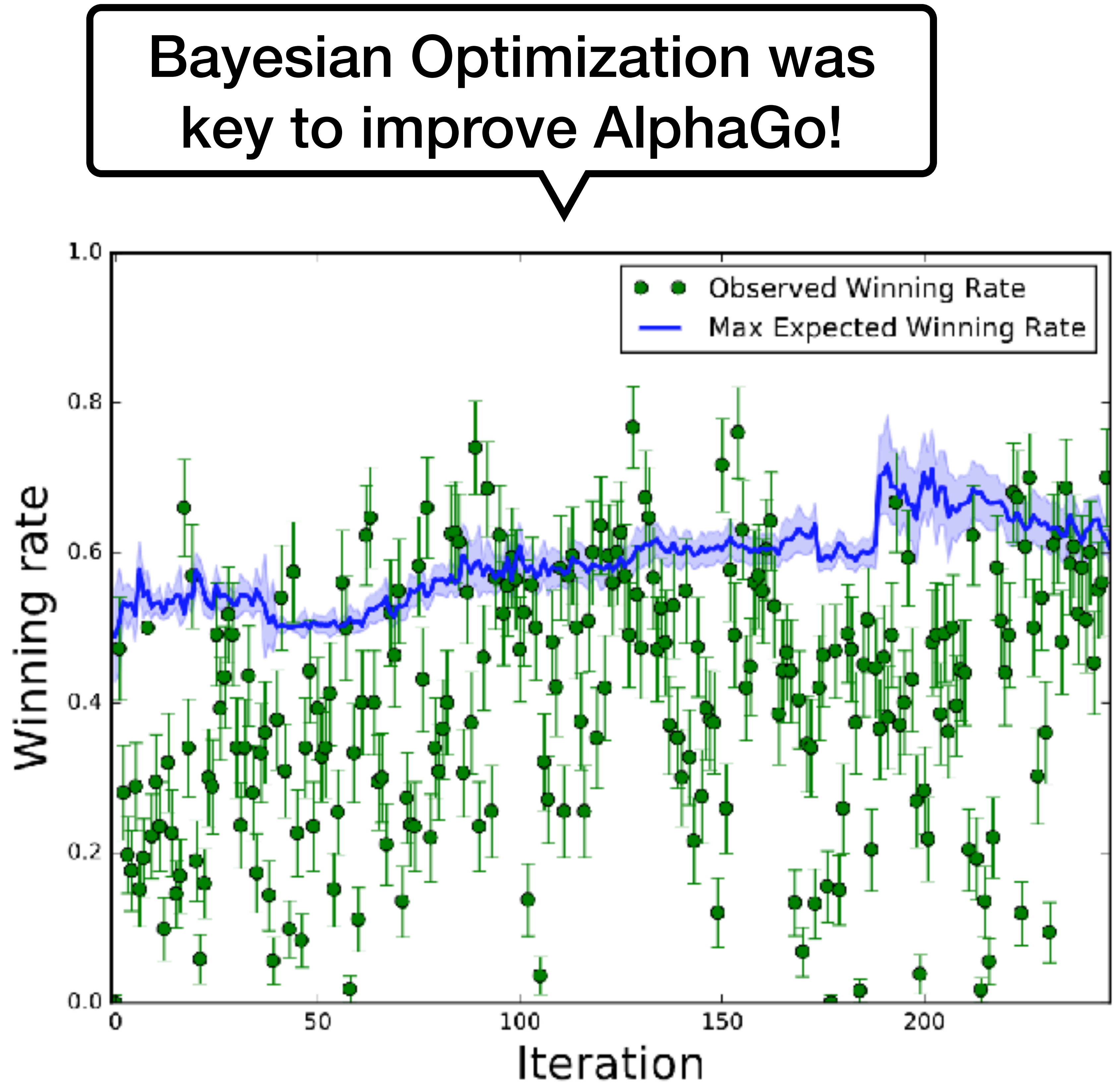
- **Transfer learning** is a subfield that **speeds up** HPO by looking at previous evaluations and tuning runs

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An example of a search space $\mathcal{X}$

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| Dropout | $[0.0, 1.0]$ | Uniform |
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- What if we had extra evaluations?

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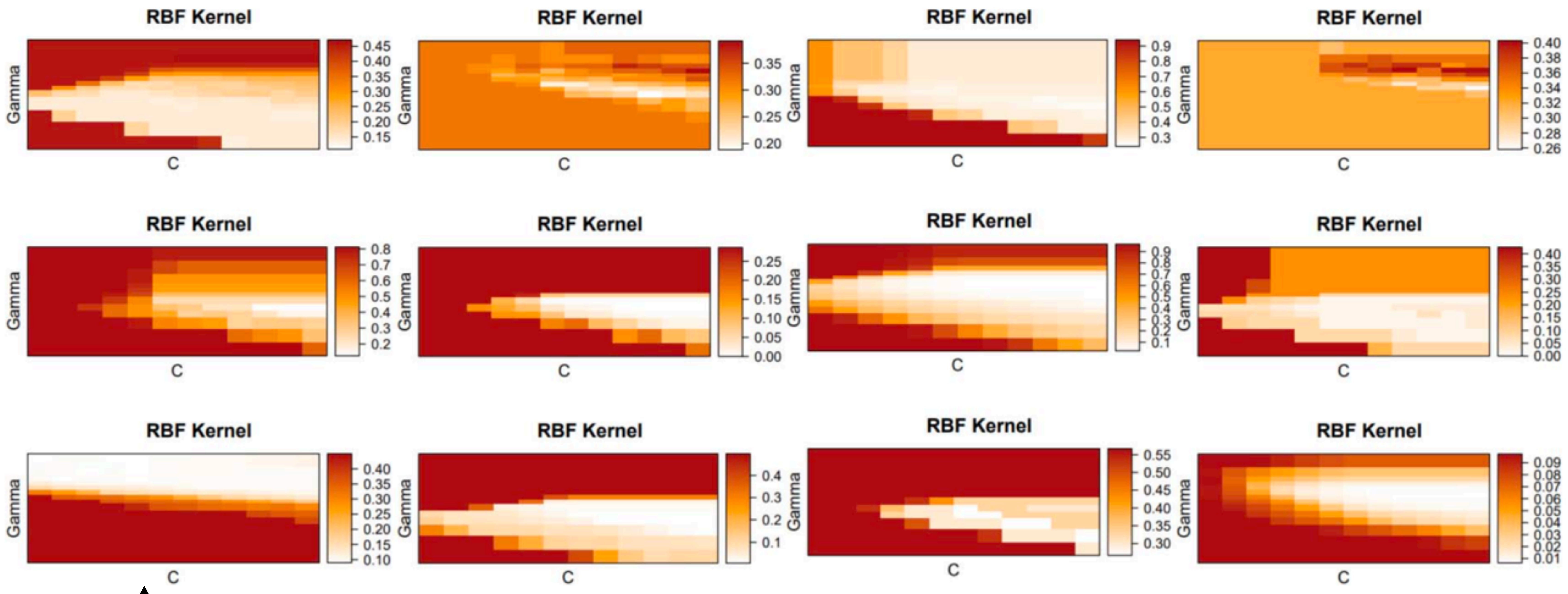
## Why we expect it to work




Response function of different datasets can look very similar.

Can we exploit the similarity between datasets?

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🤔 How to exploit past-observations to speed-up the search of a new task?

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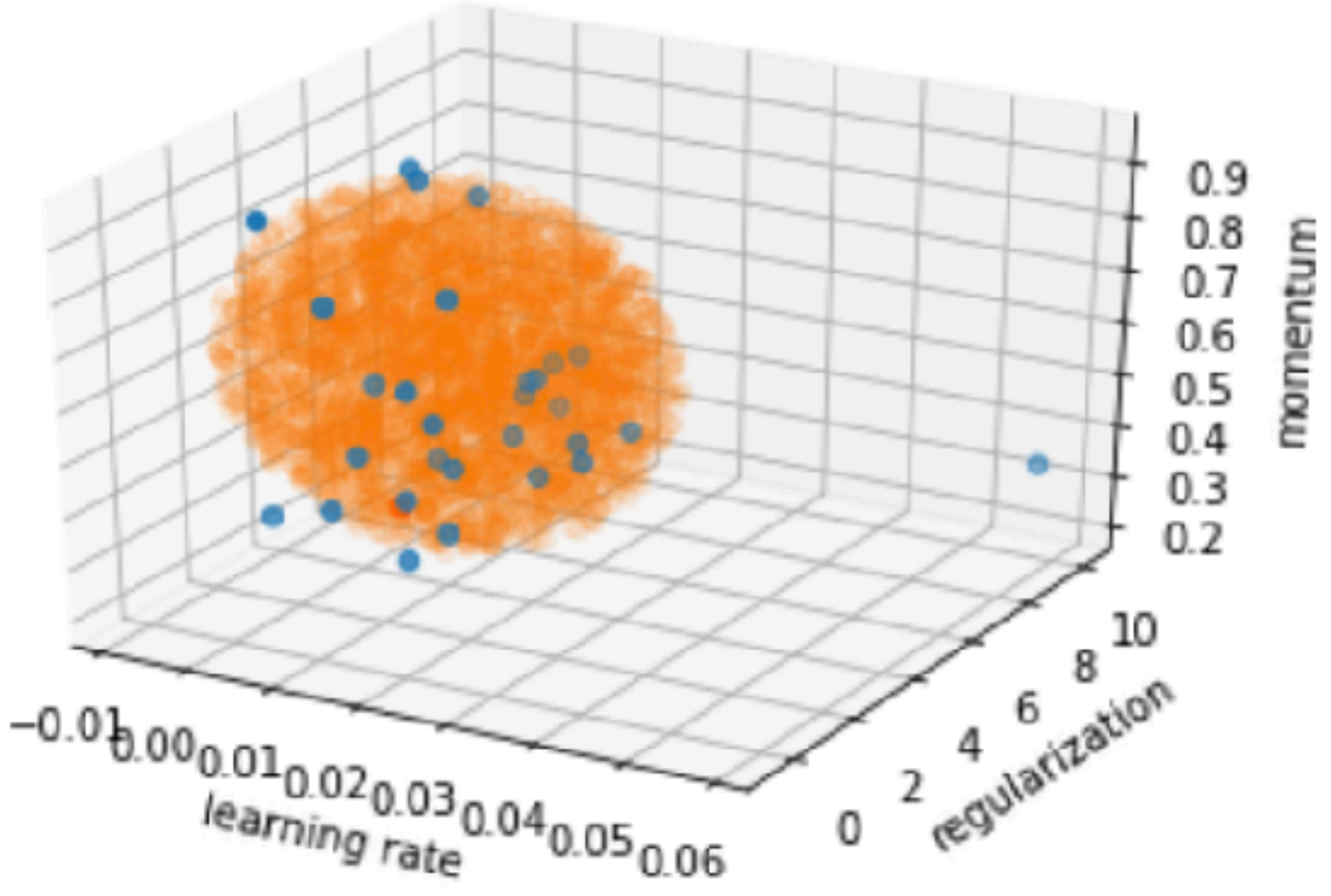


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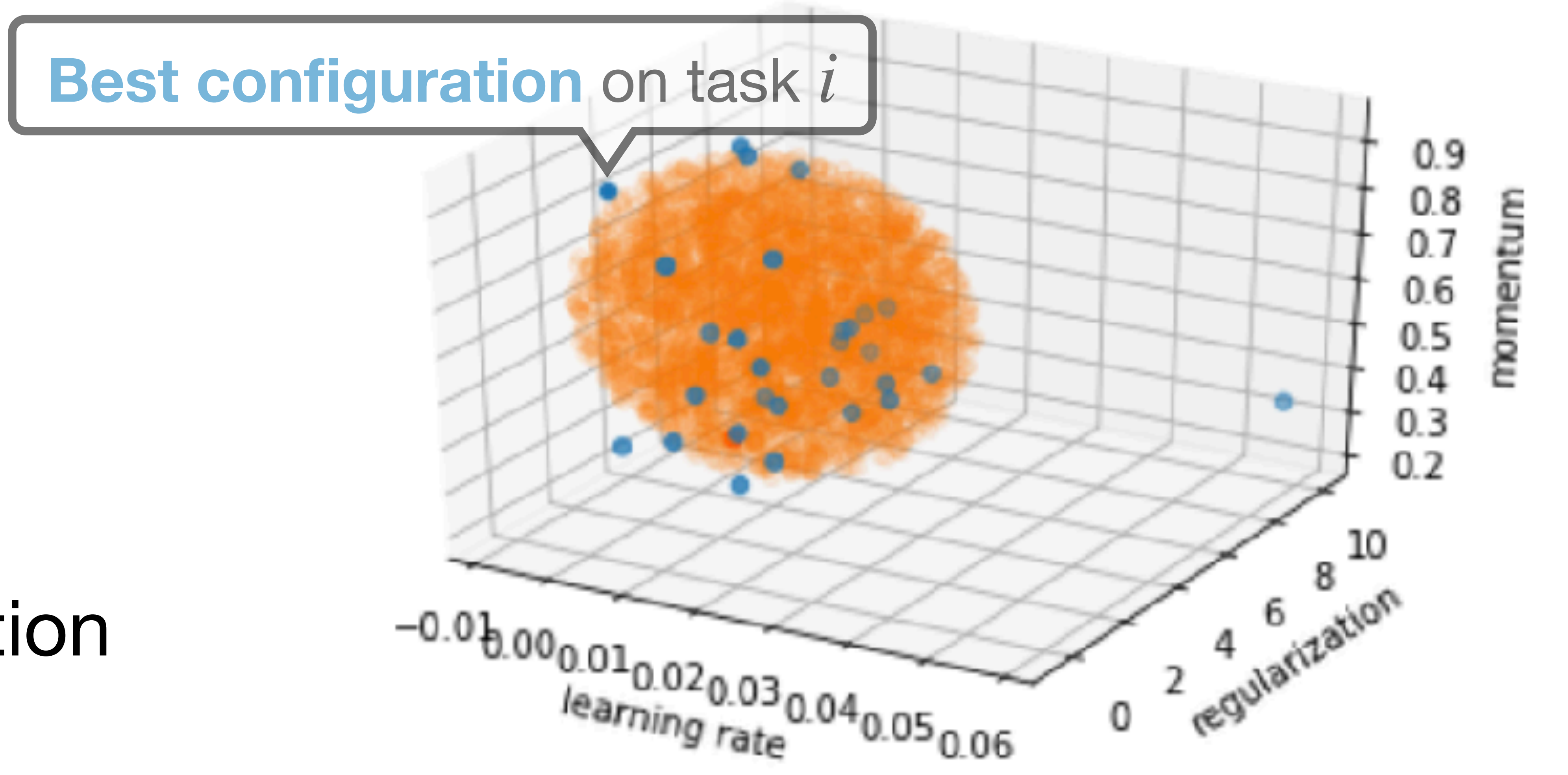


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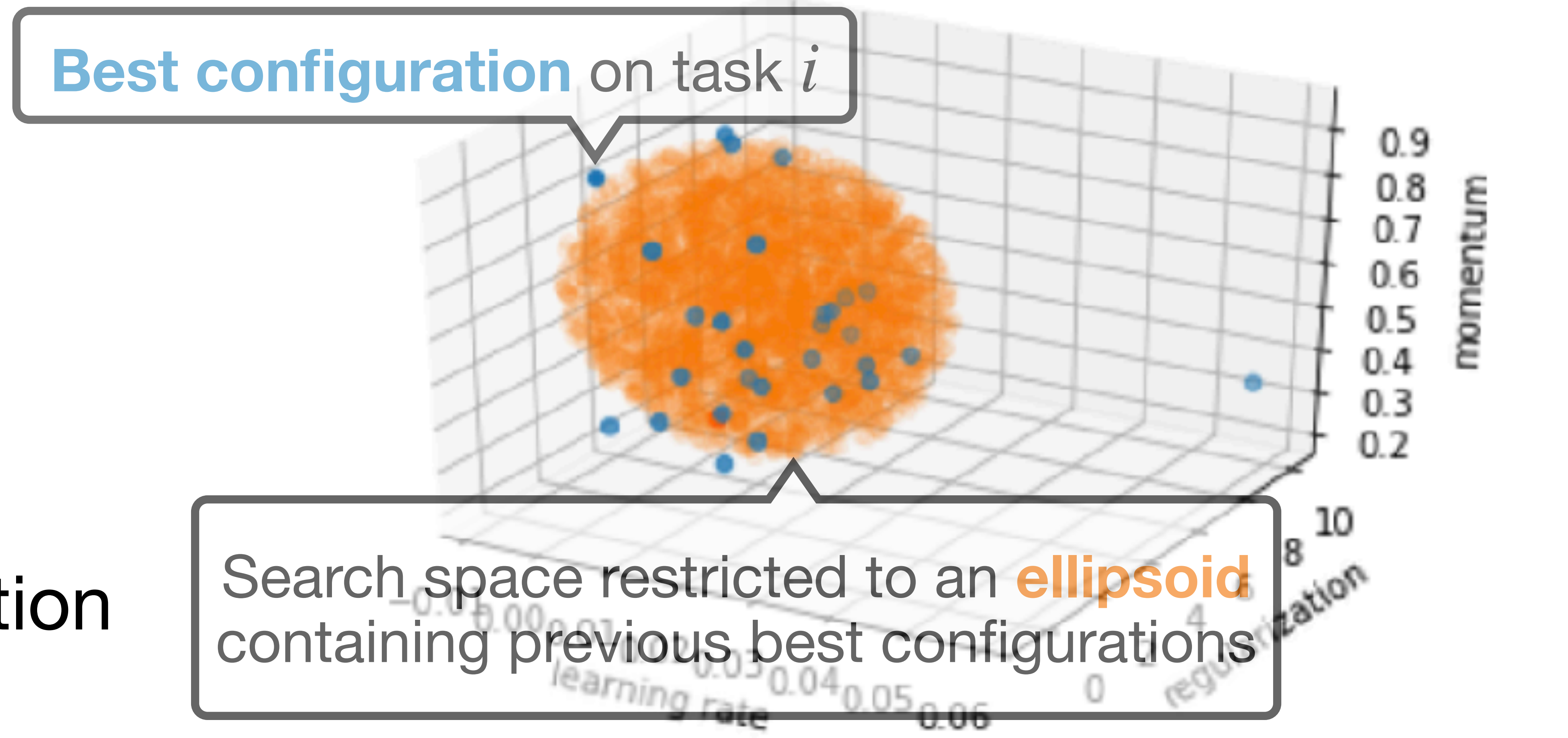


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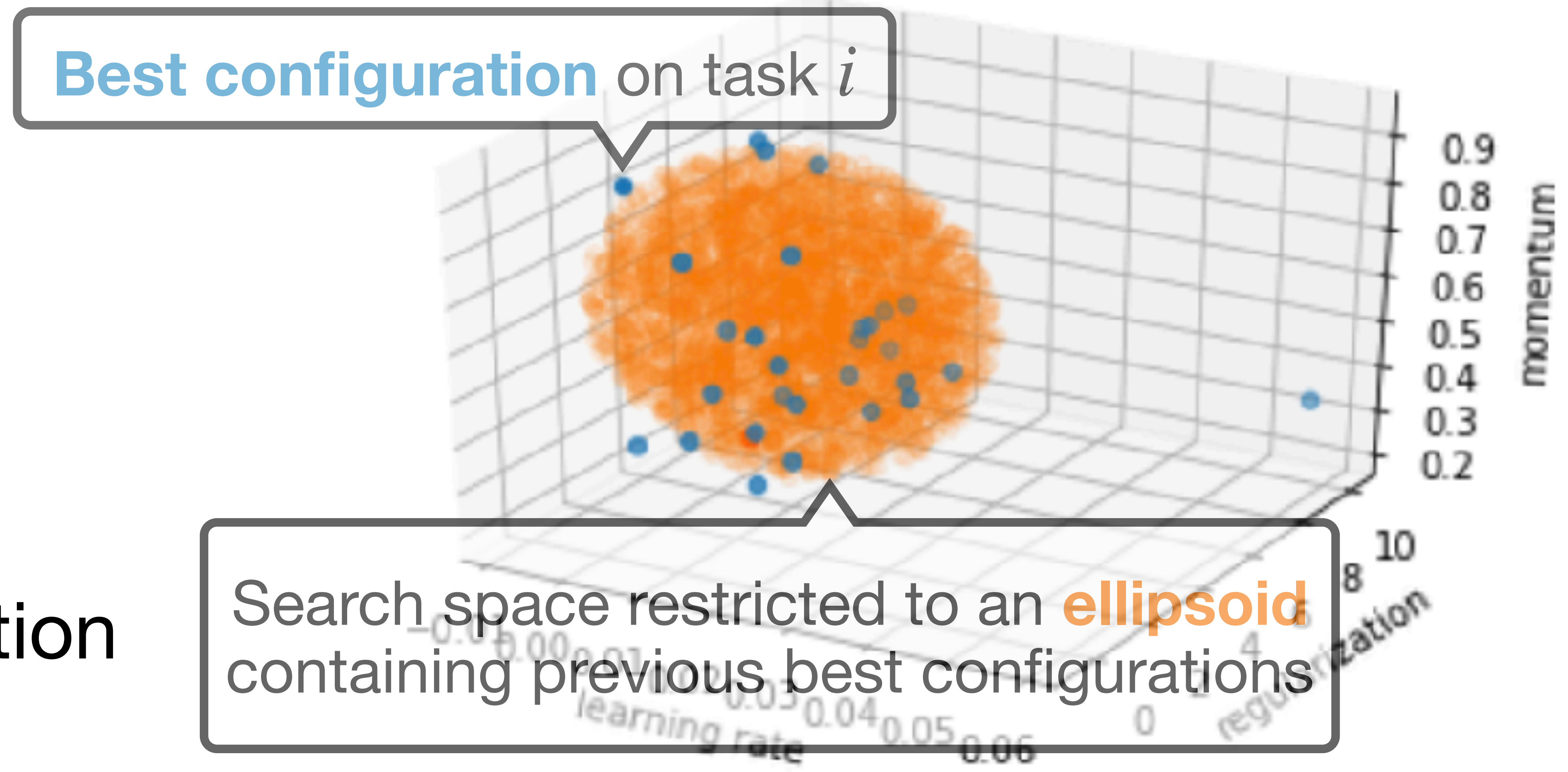


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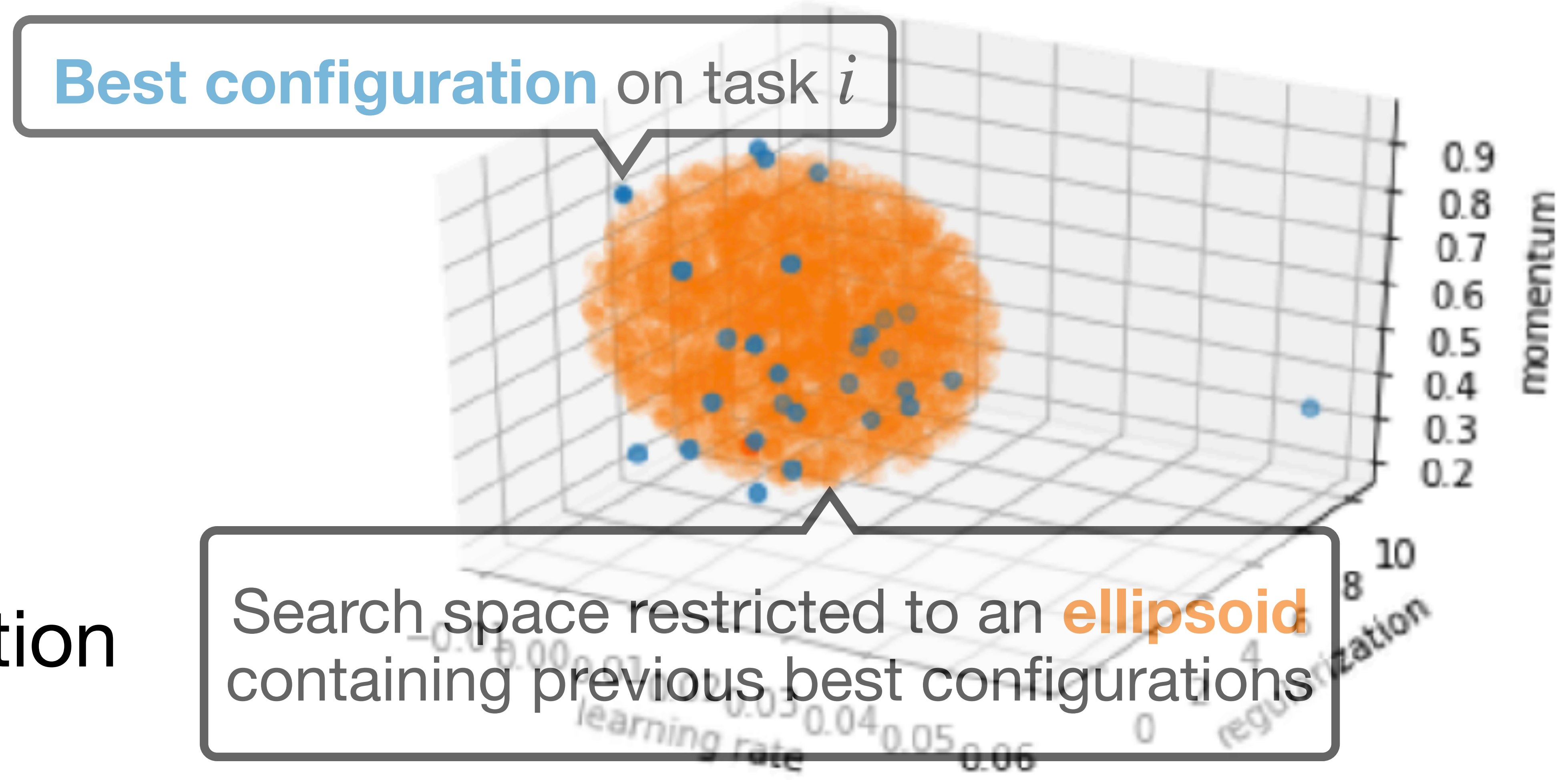


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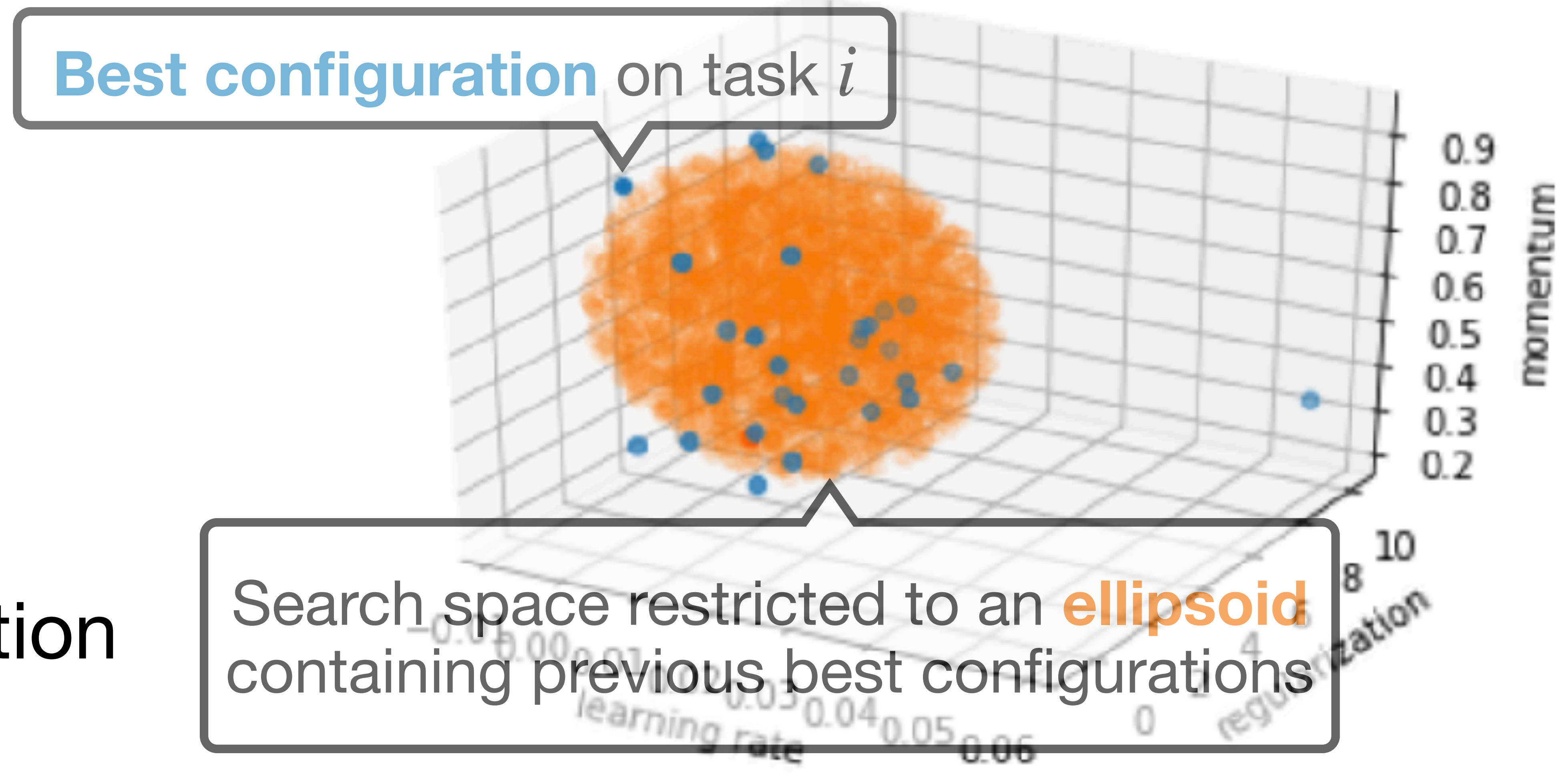


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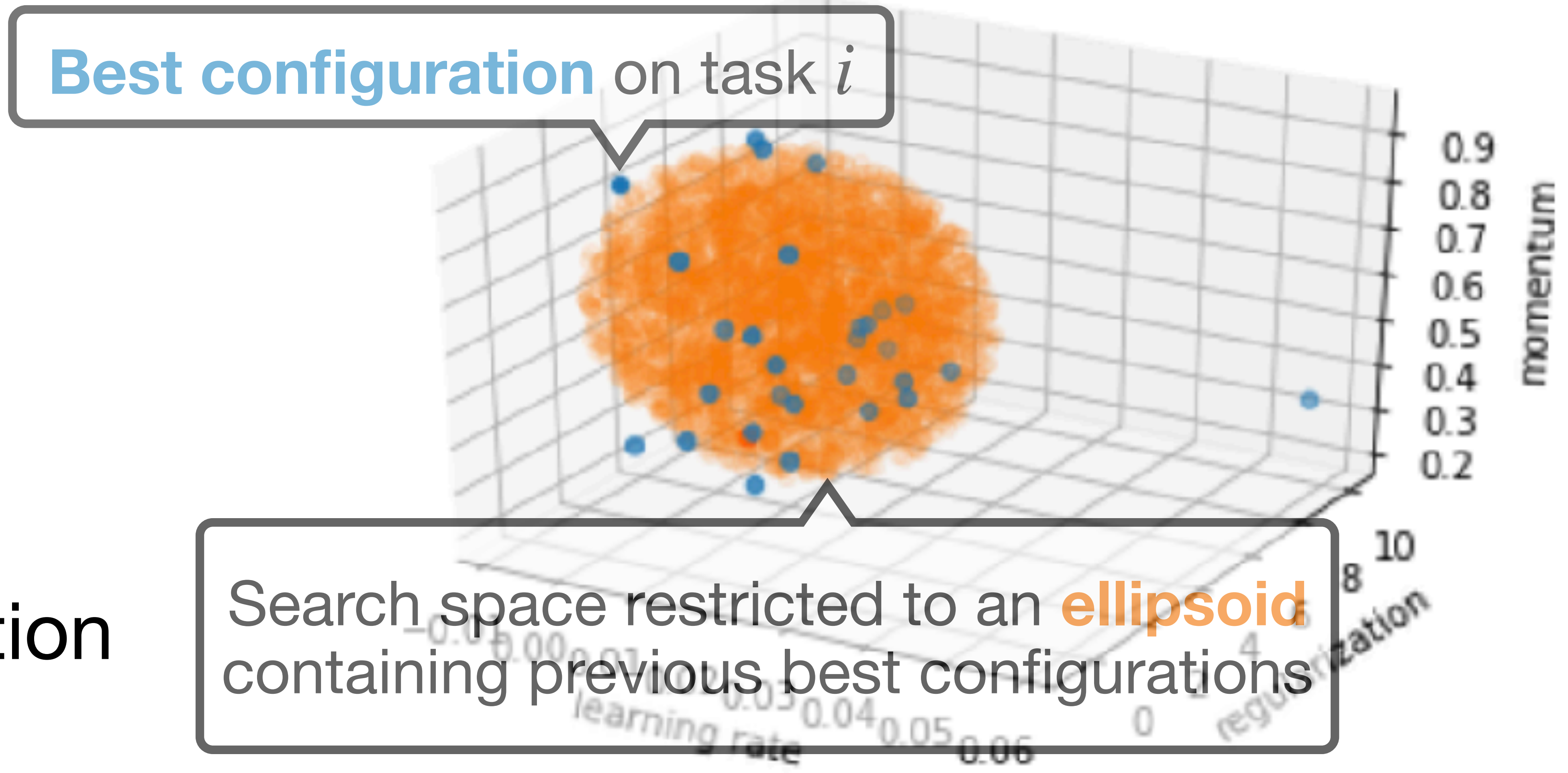


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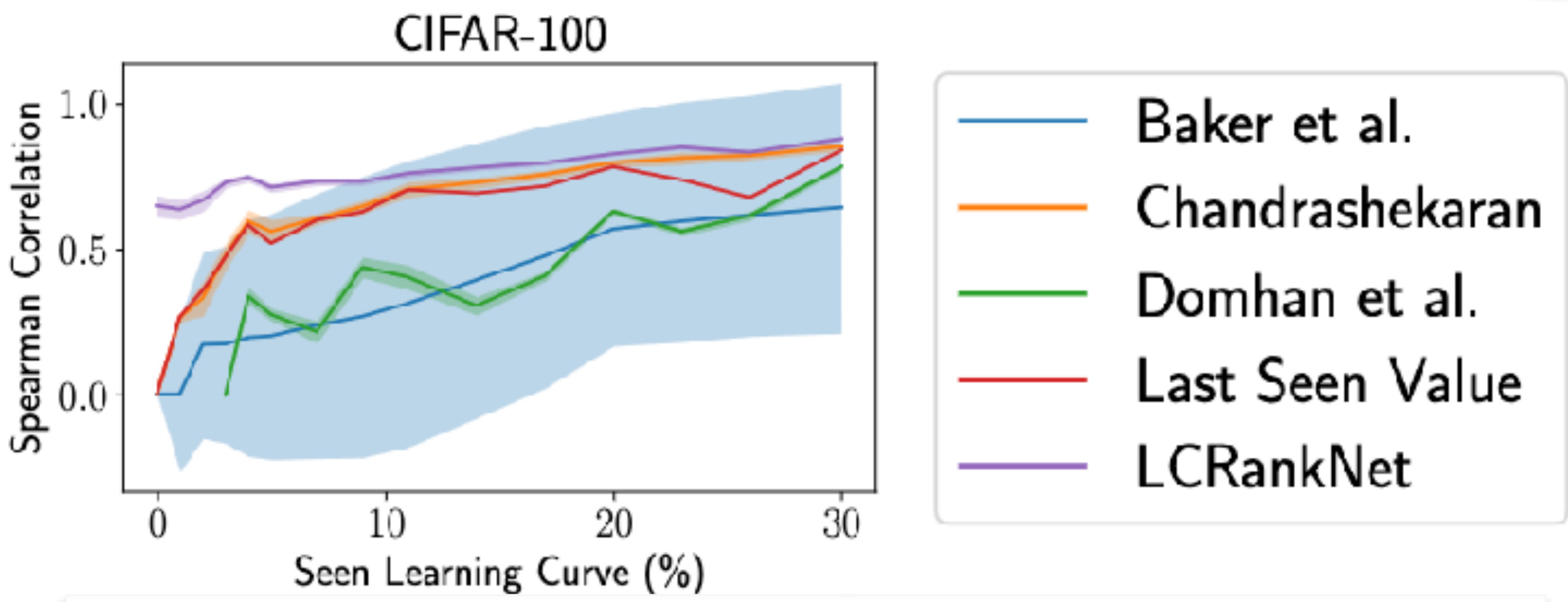


Learning curve model learned on offline evaluations allows to predict final values with high correlations [Wistuba 2020]

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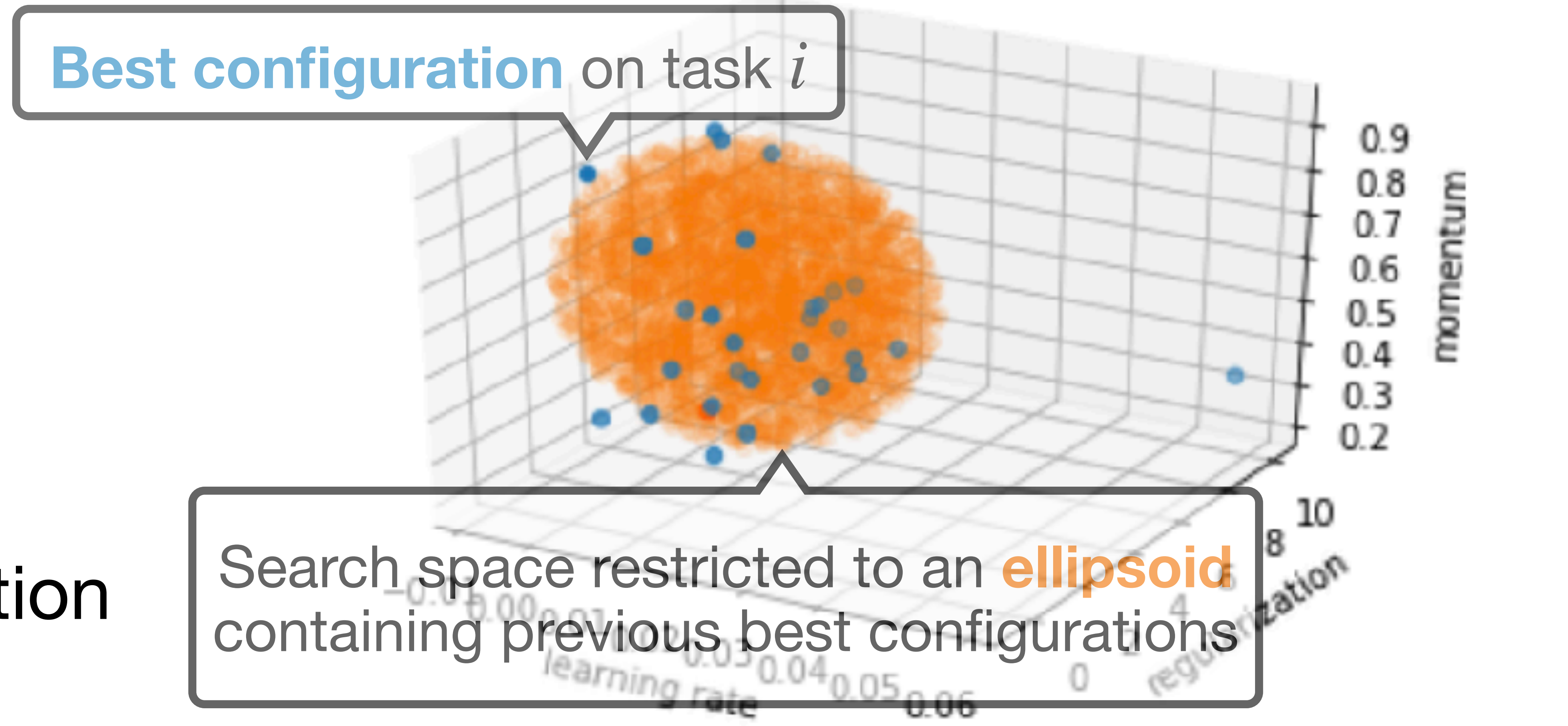


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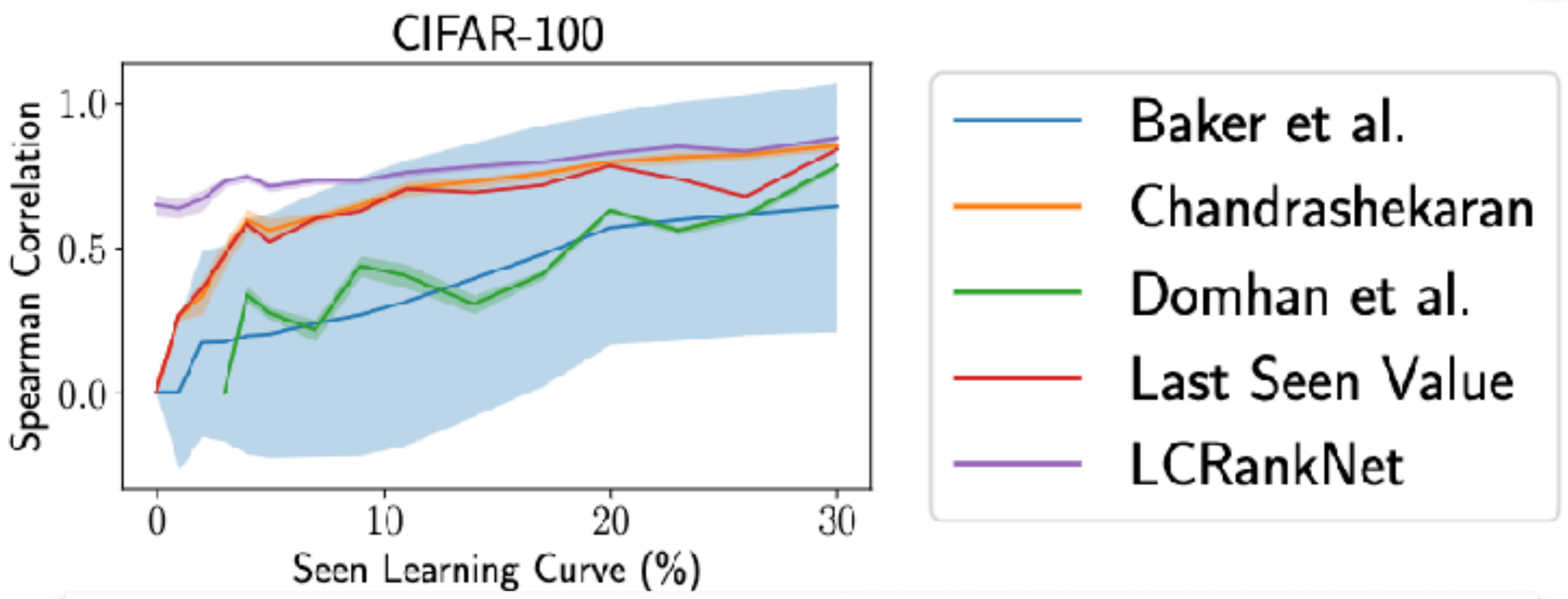


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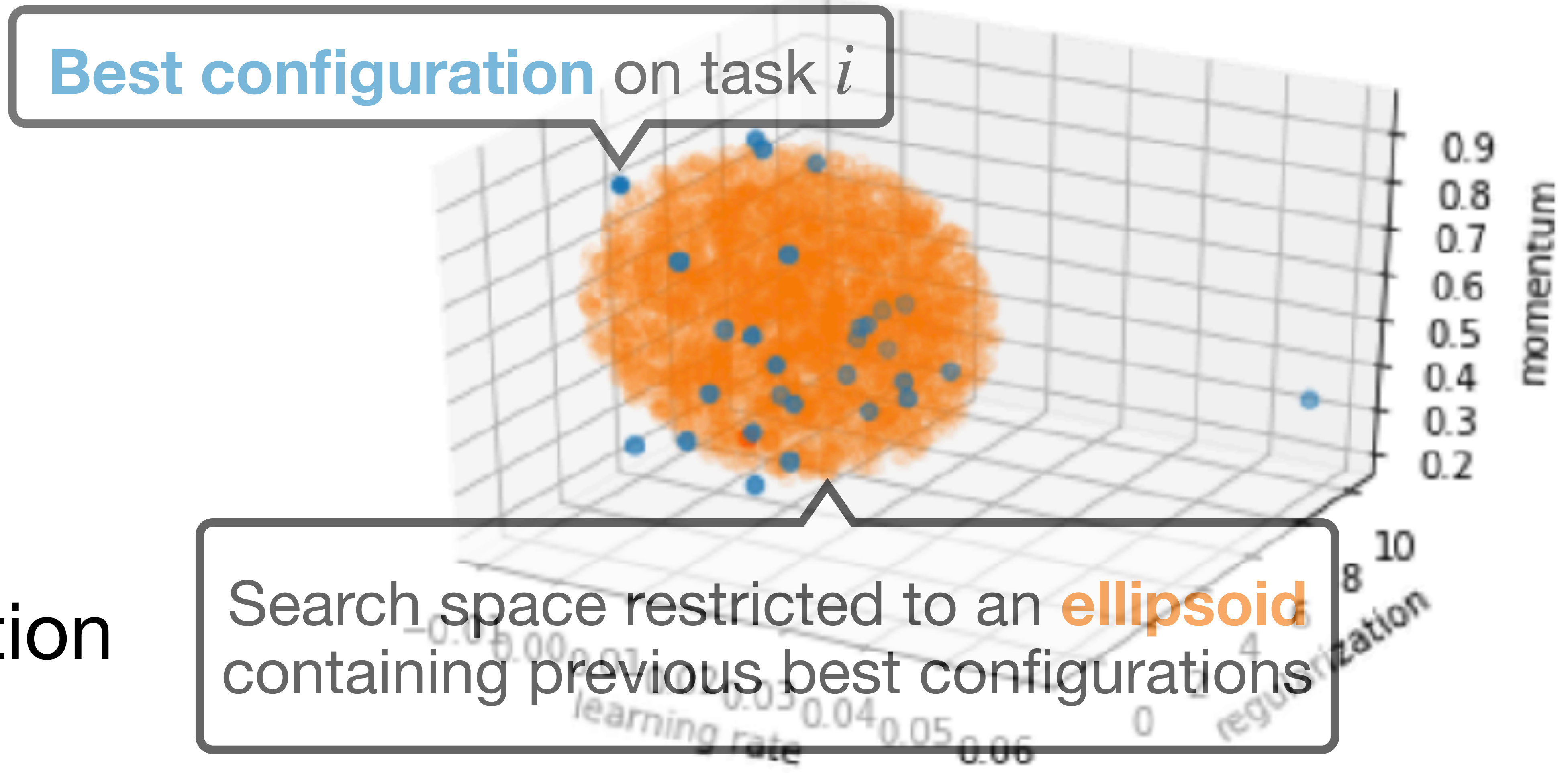


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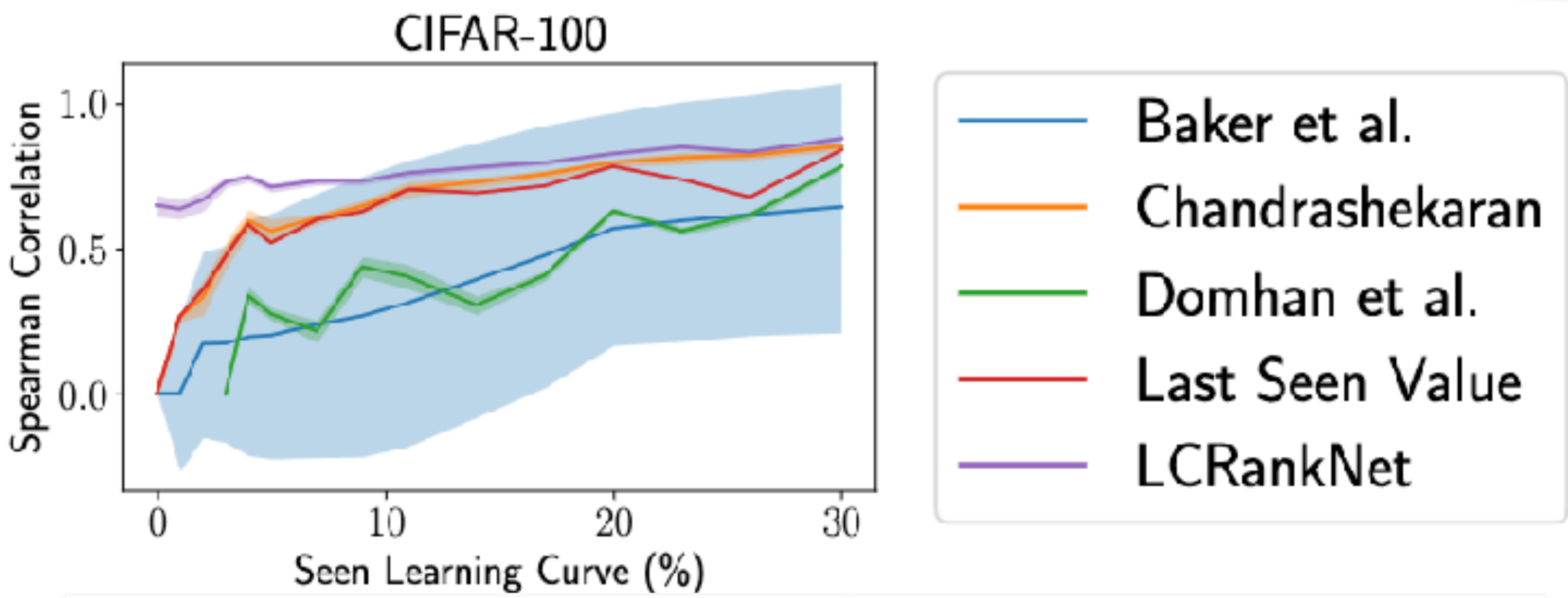


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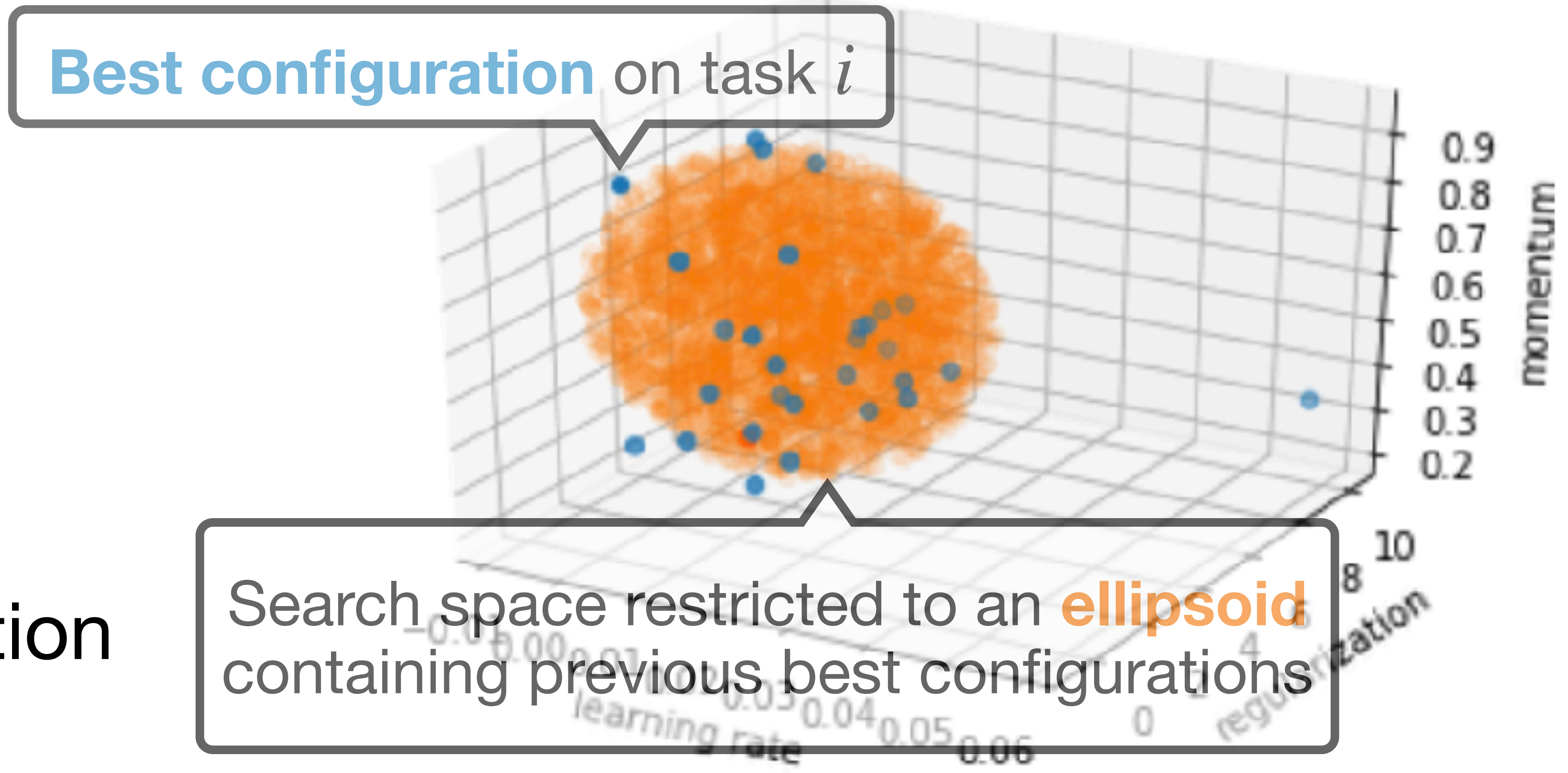


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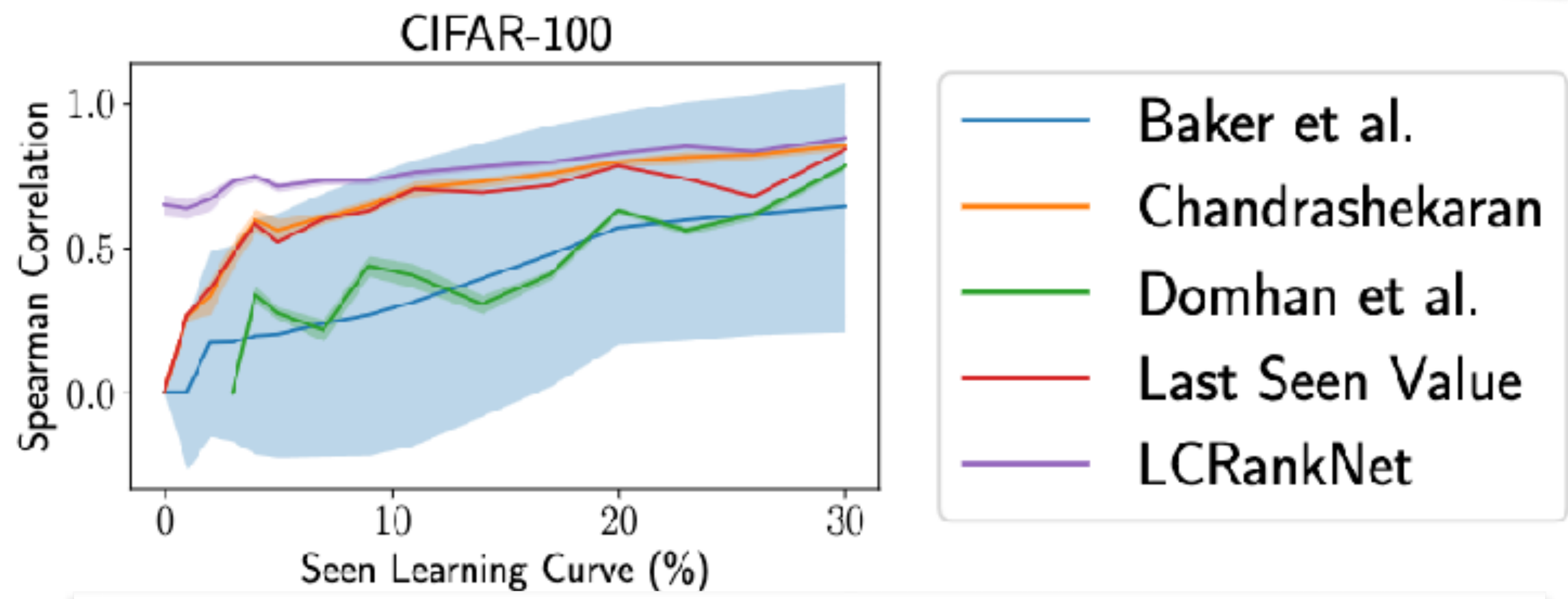


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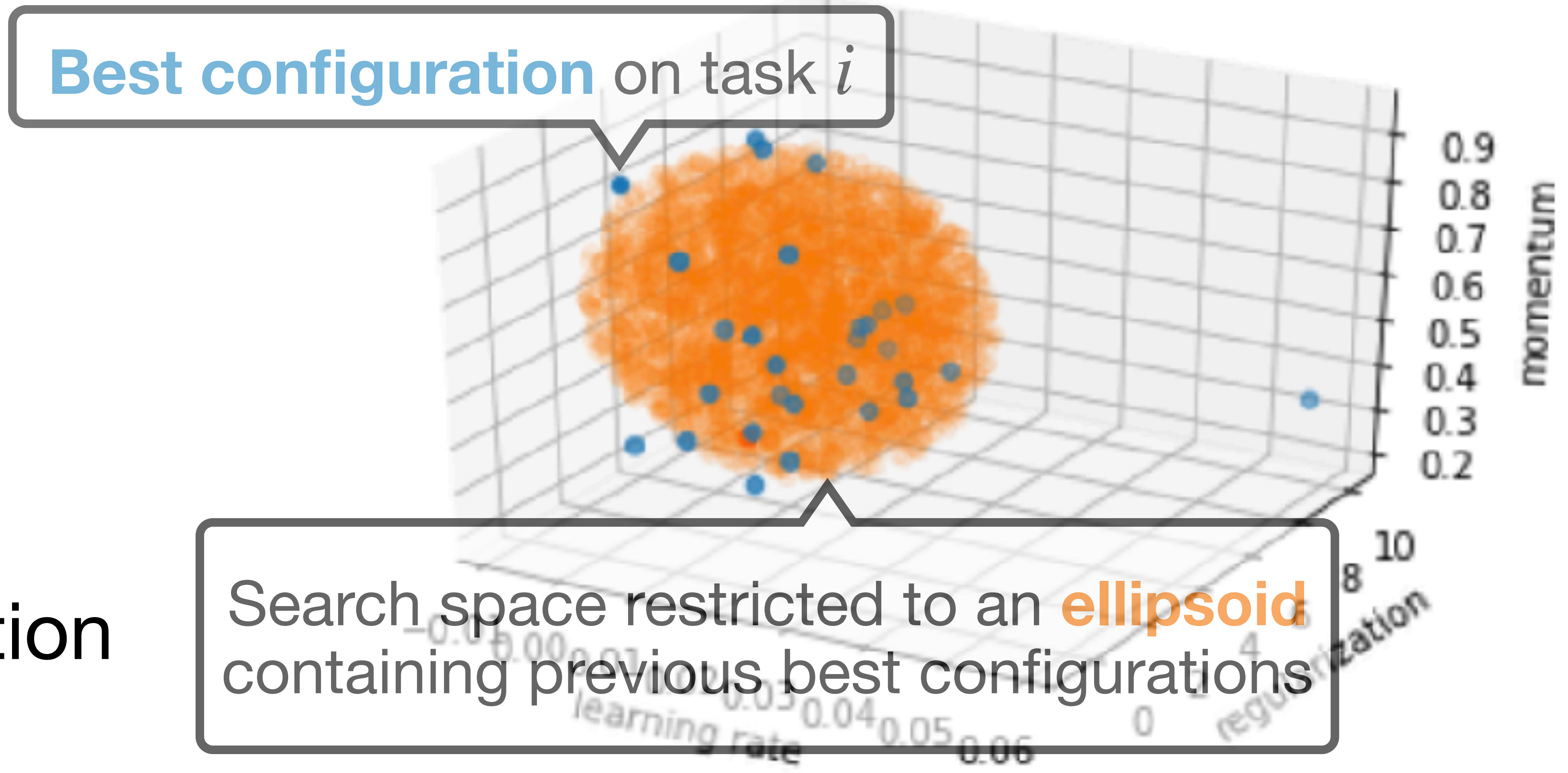


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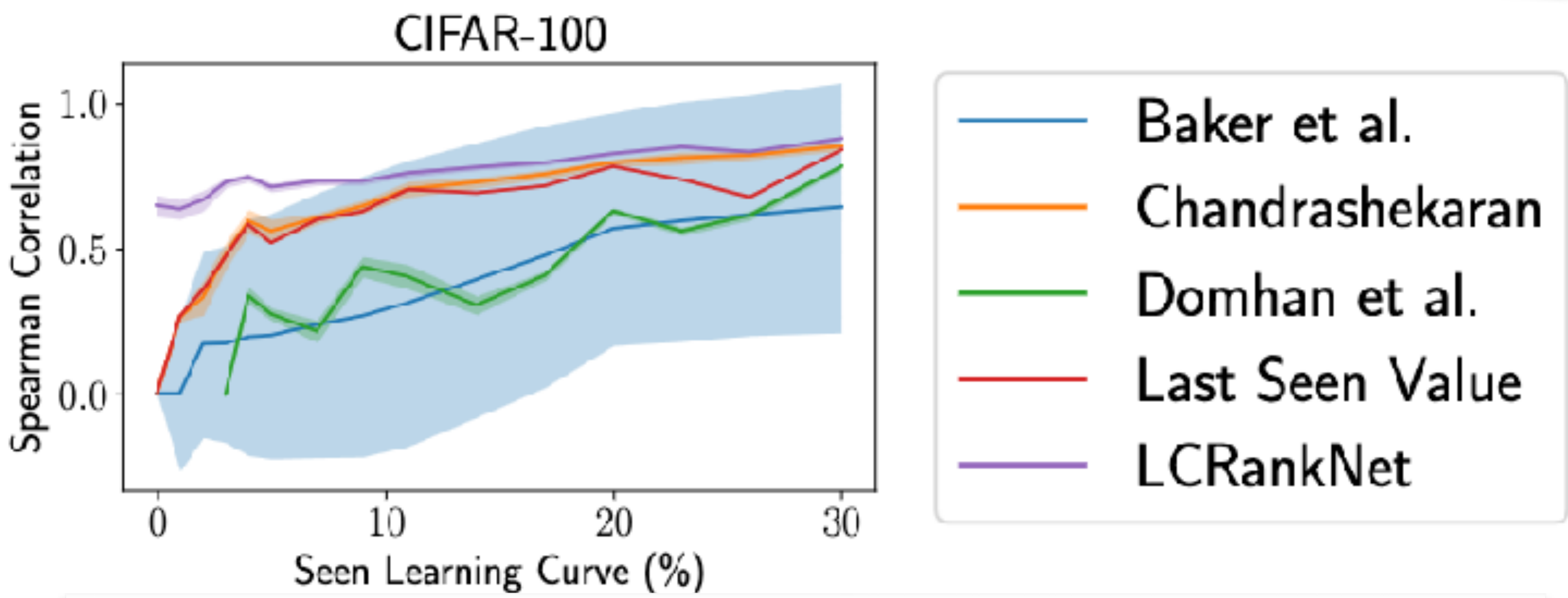


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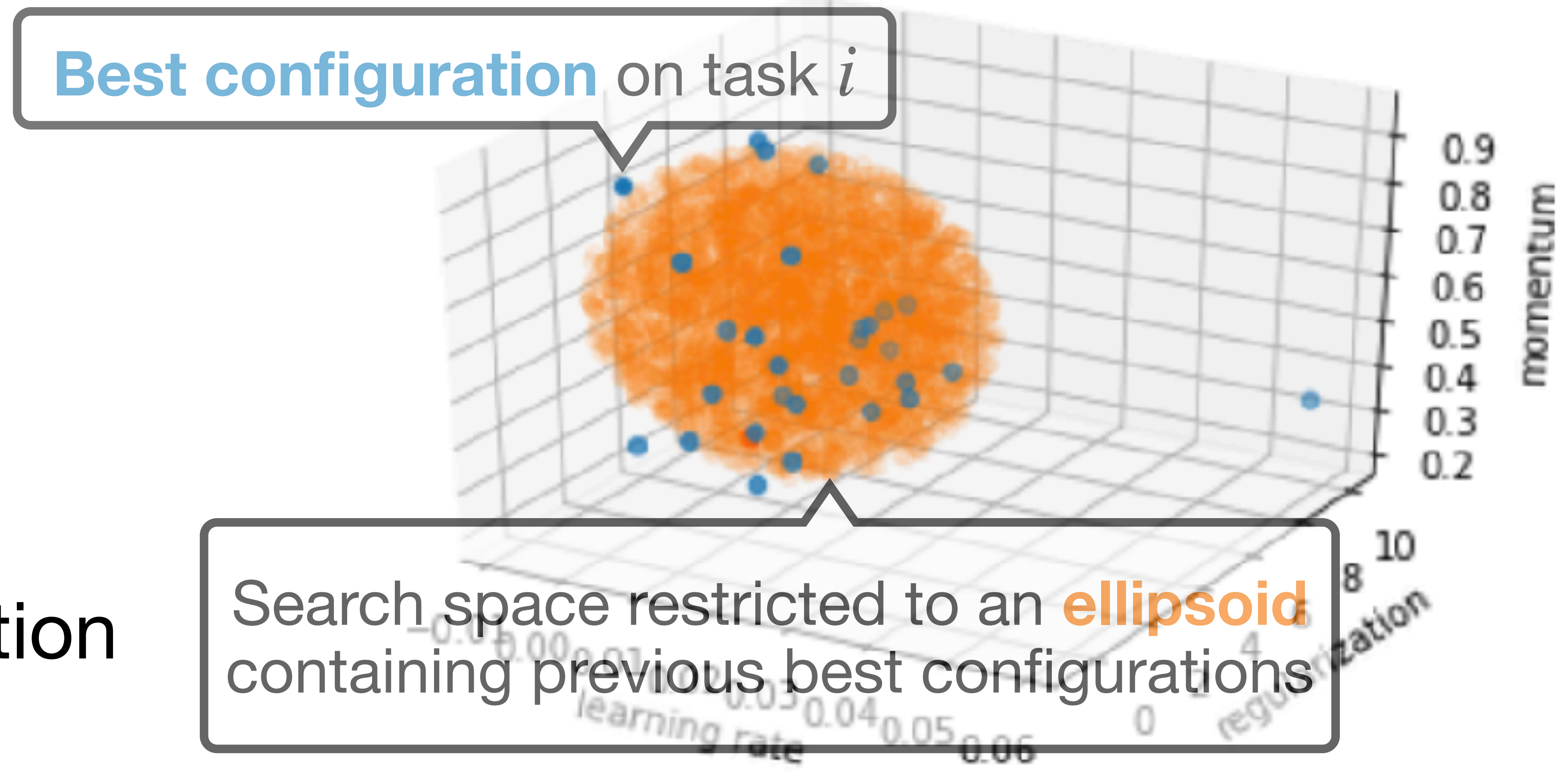


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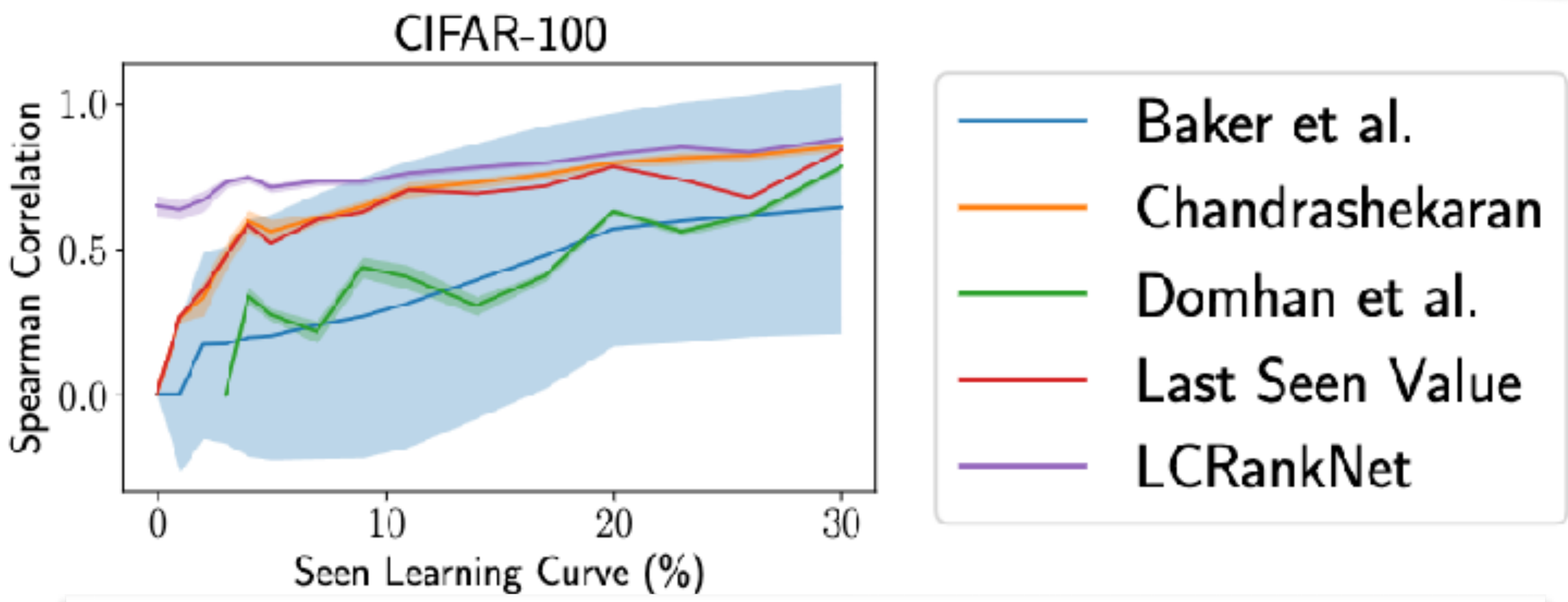


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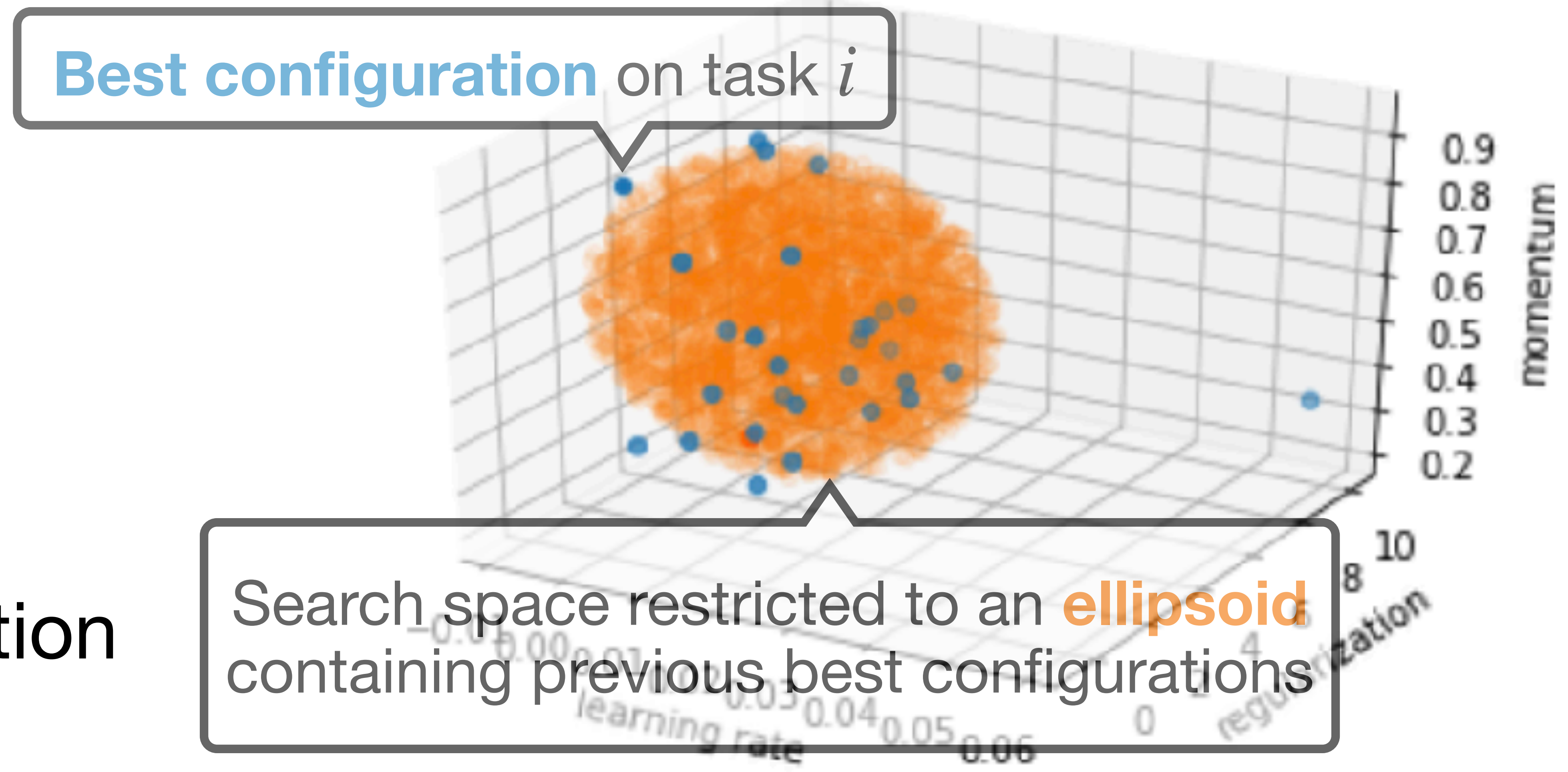


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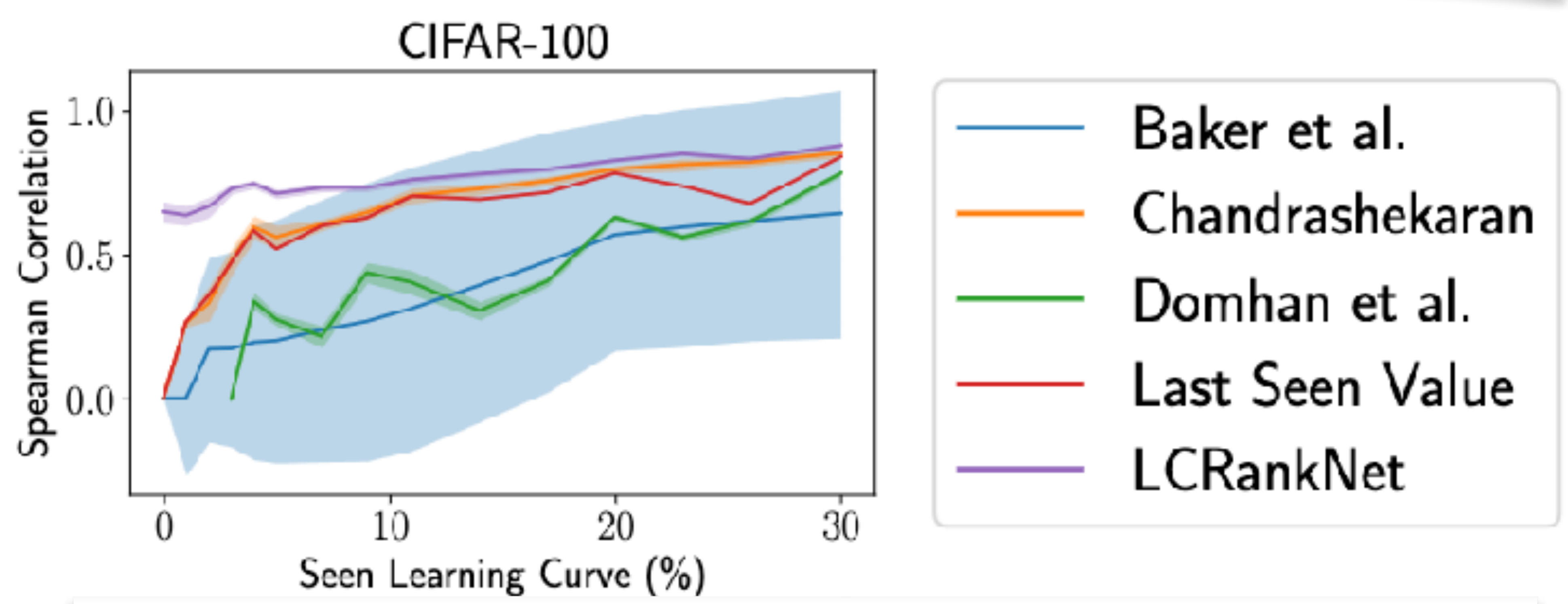


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We will focus on those methods

# Methods

## Prior based methods

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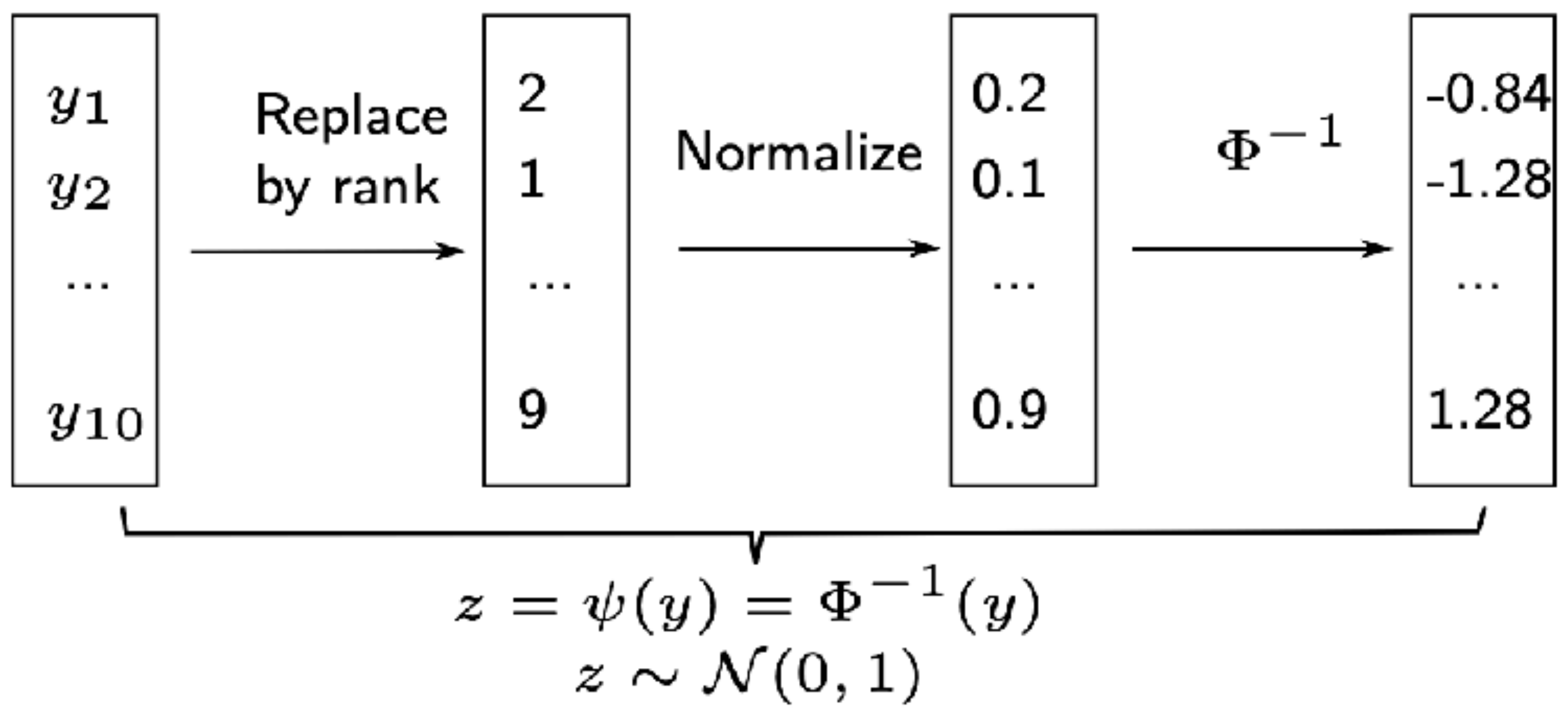

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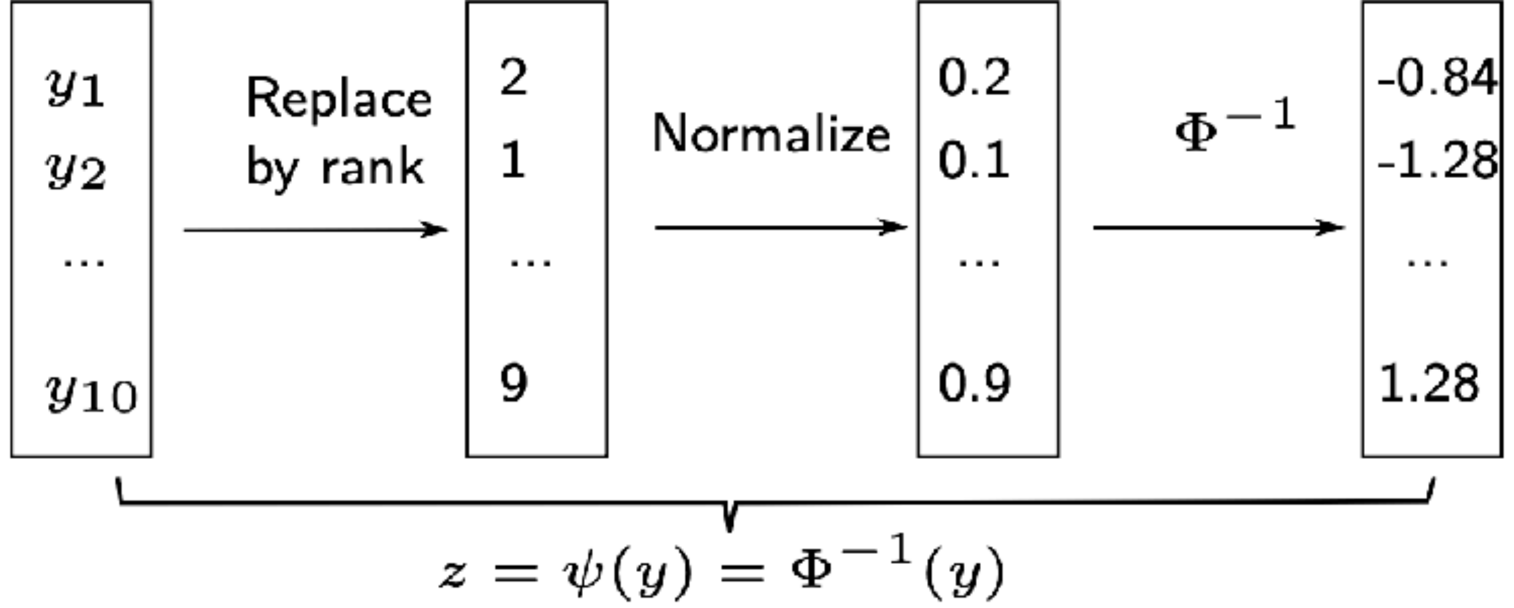


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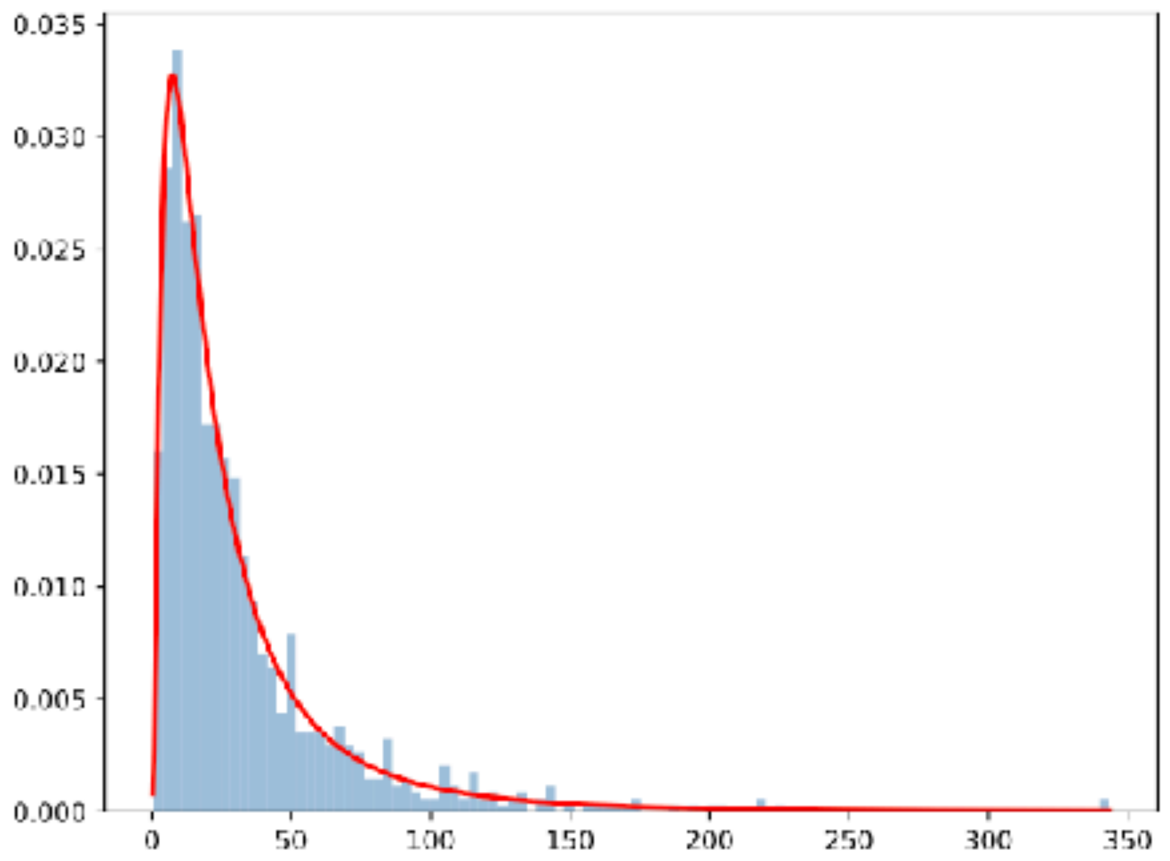
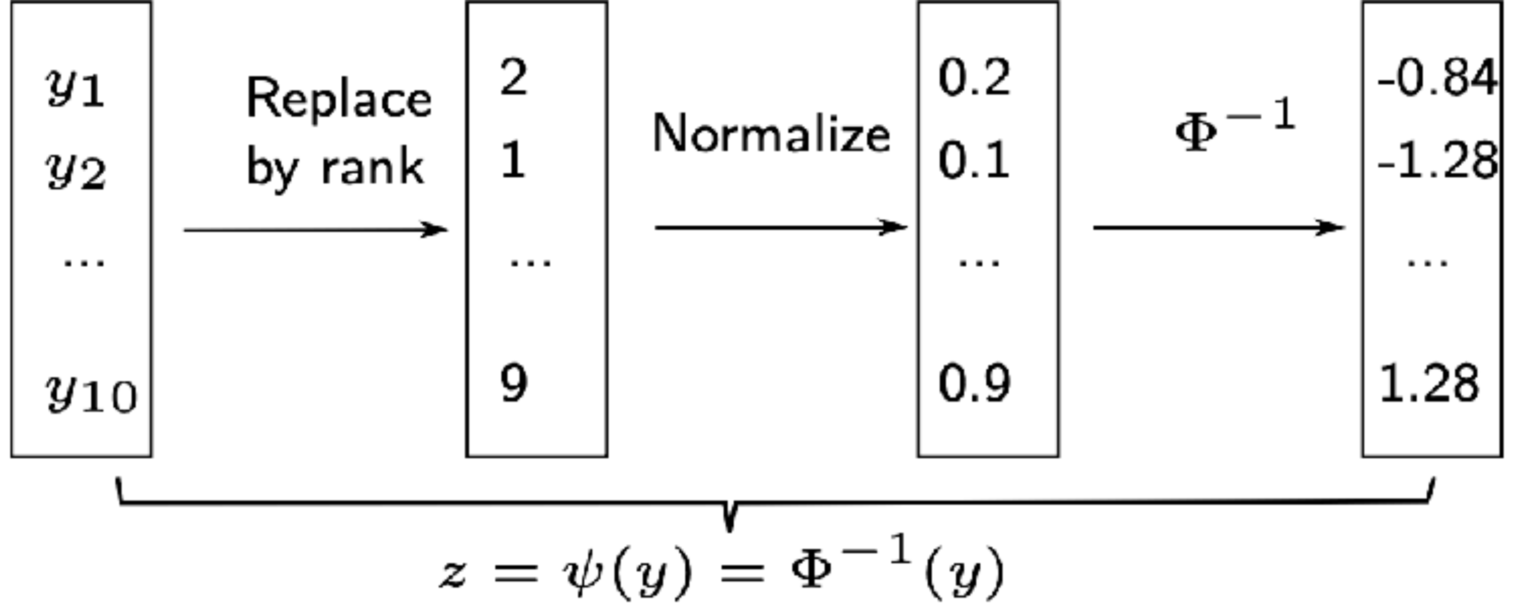



Original distribution

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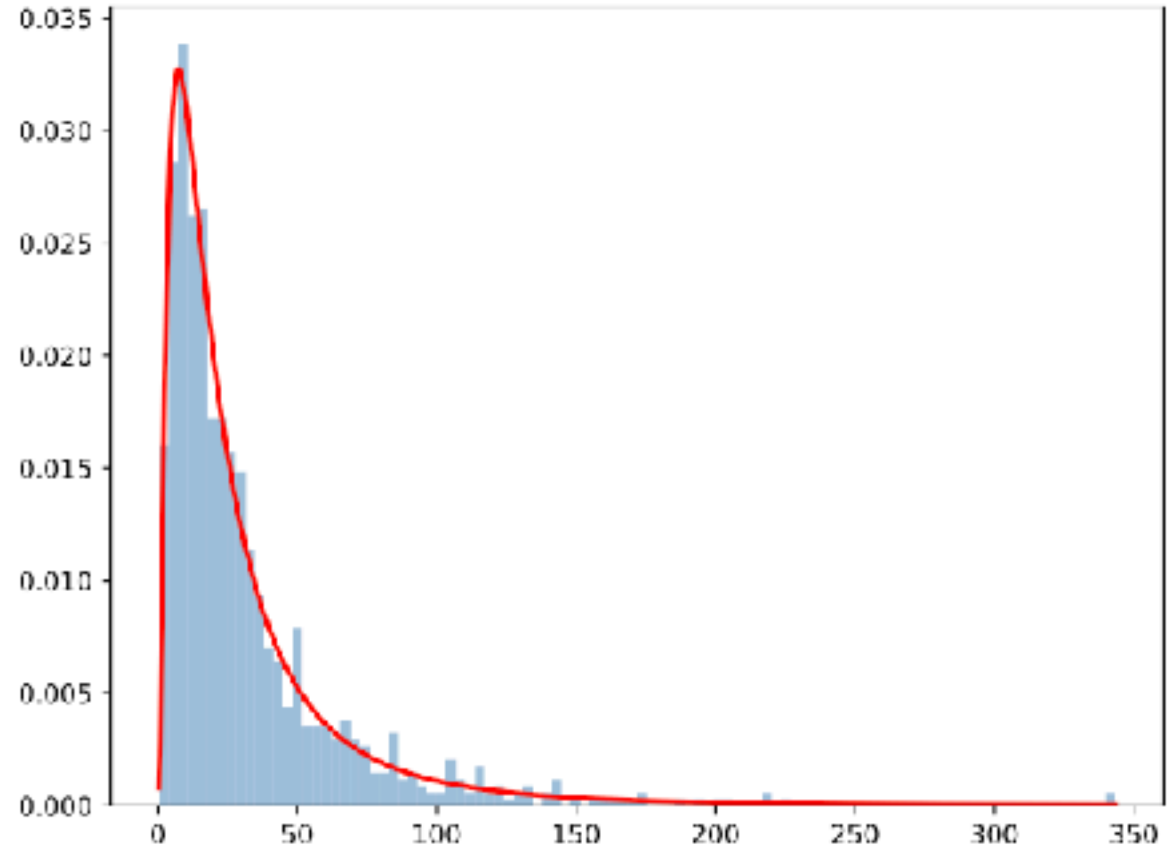


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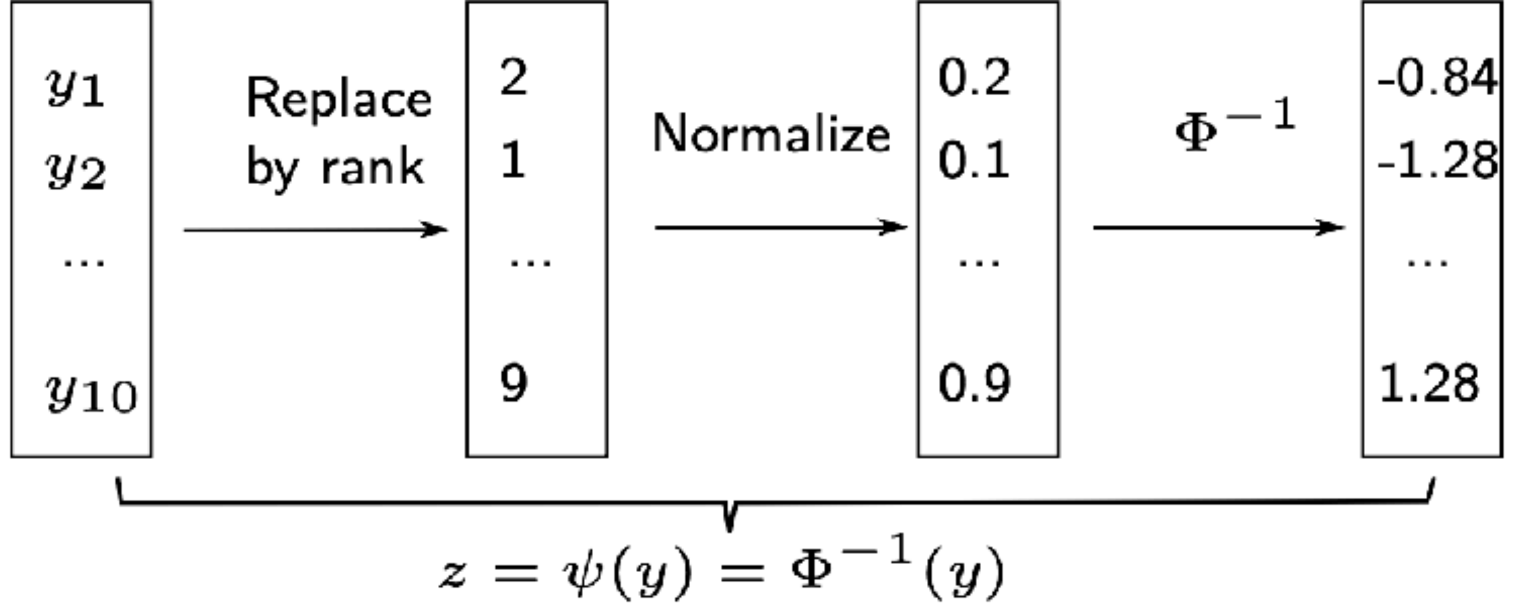


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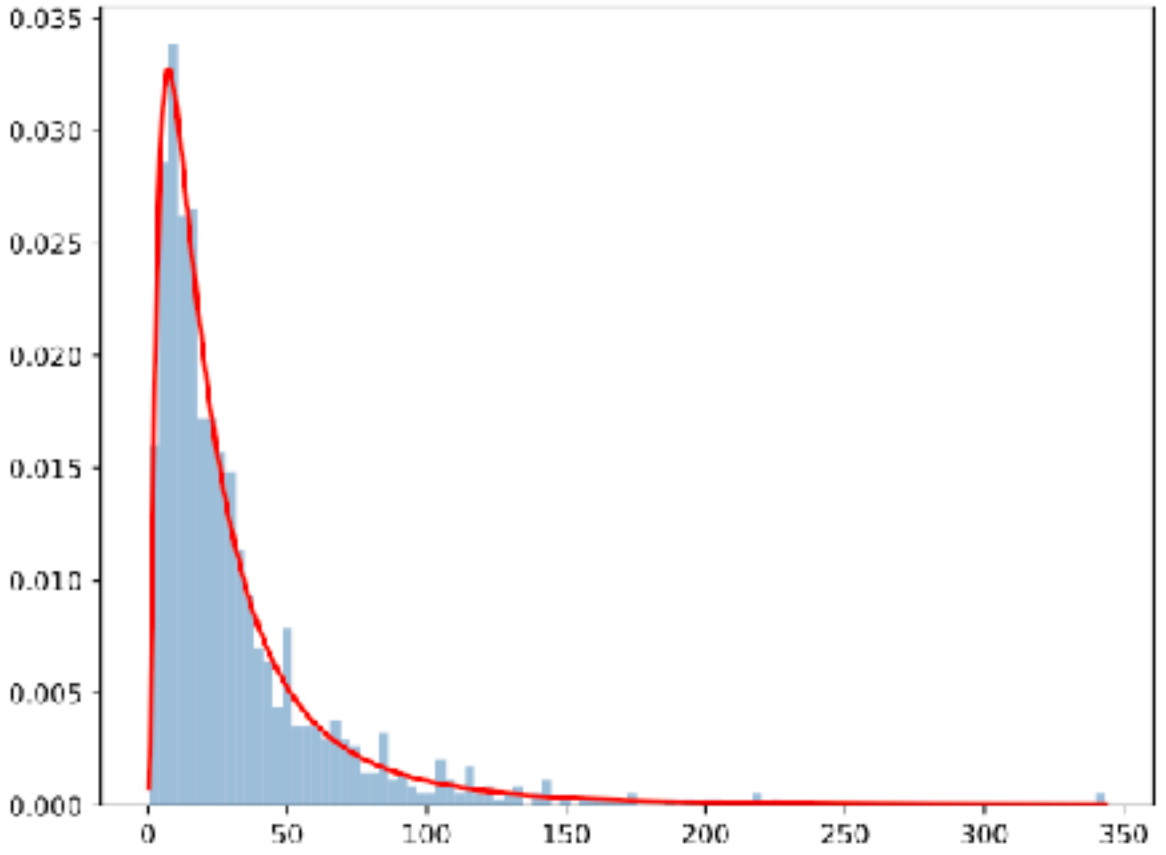


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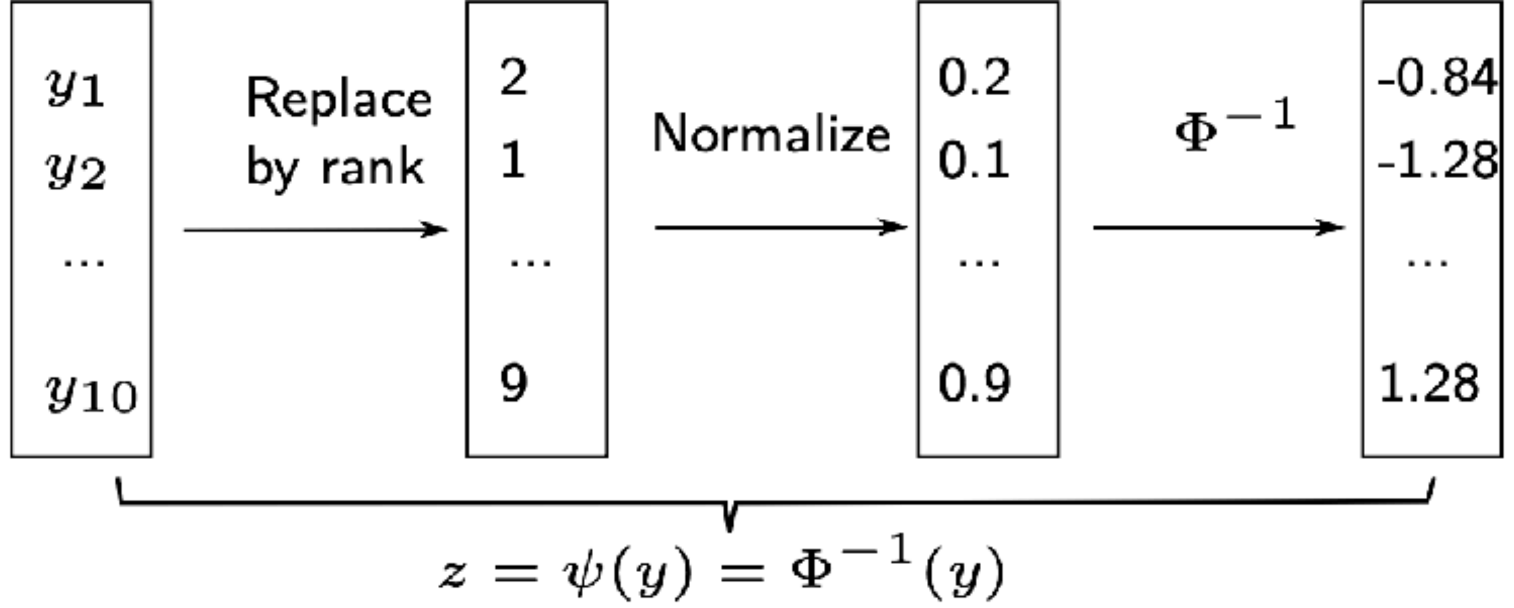


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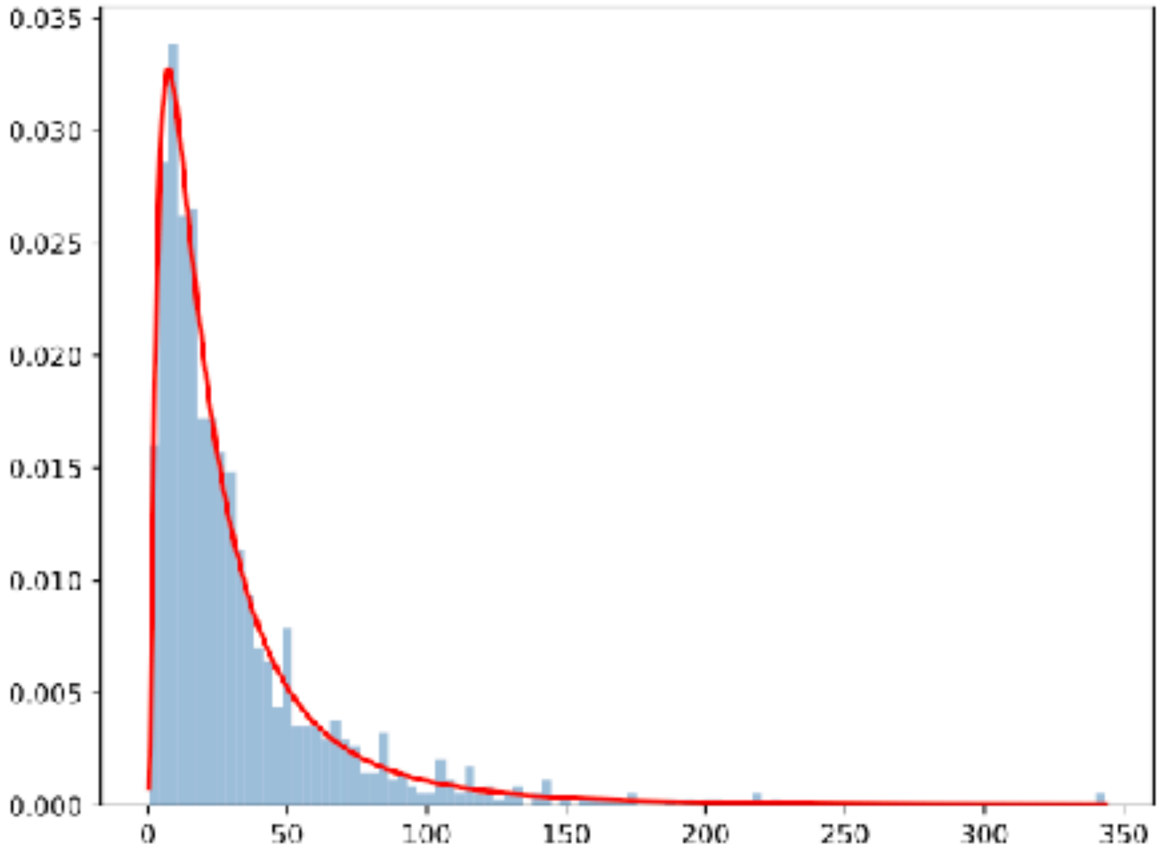

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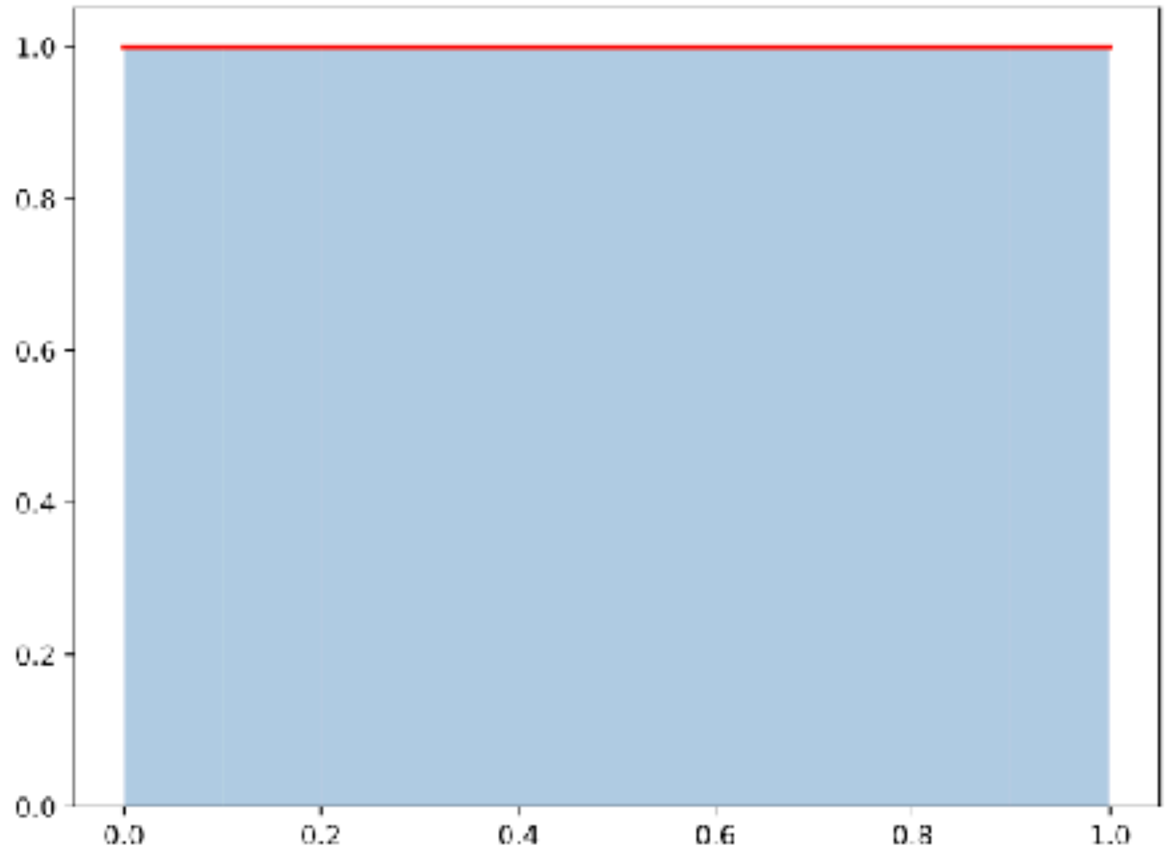

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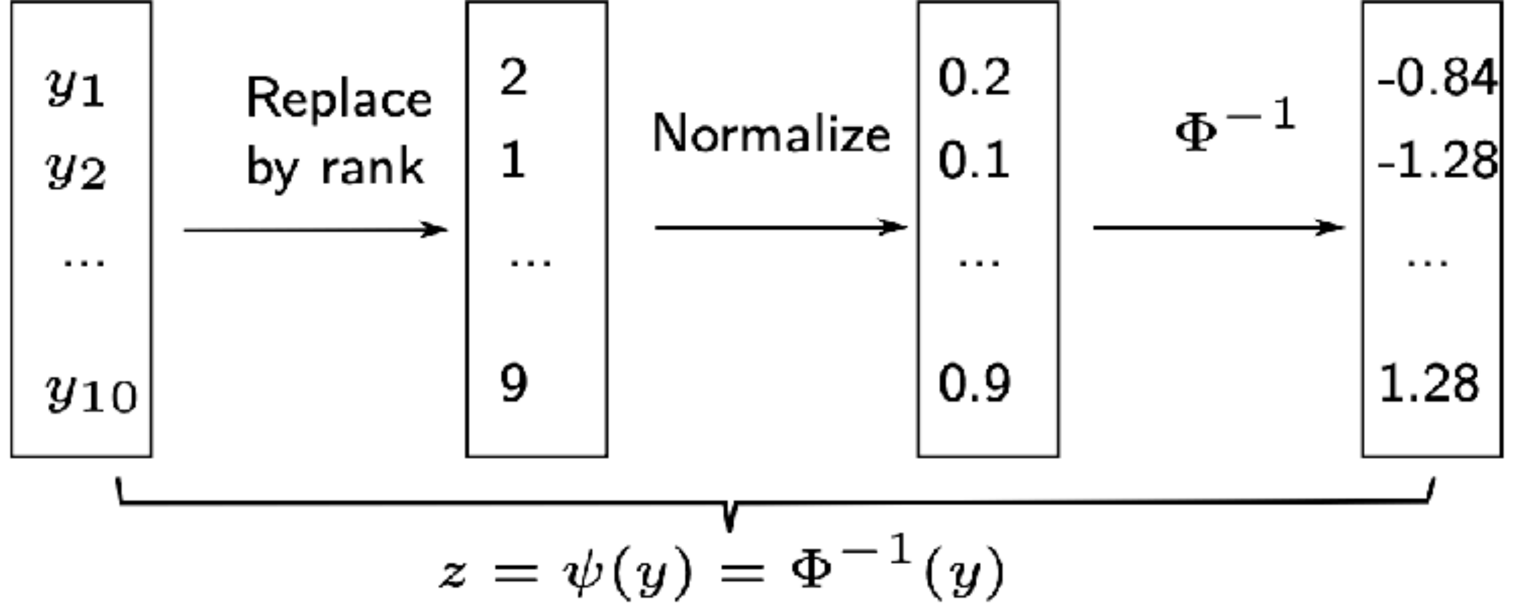


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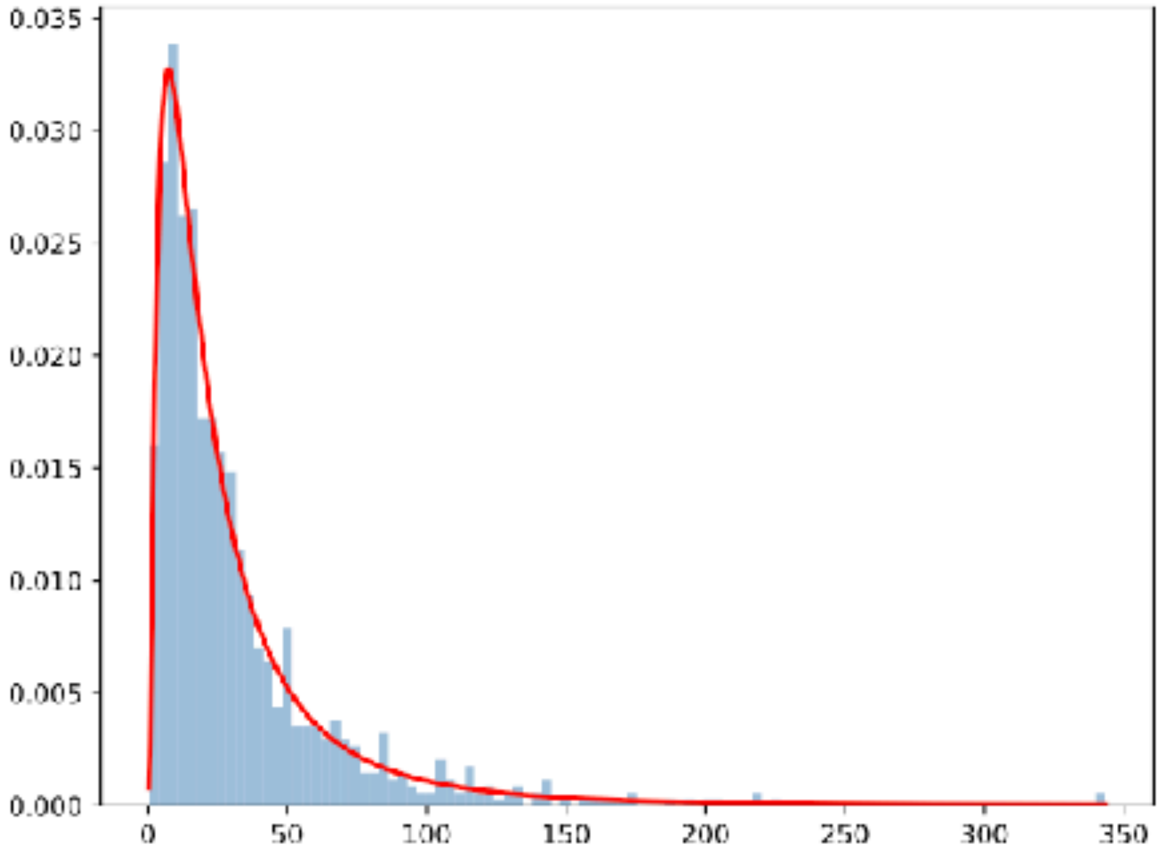


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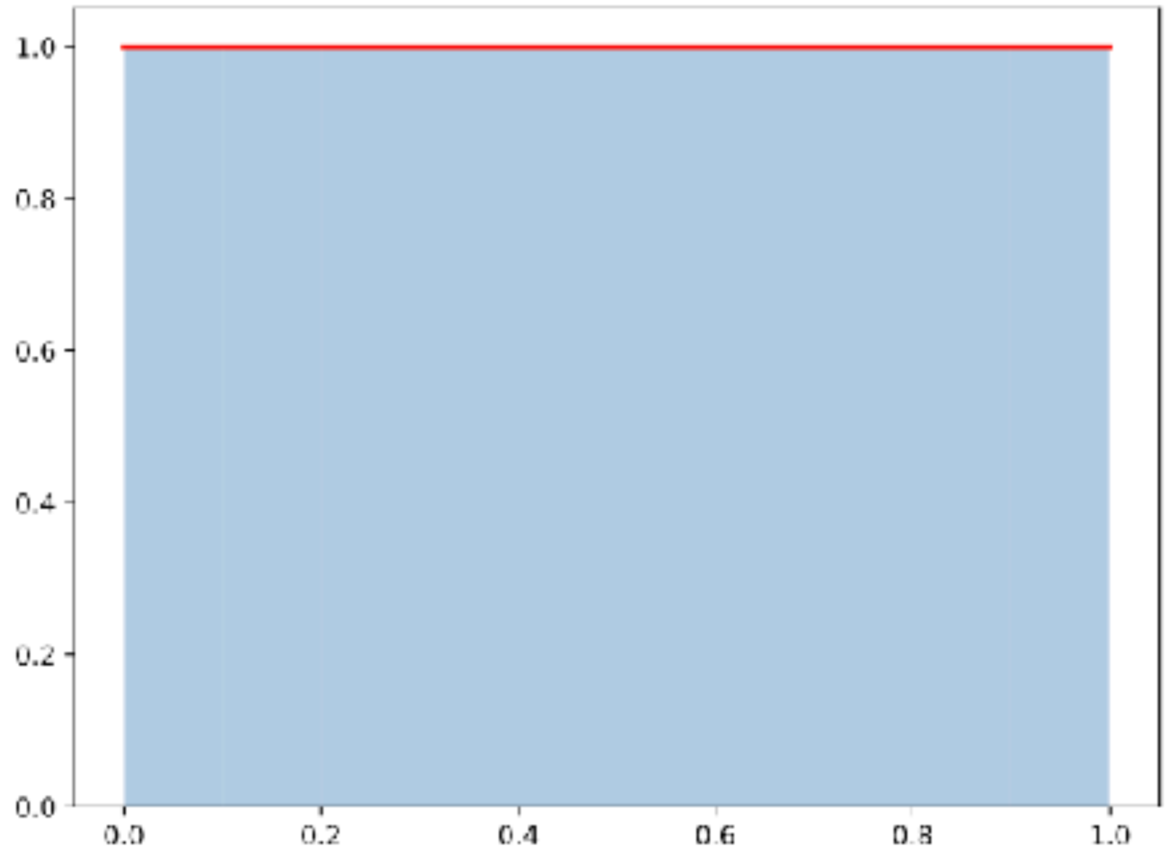


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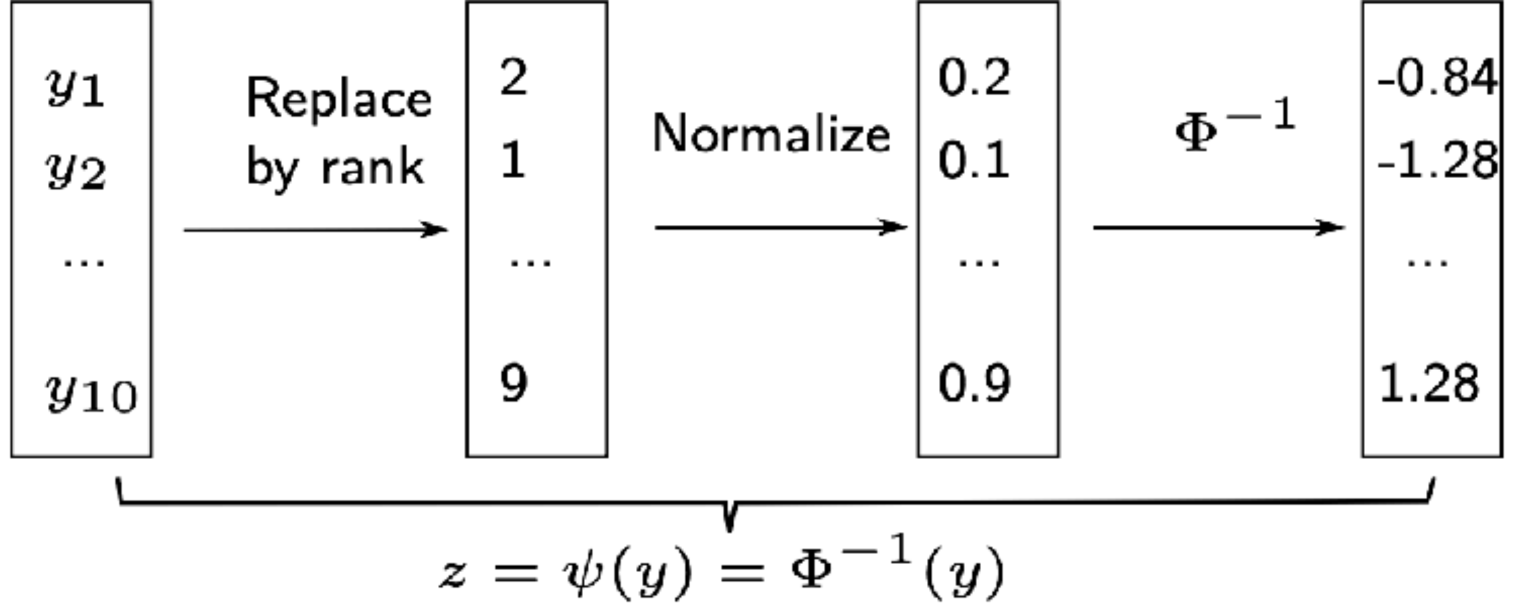


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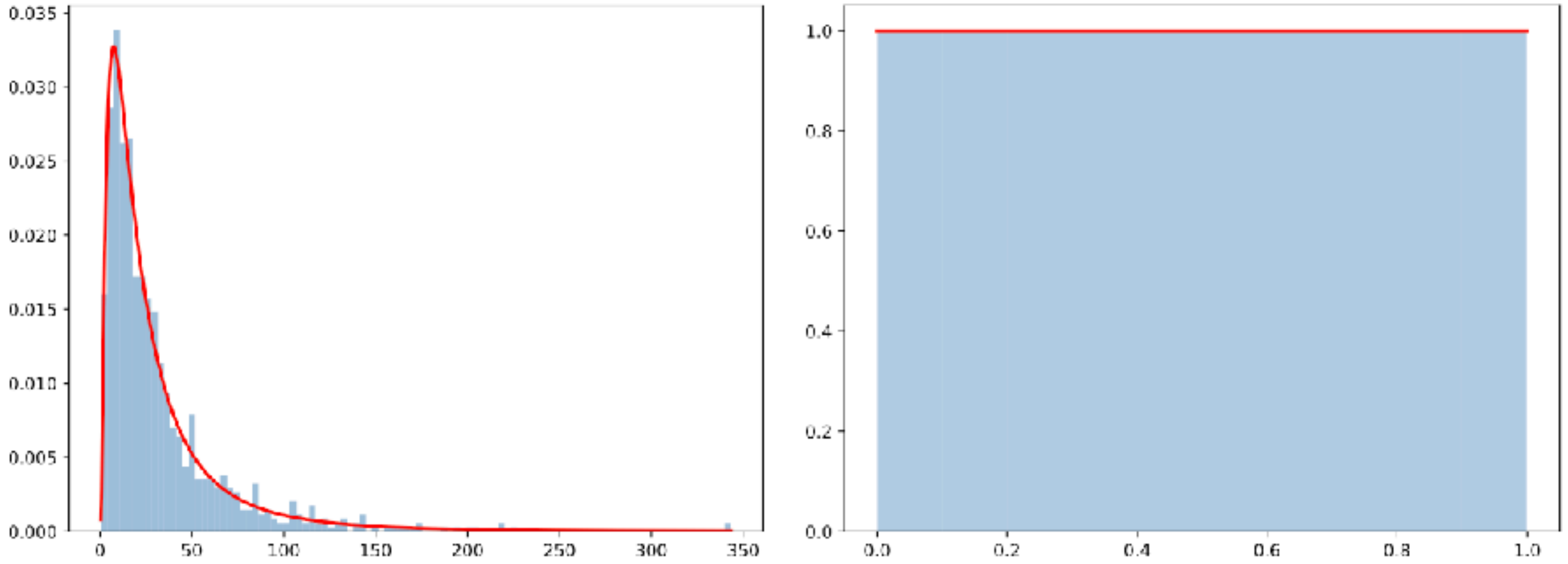

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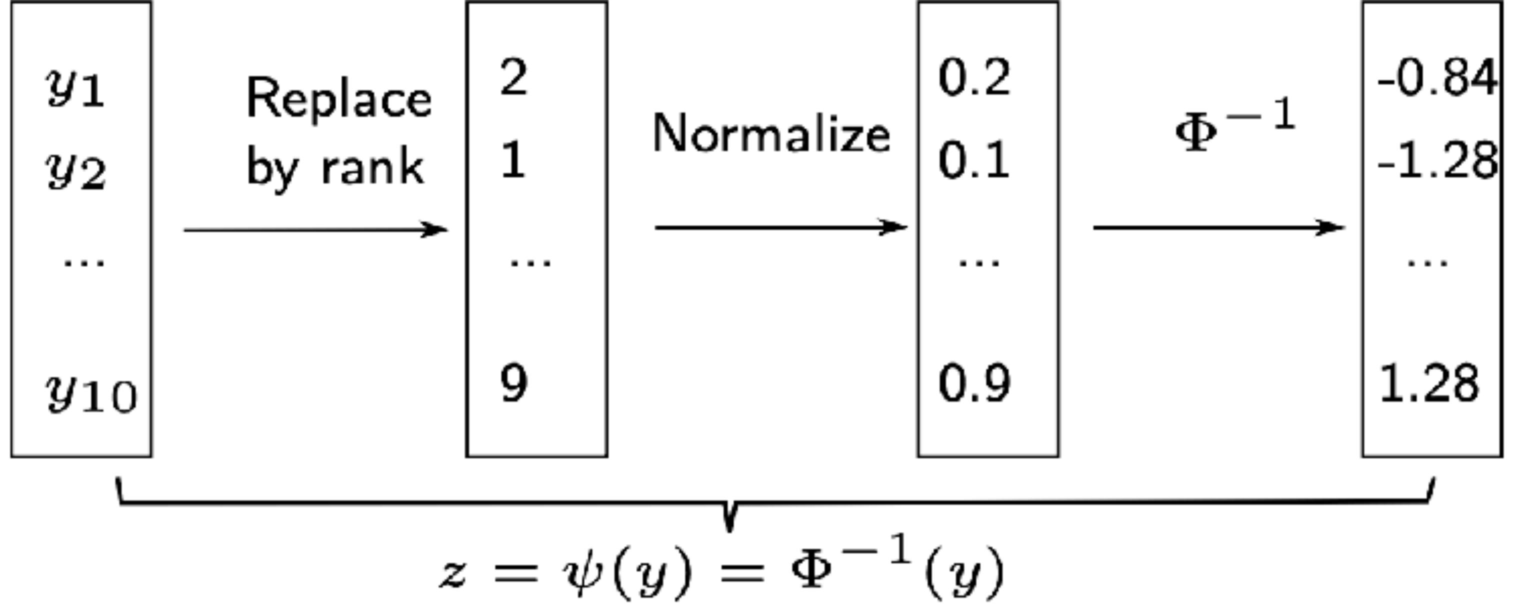


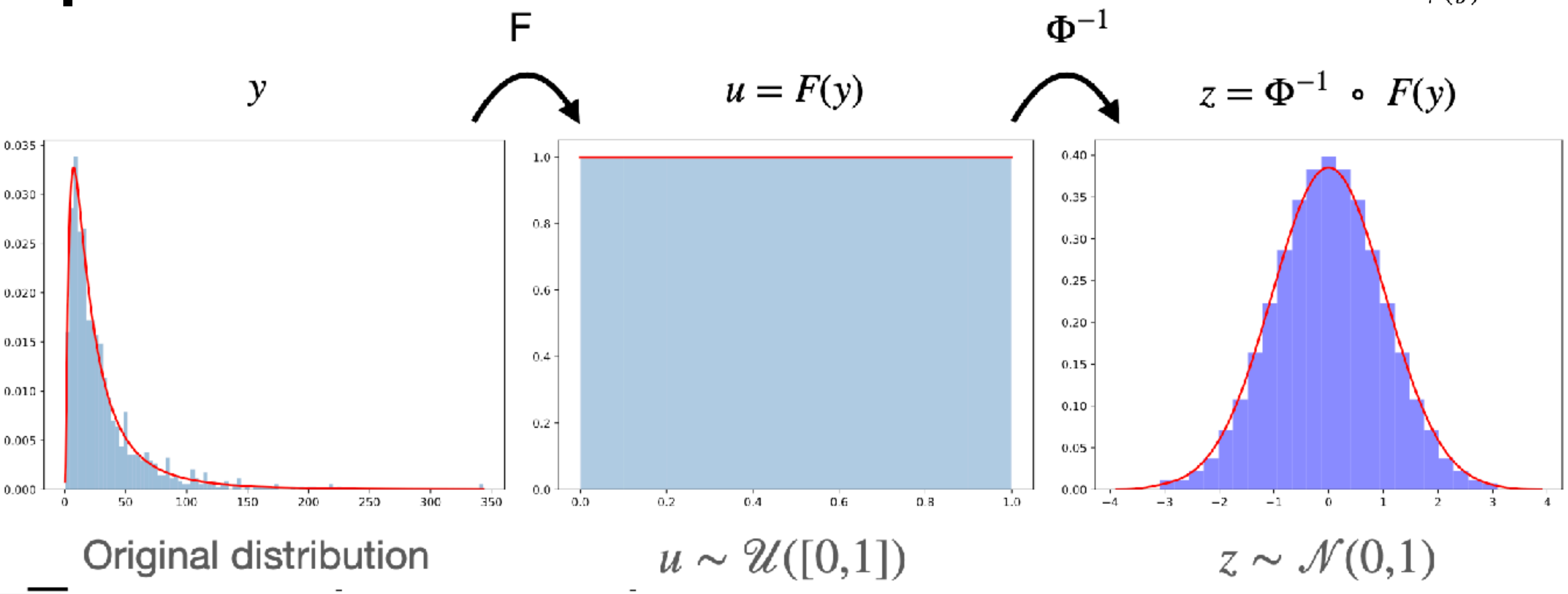


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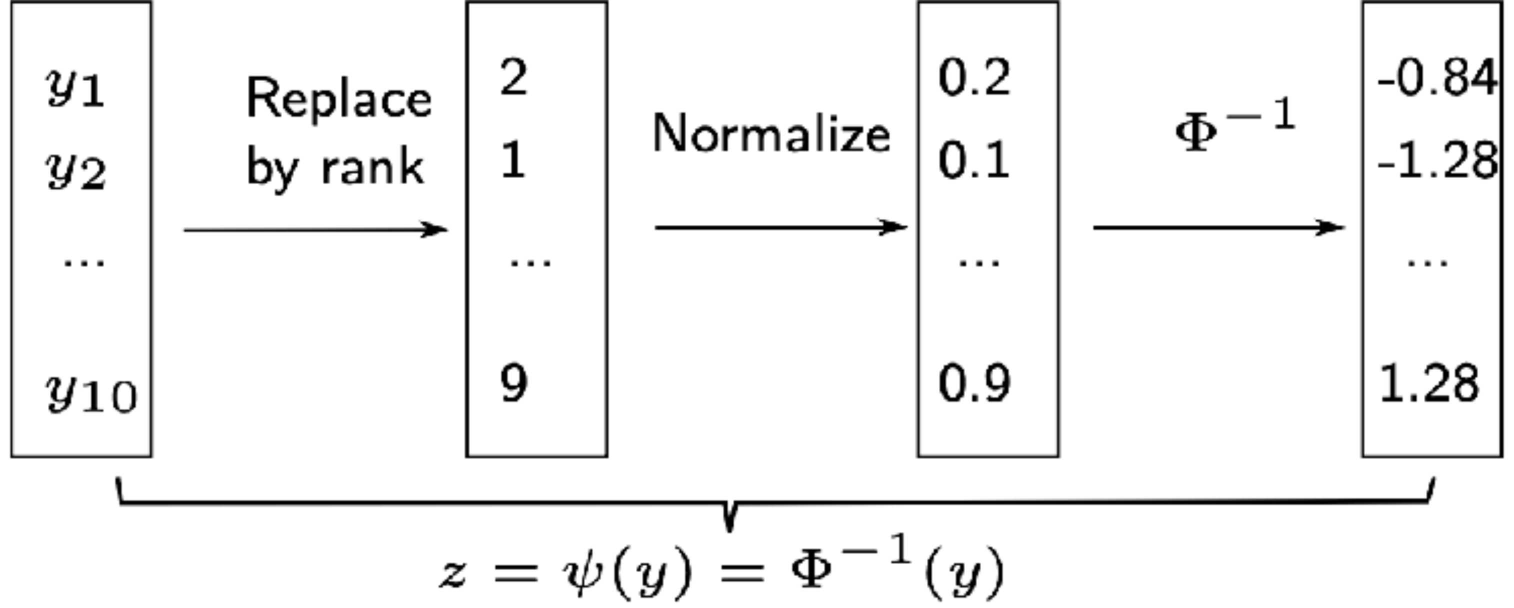


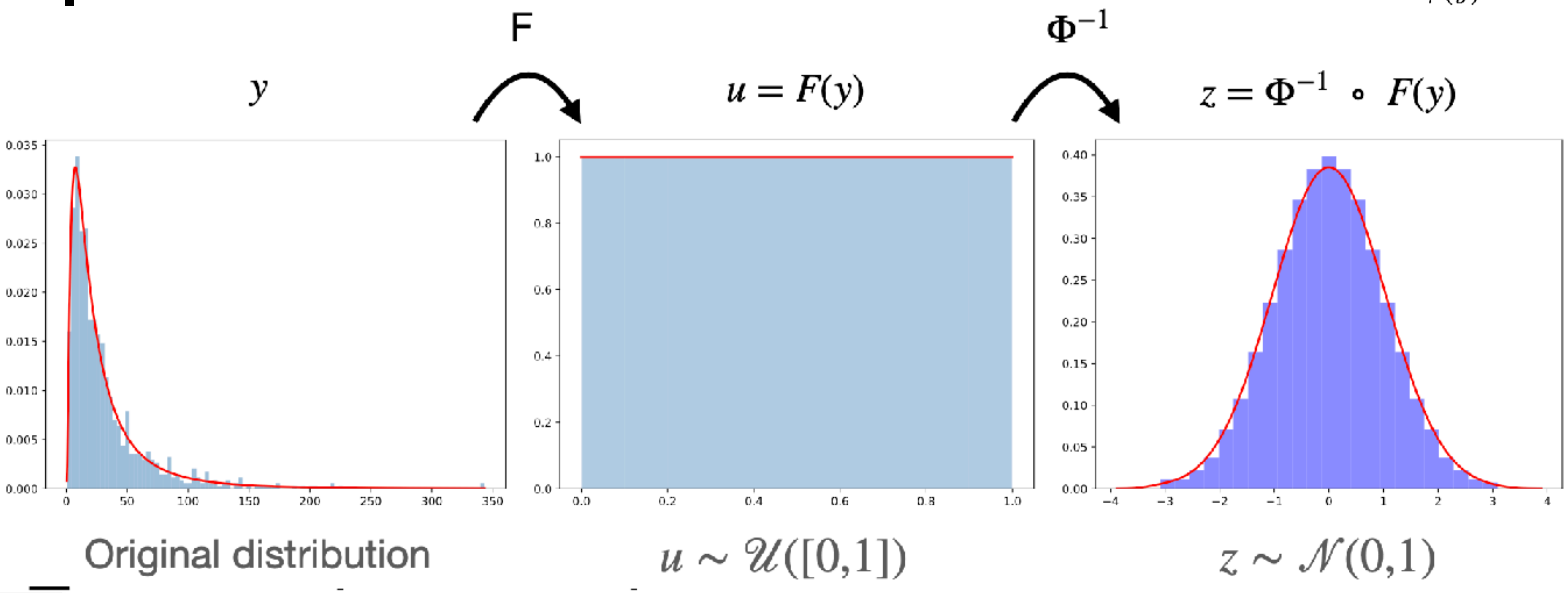


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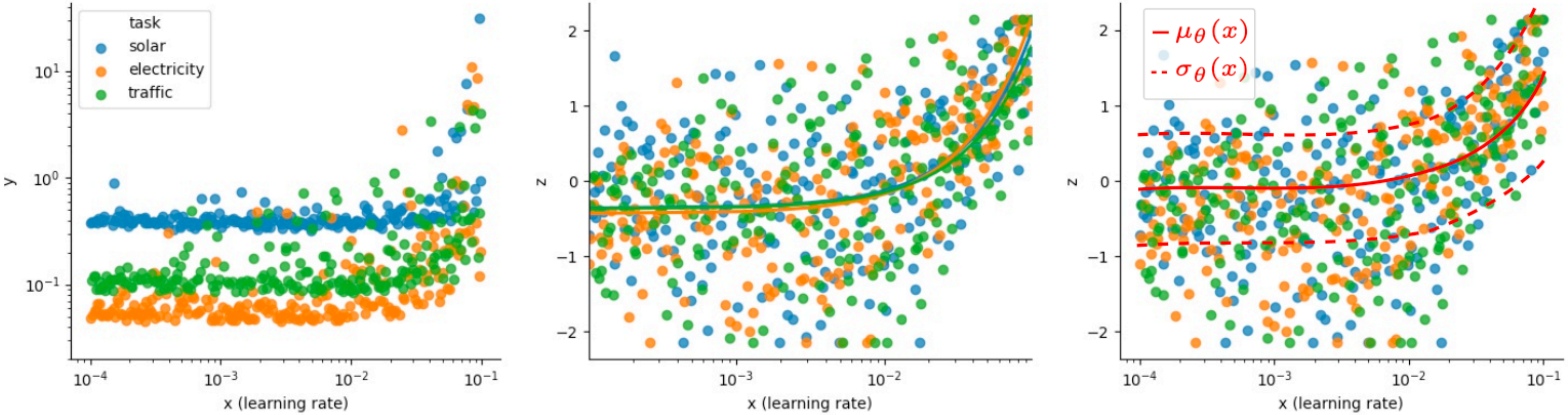
Two very nice properties of $\Psi = \Phi^{-1} \circ F$:

- 😀 $z^j = \Psi(y^j) \sim \mathcal{N}(0,1)$ (great for GP)
- 😀 Built-in invariance of $z^j$ to monotonic transformation on $y^j$

# Gaussian Copula Transform

## Learning joint representations across tasks




**Left:** Plot blackbox error $y$ in log-space against a single hyperparameter $x$ for different tasks.
**Middle:** Running mean after transforming each task objectives with $z = \psi(y) = \Phi^{-1} \circ F(y)$.
**Right:** Illustrative plot of possible mean/variance fit of a model $\mu_\theta(x), \sigma_\theta(x)$ trained jointly on all tasks with shared parameters $\theta$.

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- Outline:

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Standard
Gaussian Process

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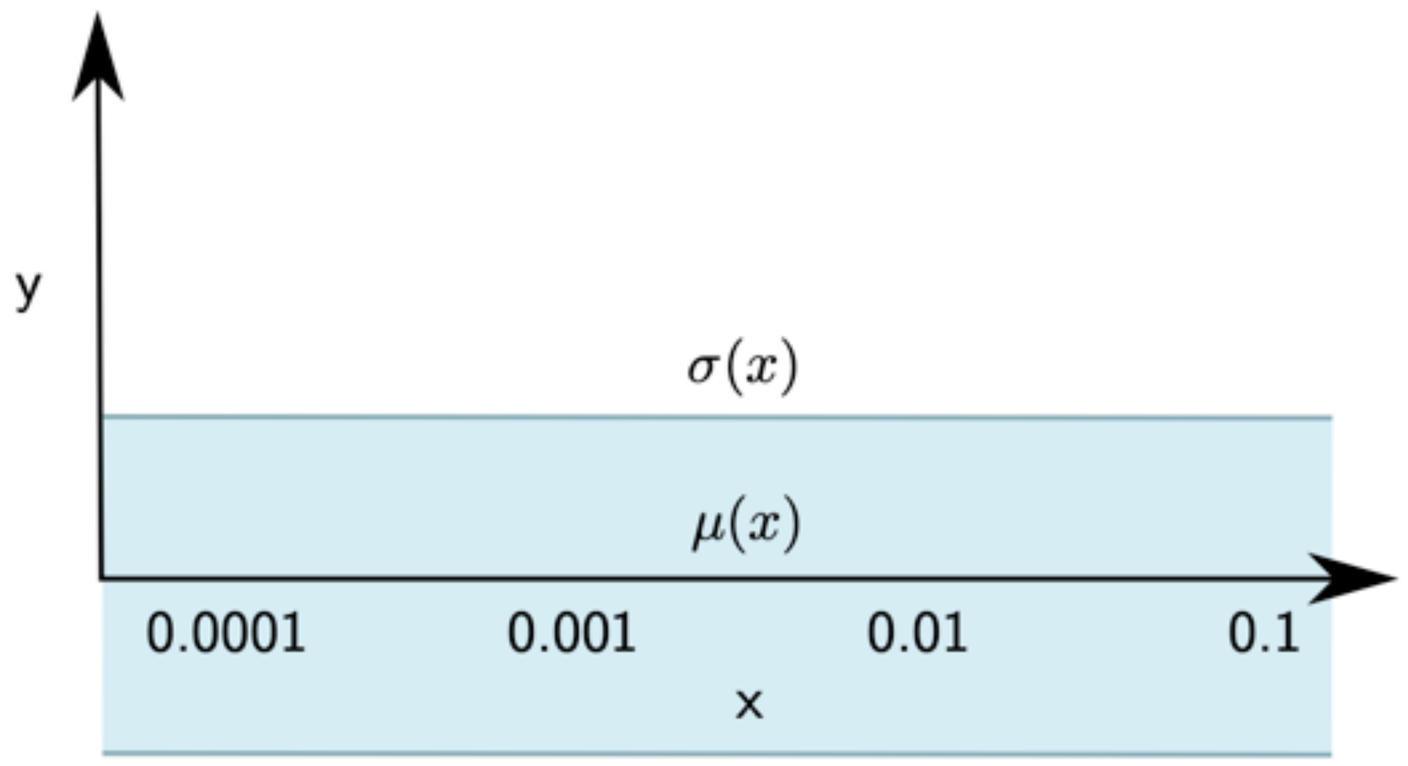


Standard
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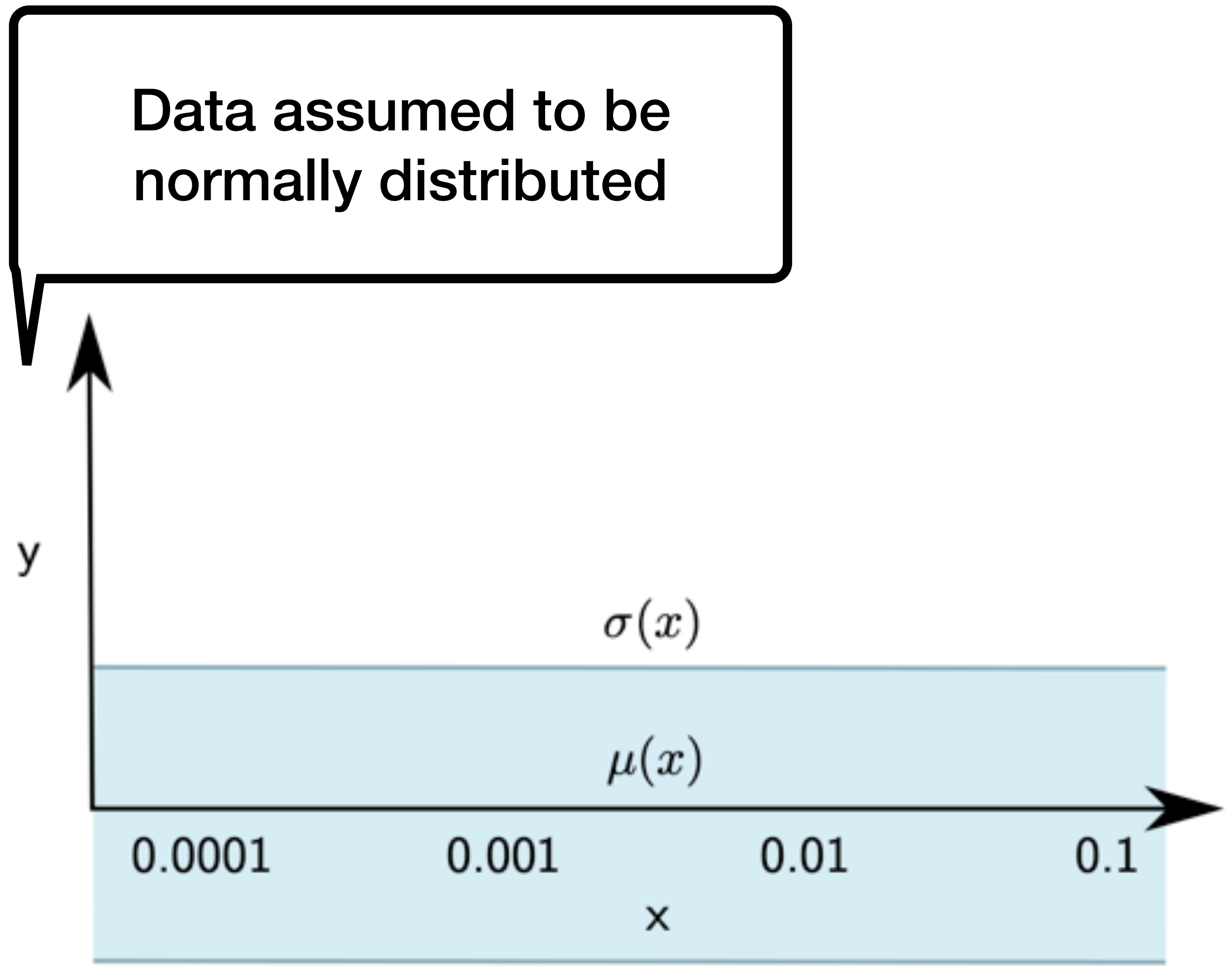


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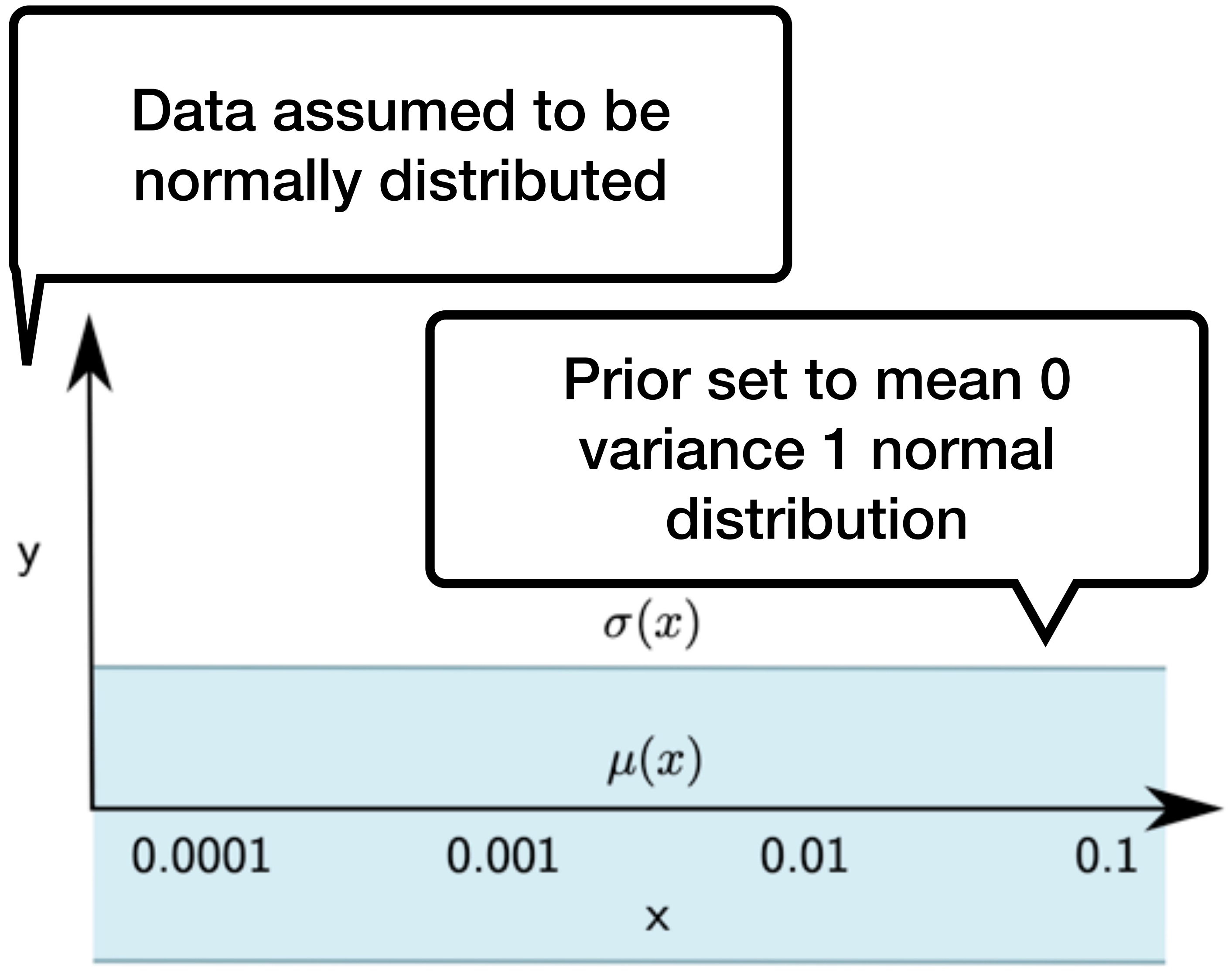


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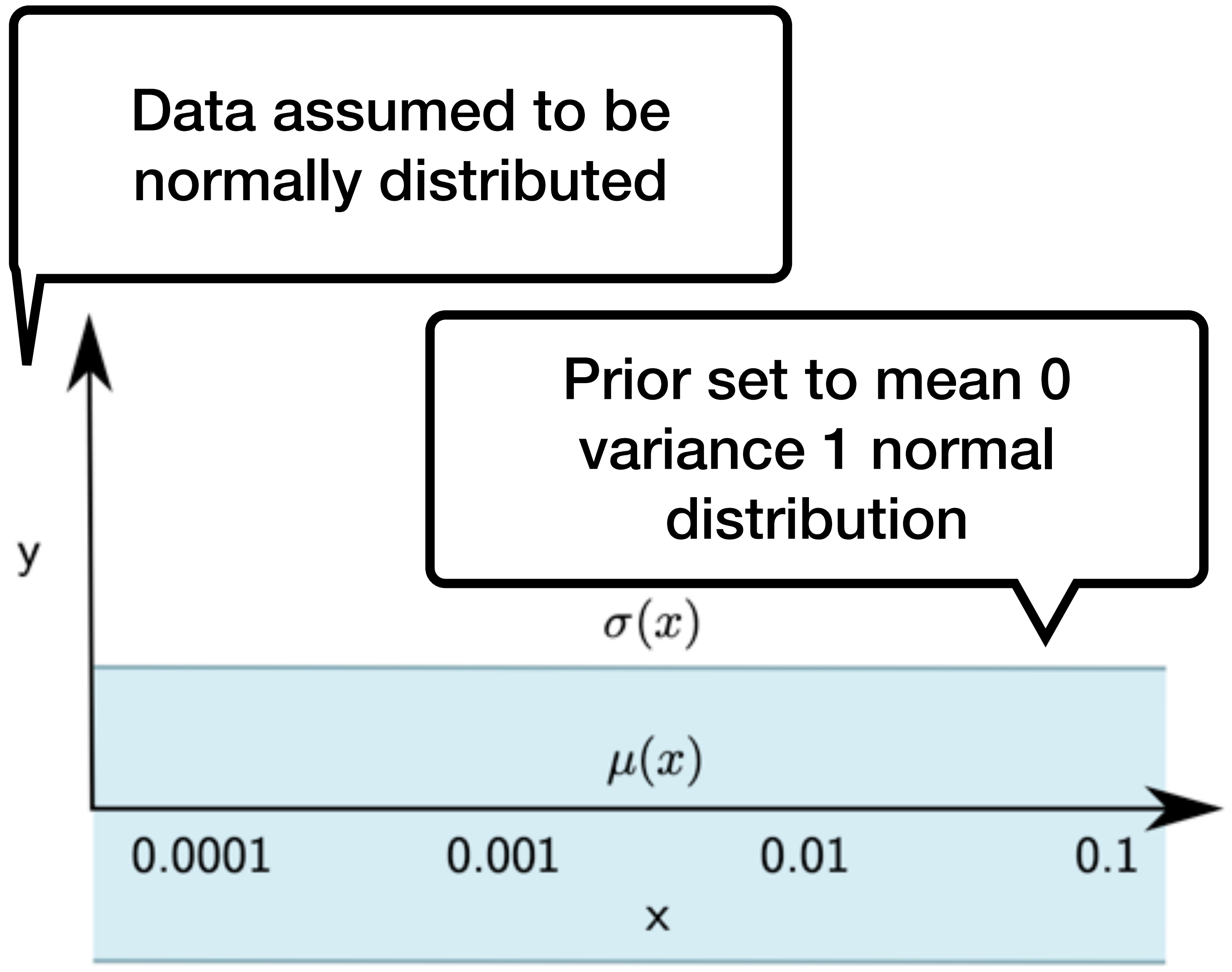


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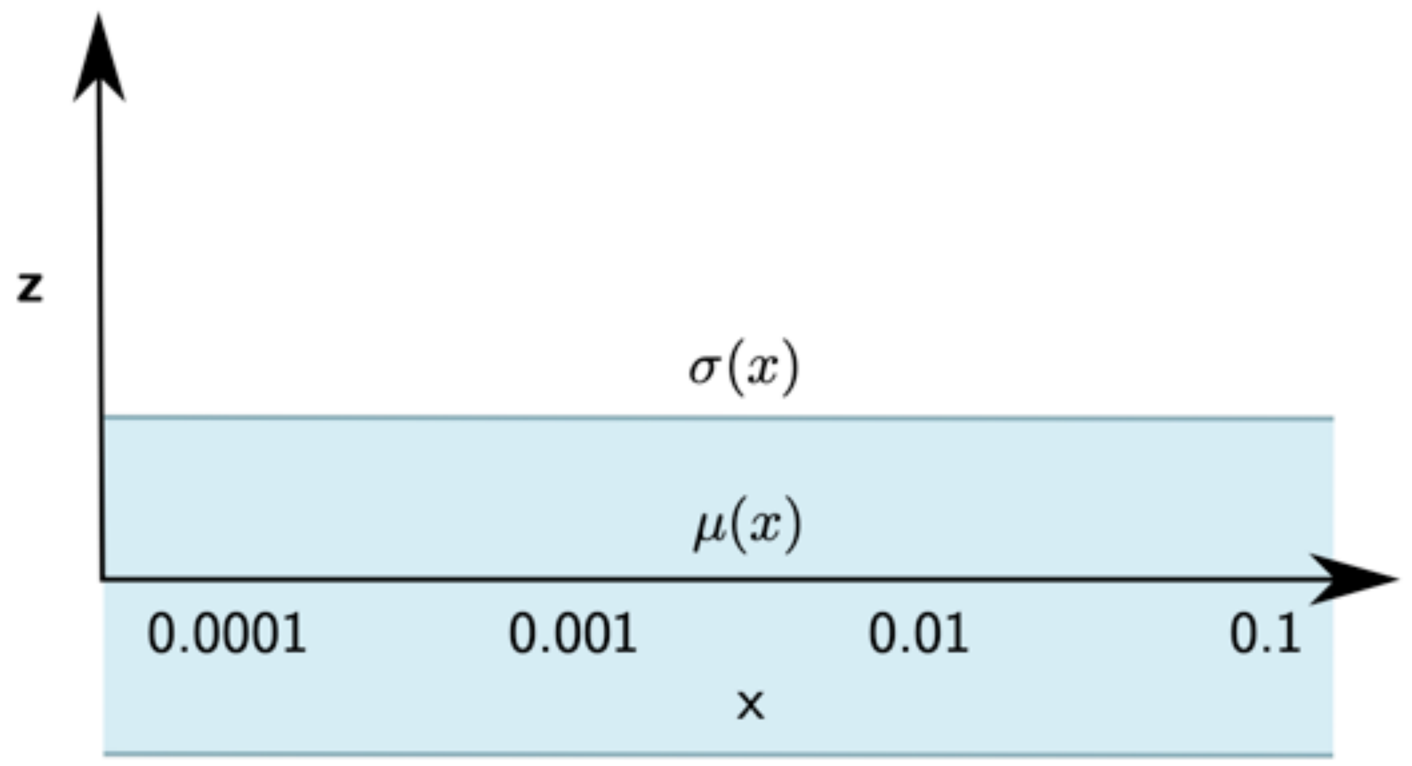


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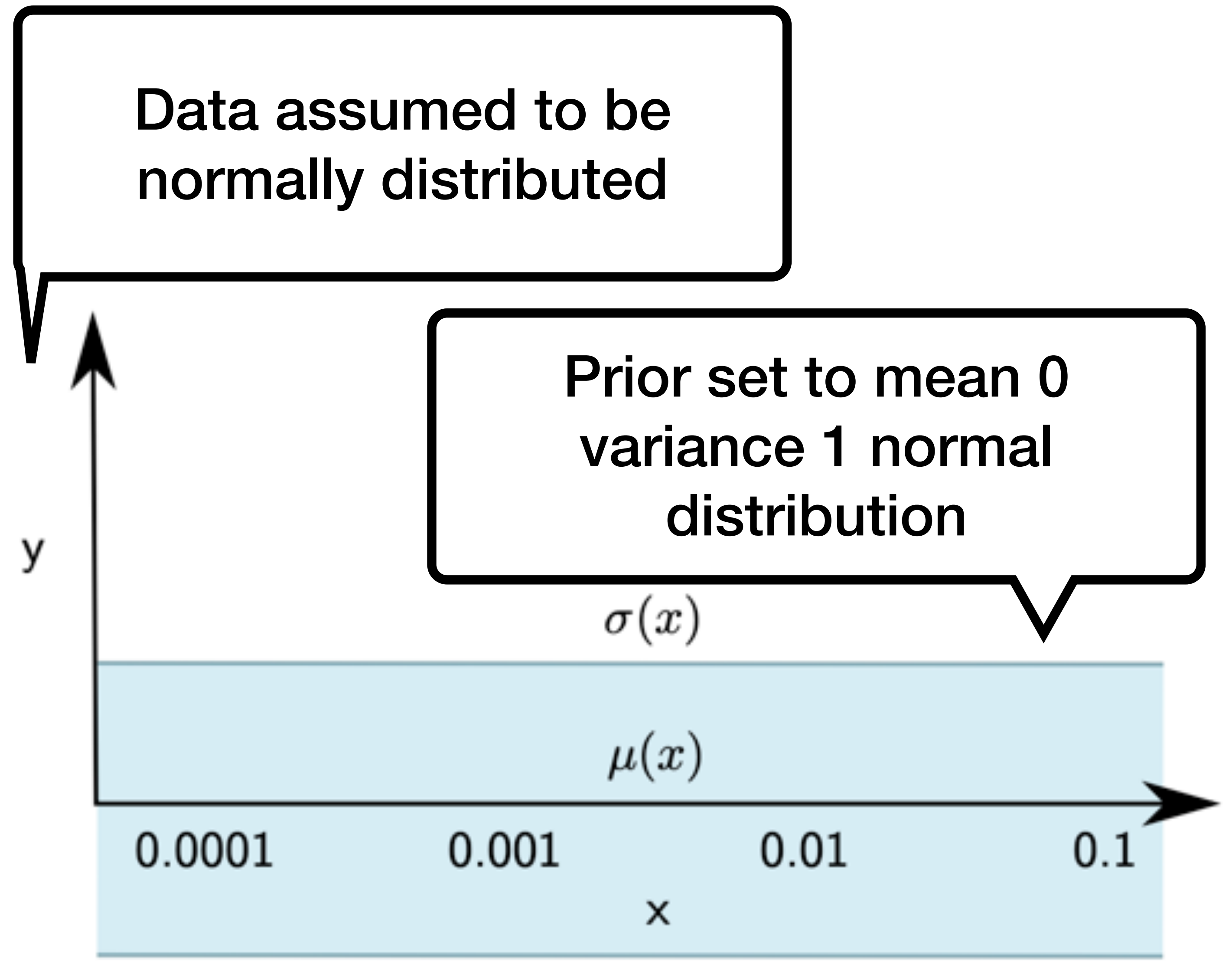


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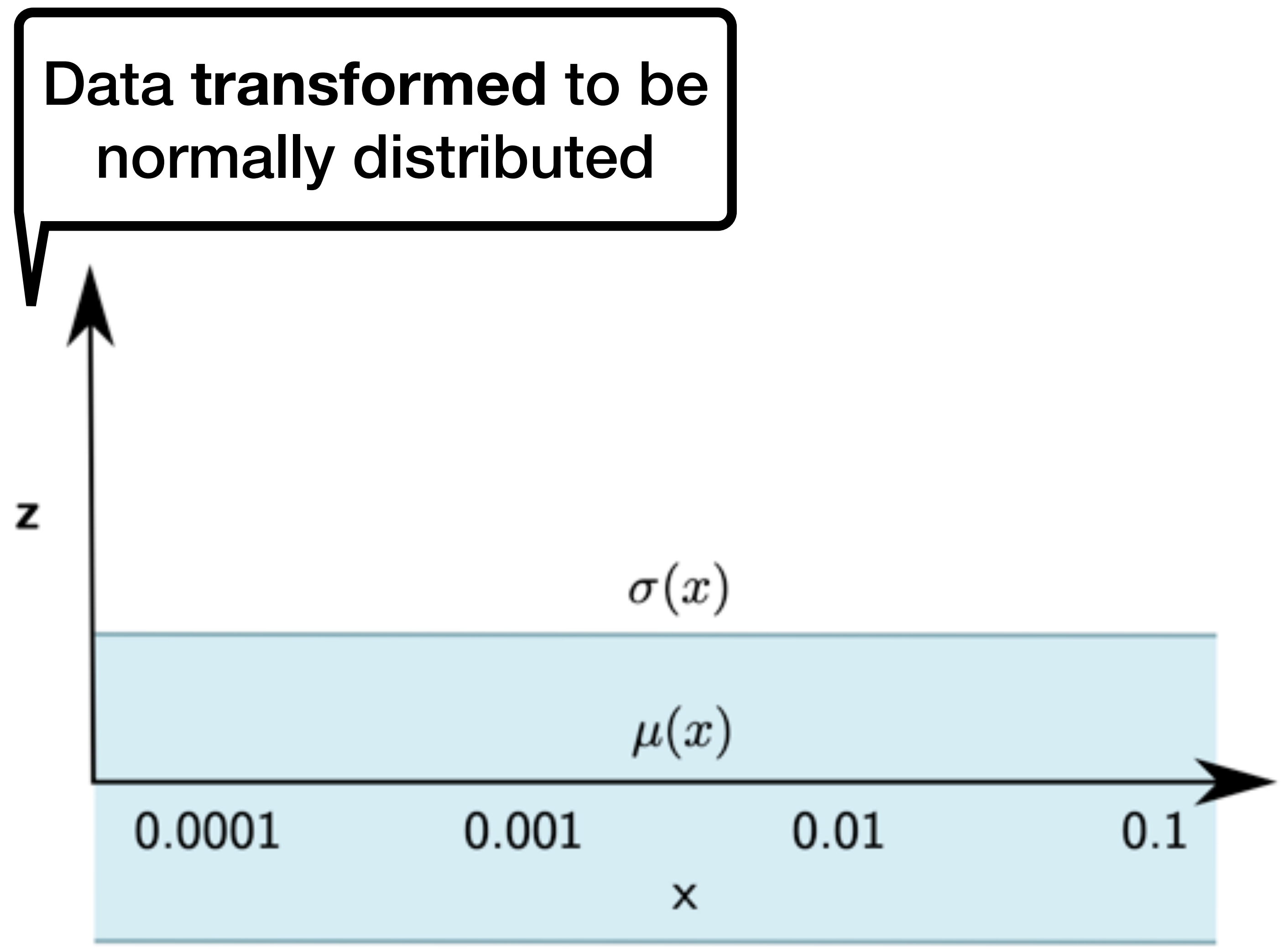


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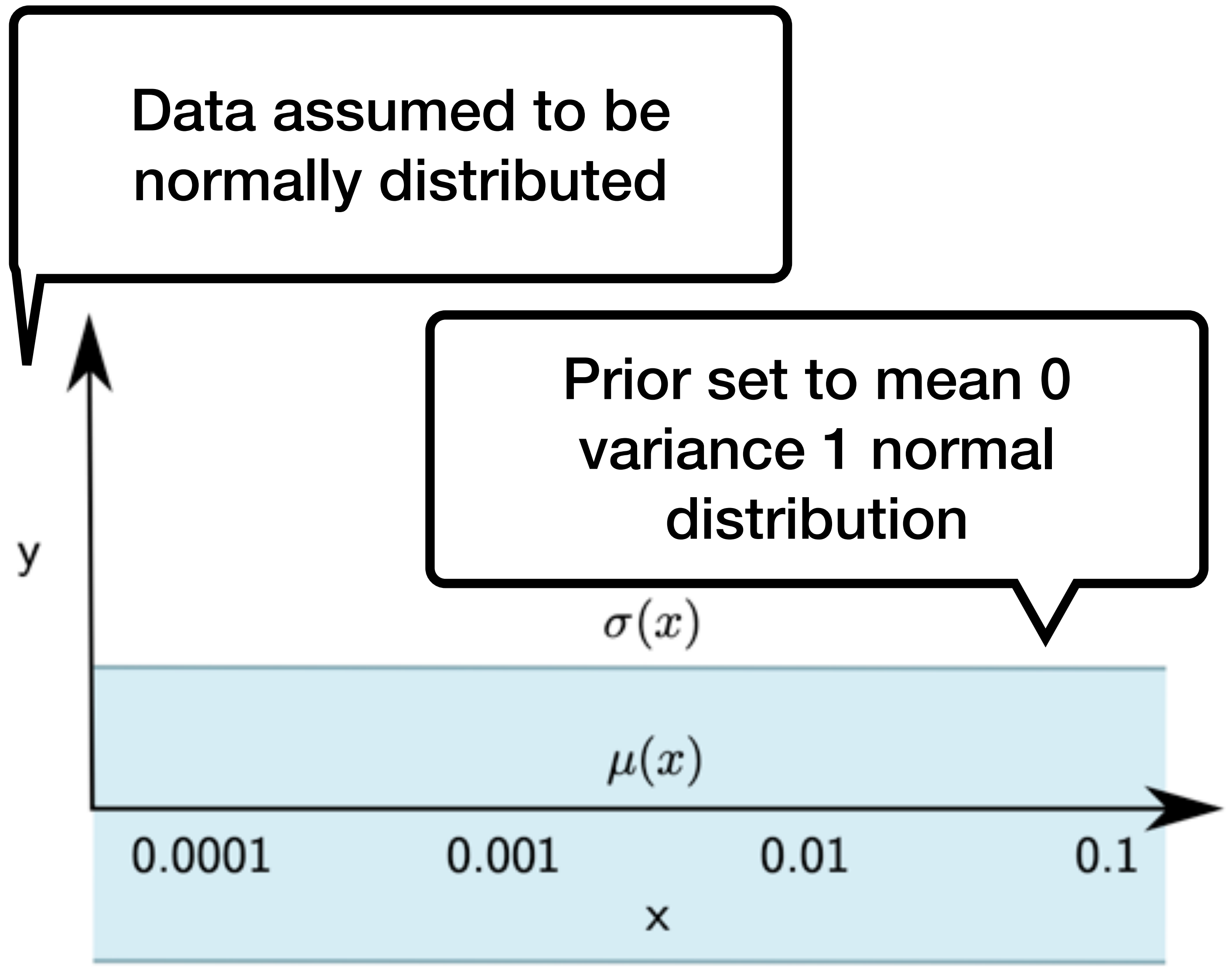


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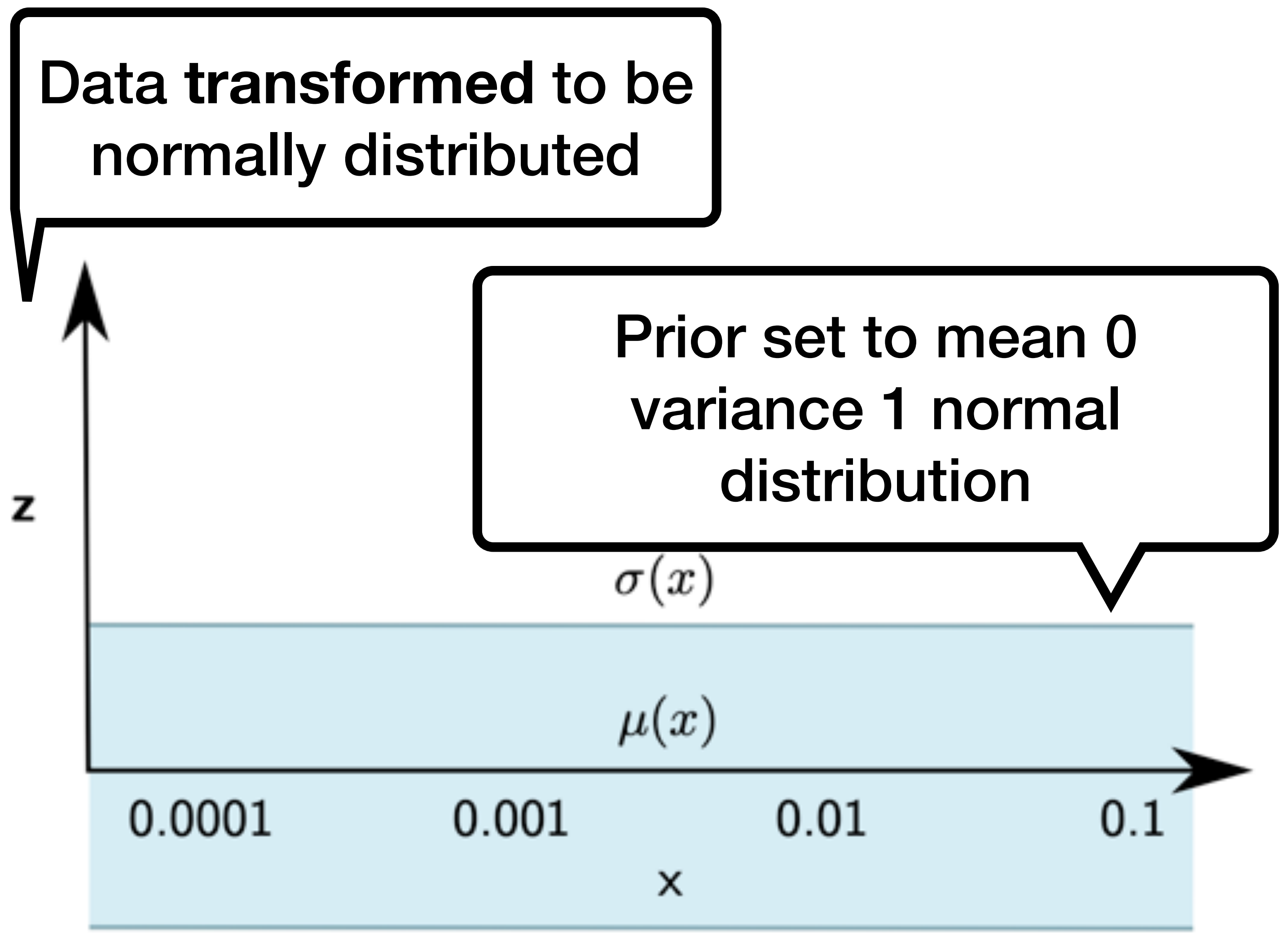


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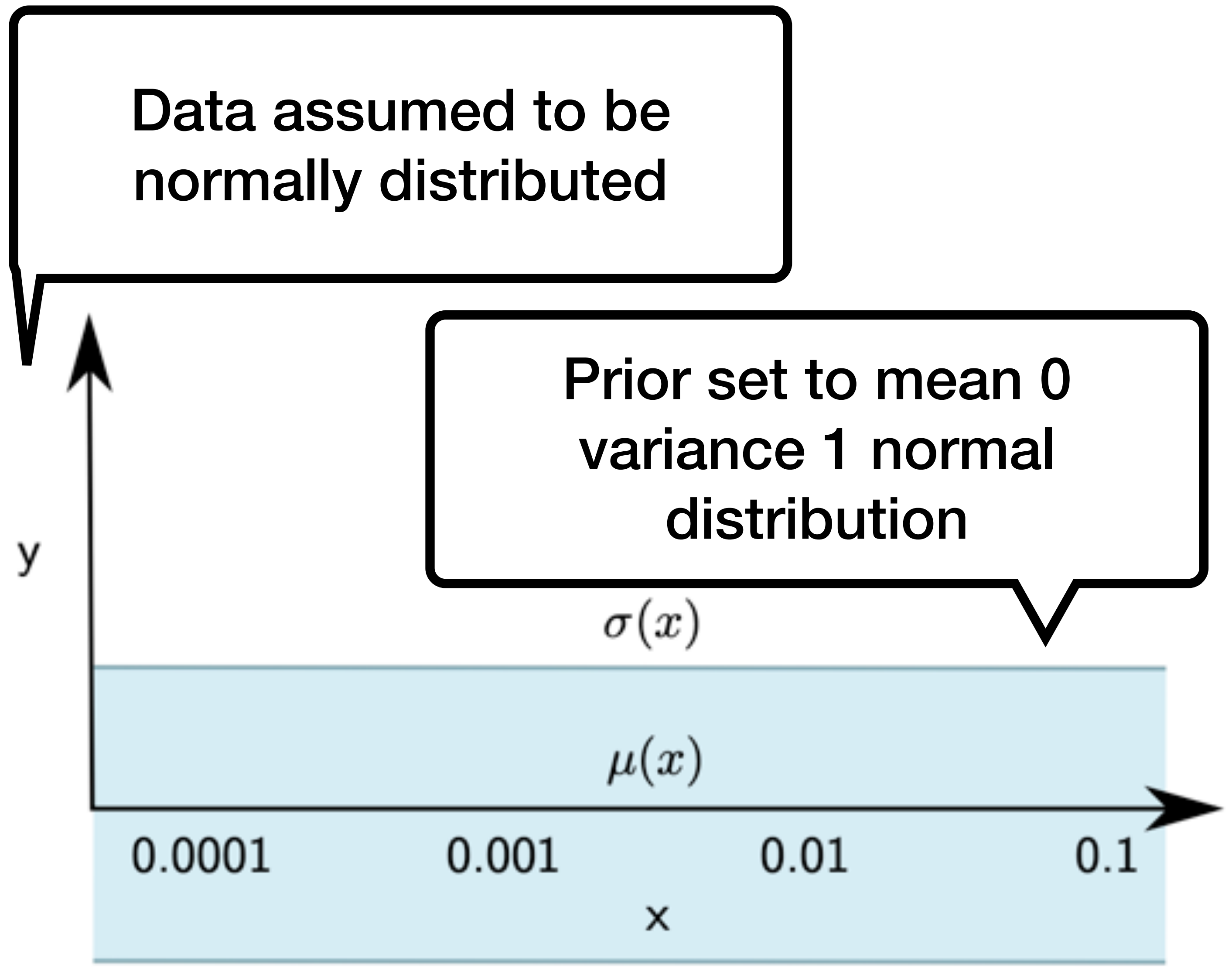


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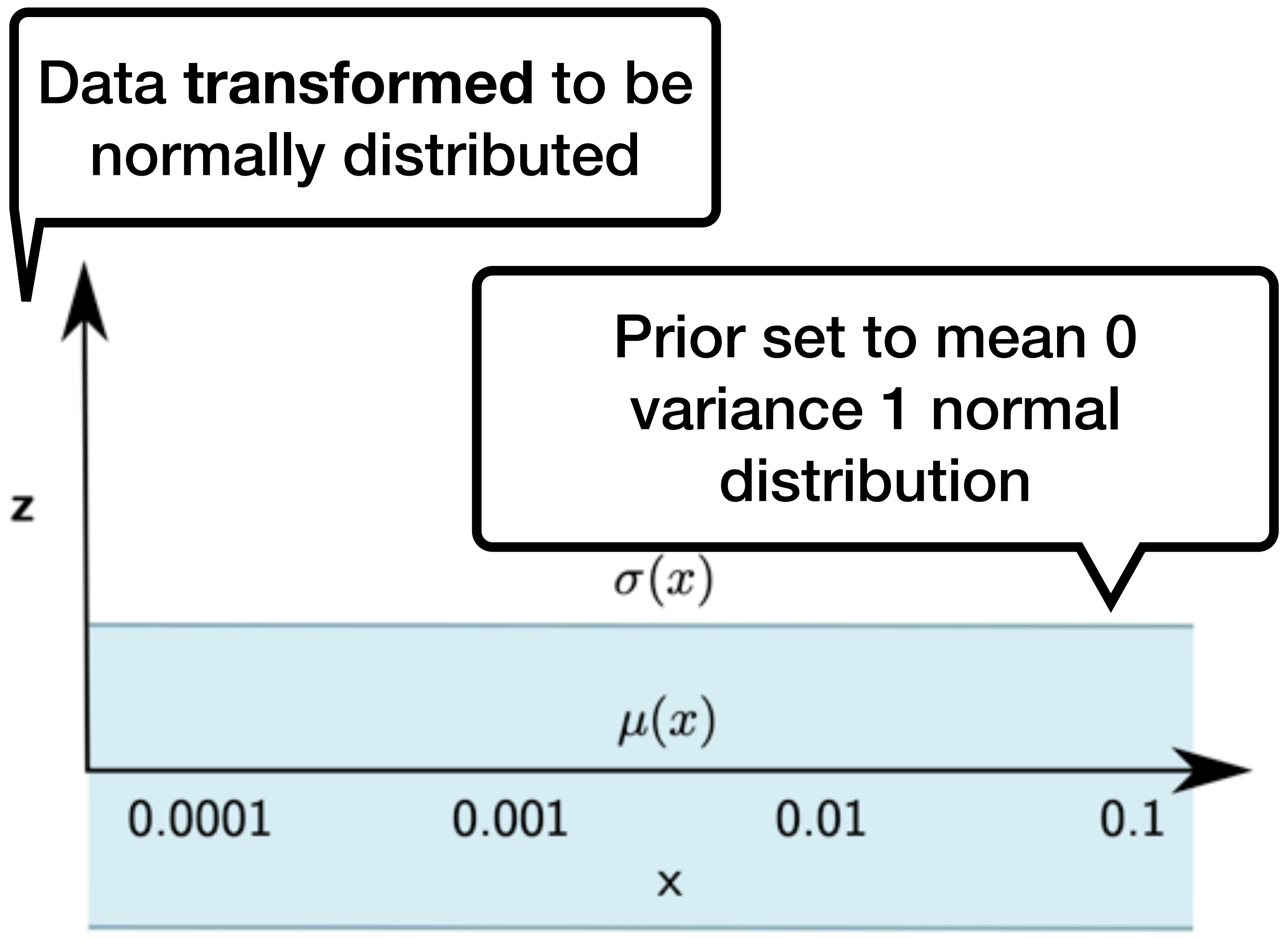


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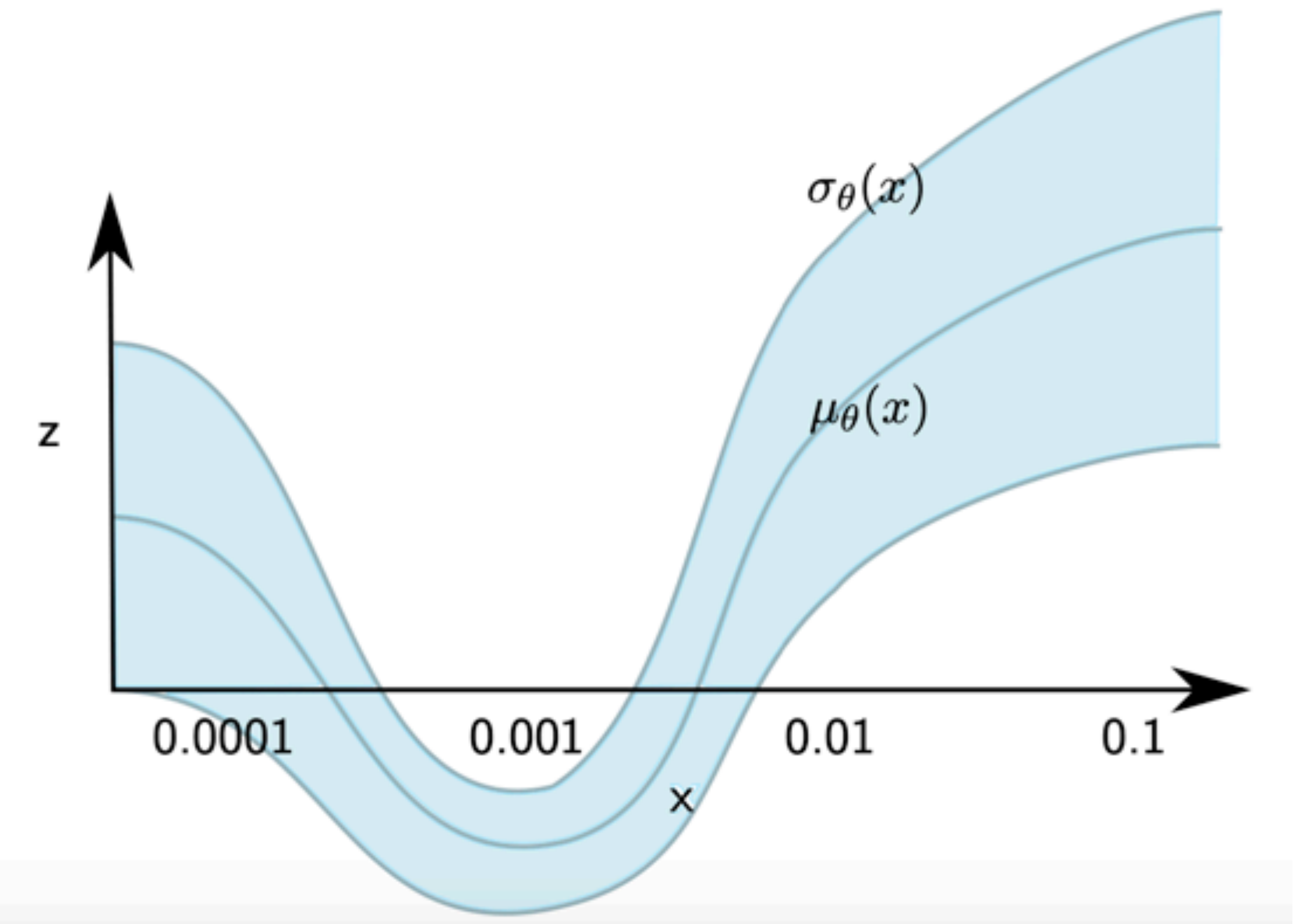


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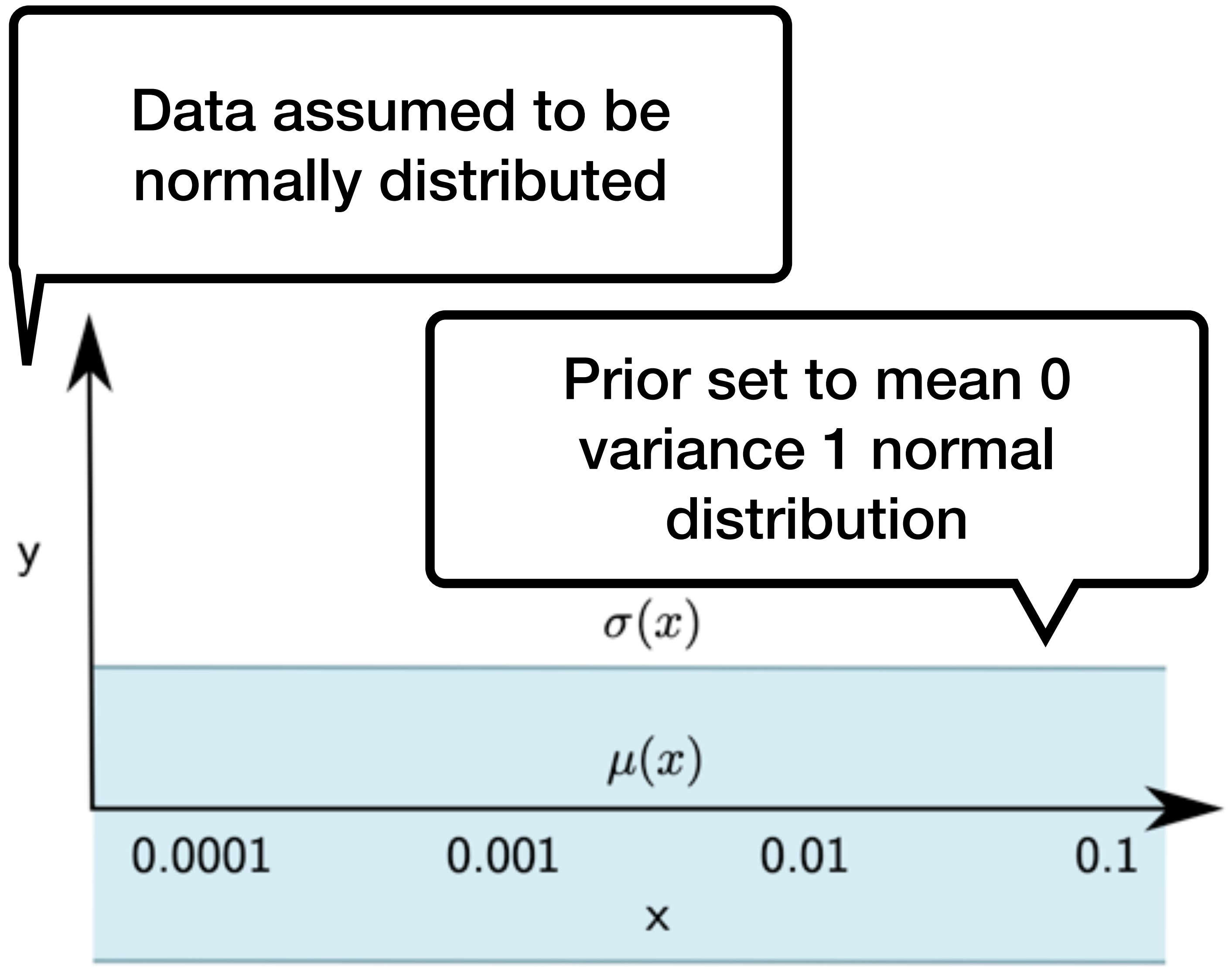


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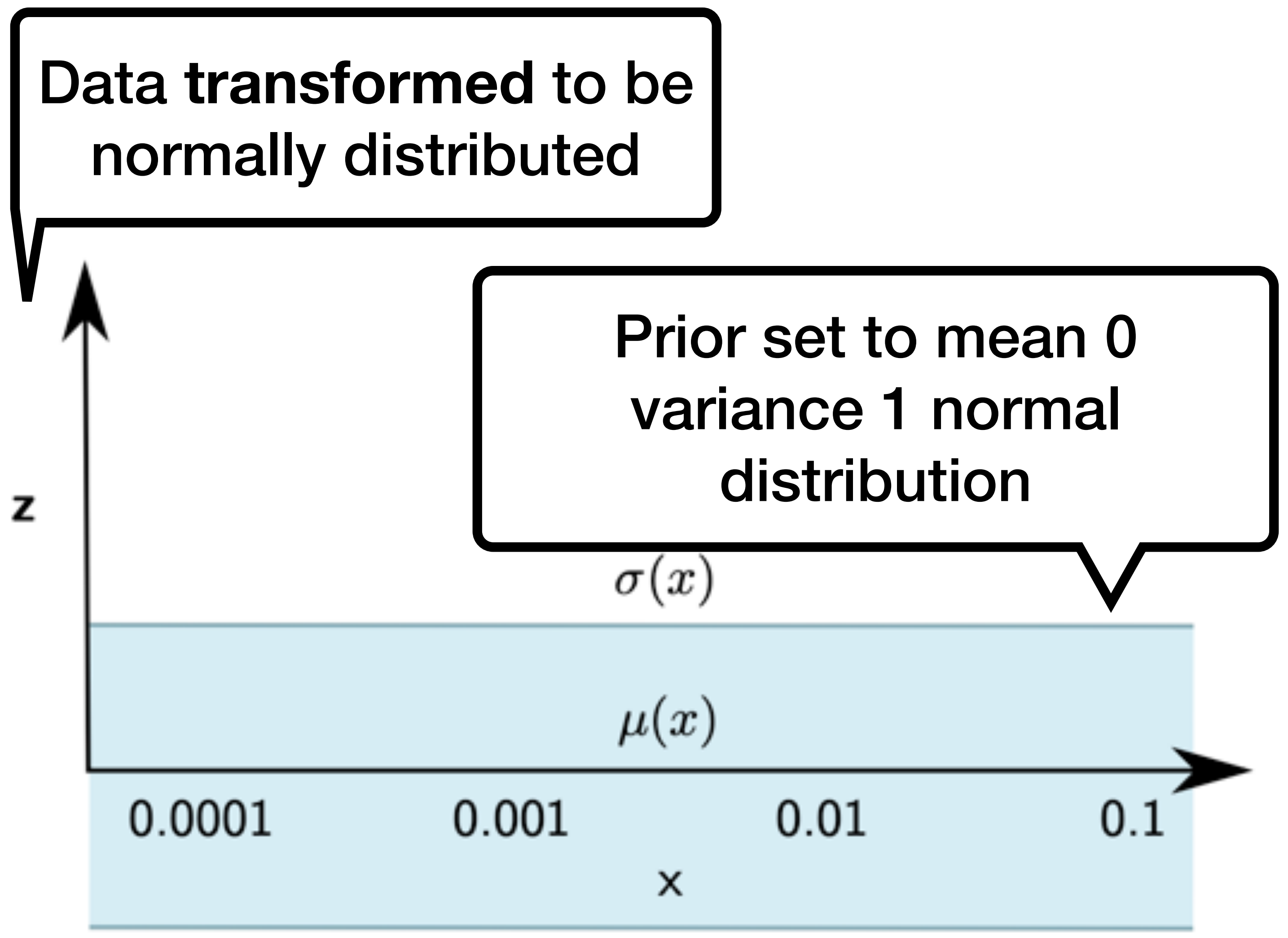


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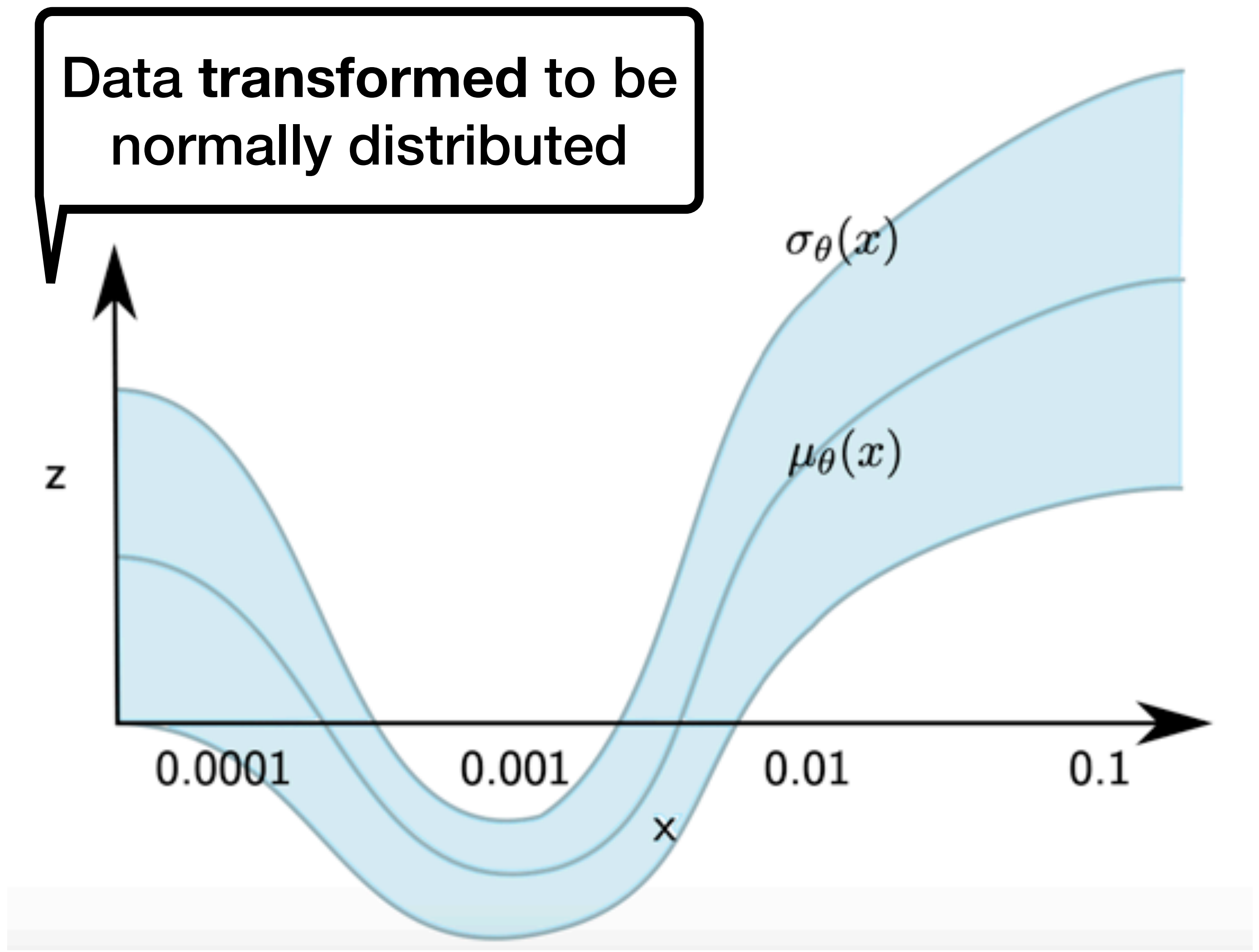


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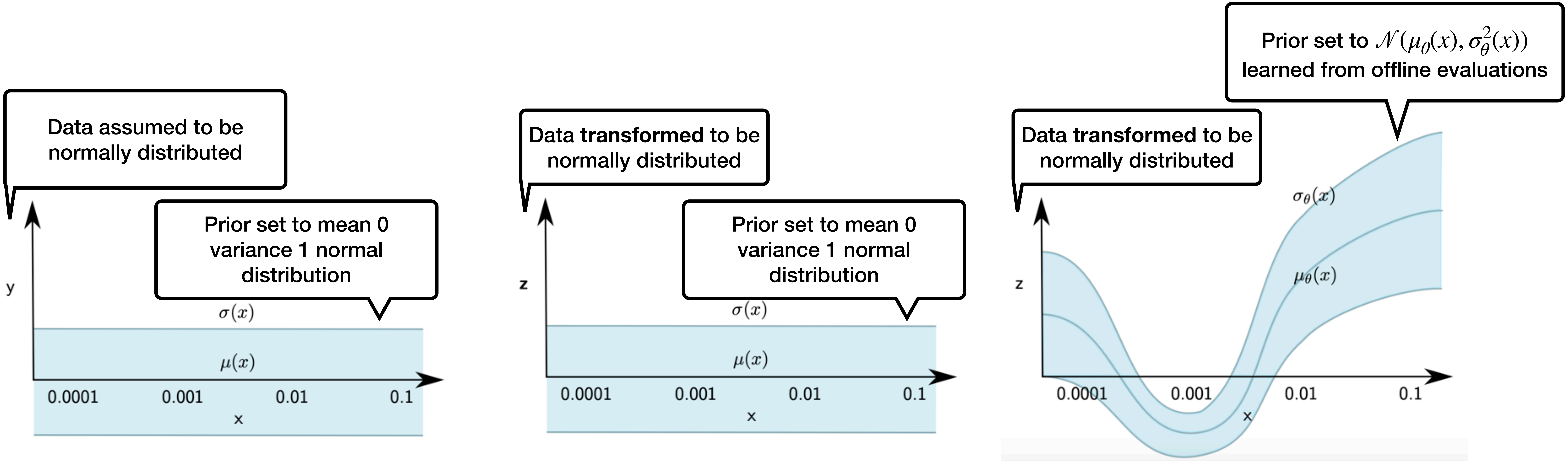


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| blackbox | # tasks | # hyperparameters | # evaluations/task | objective |
|---|---|---|---|---|
| DeepAR | 11 | 6 | $\sim$ 220 | quantile loss |
| FCNET | 4 | 9 | 62208 | MSE |
| XGBoost | 9 | 9 | 5000 | 1-AUC |
| NAS | 3 | 6 | 46875 | accuracy |

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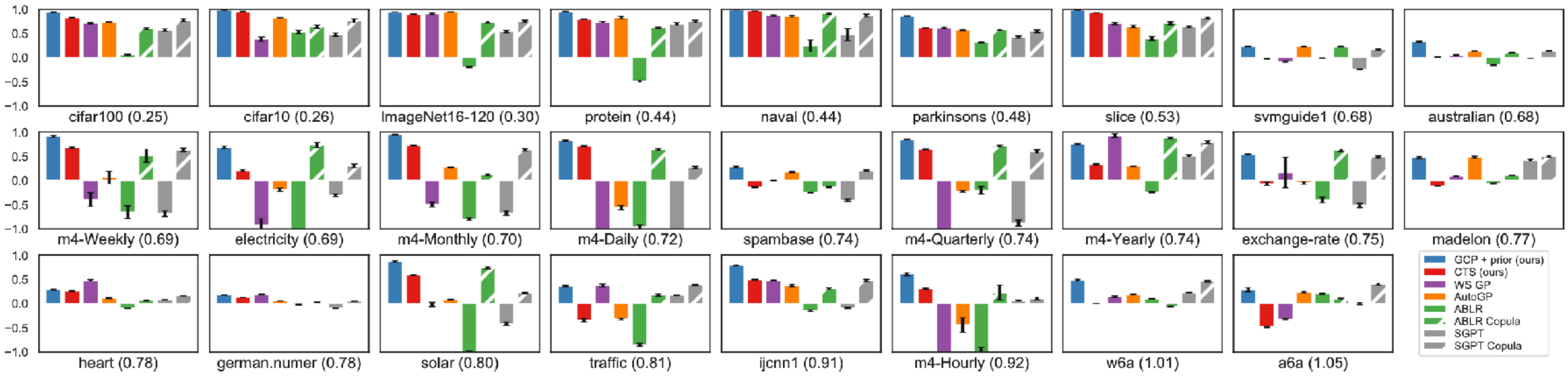


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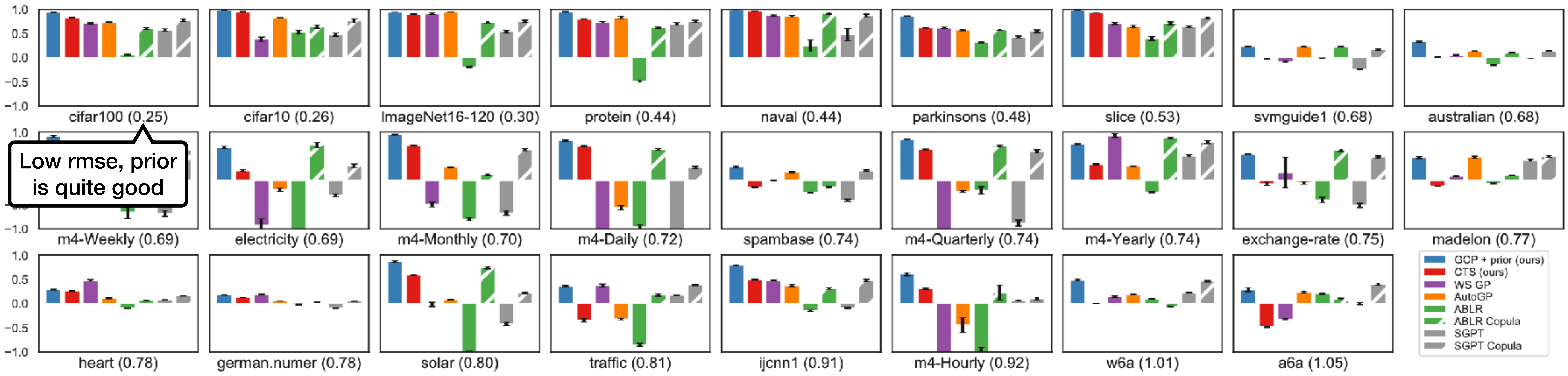


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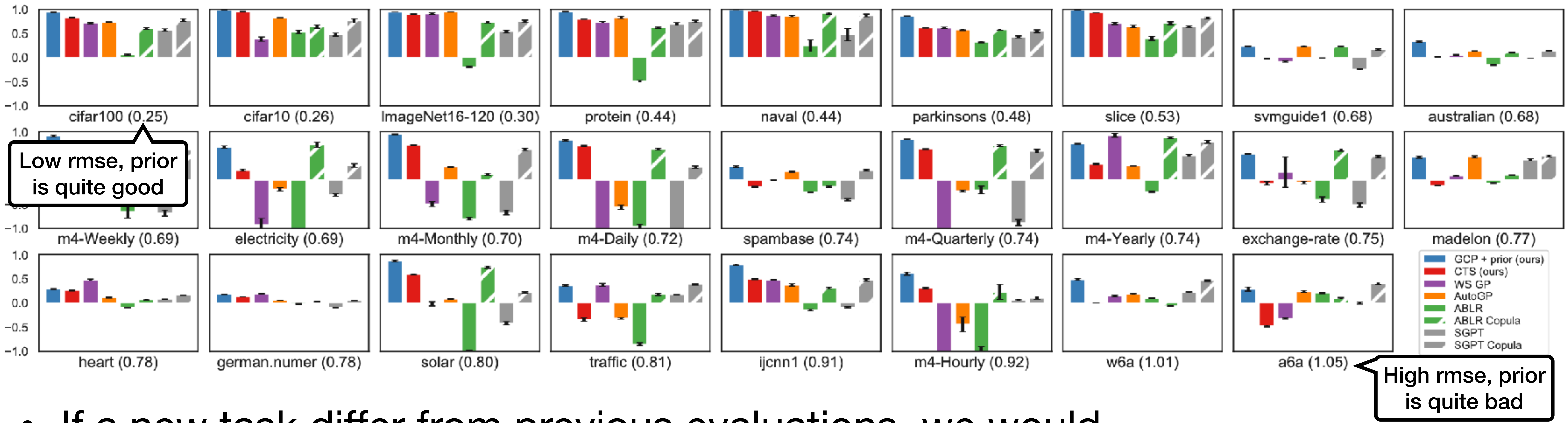


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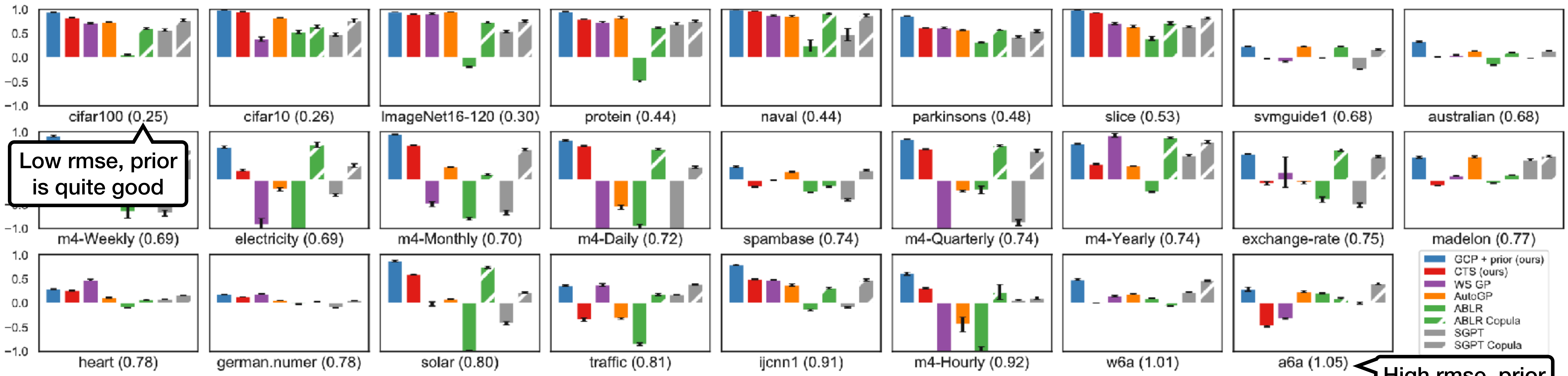


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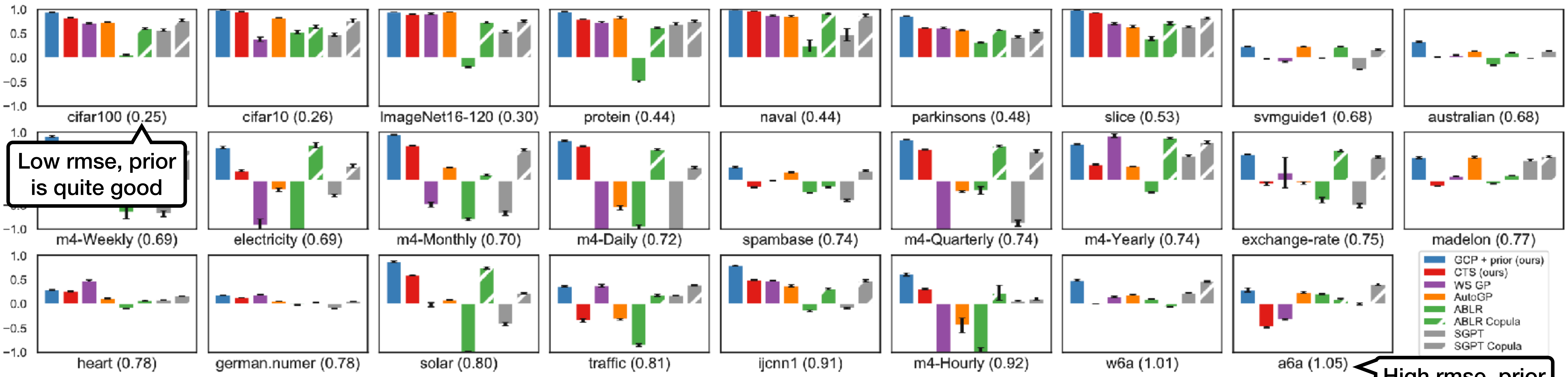


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… as opposed to CTS that just exploits prior from transfer learning

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🤔 **Could we avoid the need of offline evaluations, perhaps the user knows some good prior distribution?**

# Theoretical analysis

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**On the Optimality Gap of Warm-Started Hyperparameter Optimization**

**Parikshit Ram**[1]

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**Abstract** We study the general framework of warm-started hyperparameter optimization (HPO) where we have some source datasets (tasks) on which we have already performed HPO, and we wish to leverage the results of these HPO to warm-start the HPO on an unseen target dataset and perform few-shot HPO. Various meta-learning schemes have been proposed over the last decade (and more) for this problem. In this paper, we theoretically analyse the optimality gap of the hyperparameter obtained via such warm-started few-shot HPO, and provide novel results for multiple existing meta-learning schemes. We show how these results allow us identify situations where certain schemes have advantage over others.

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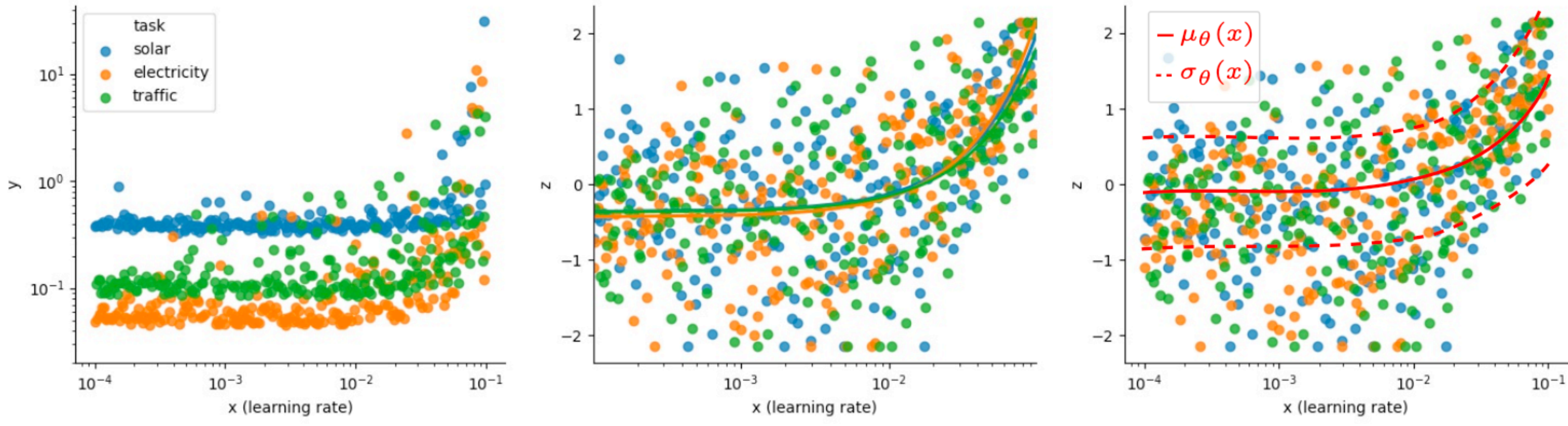


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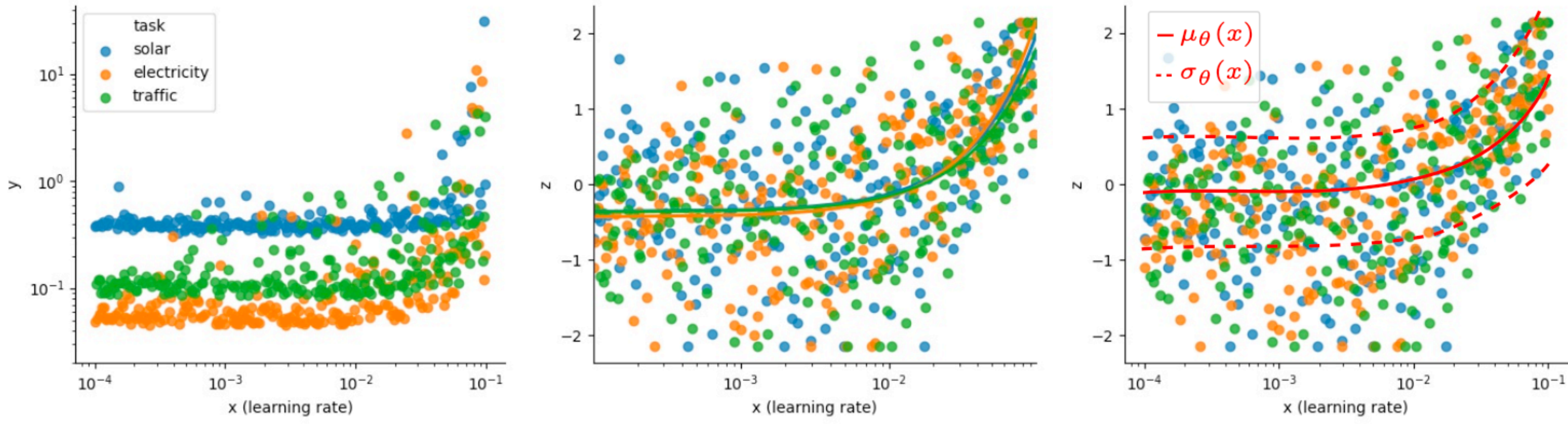


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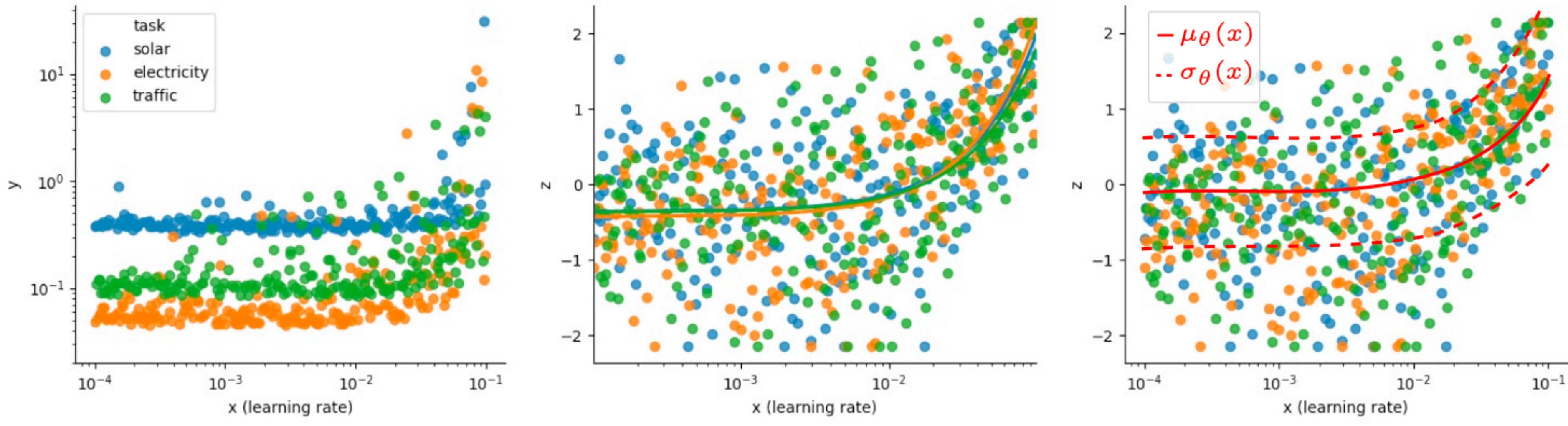


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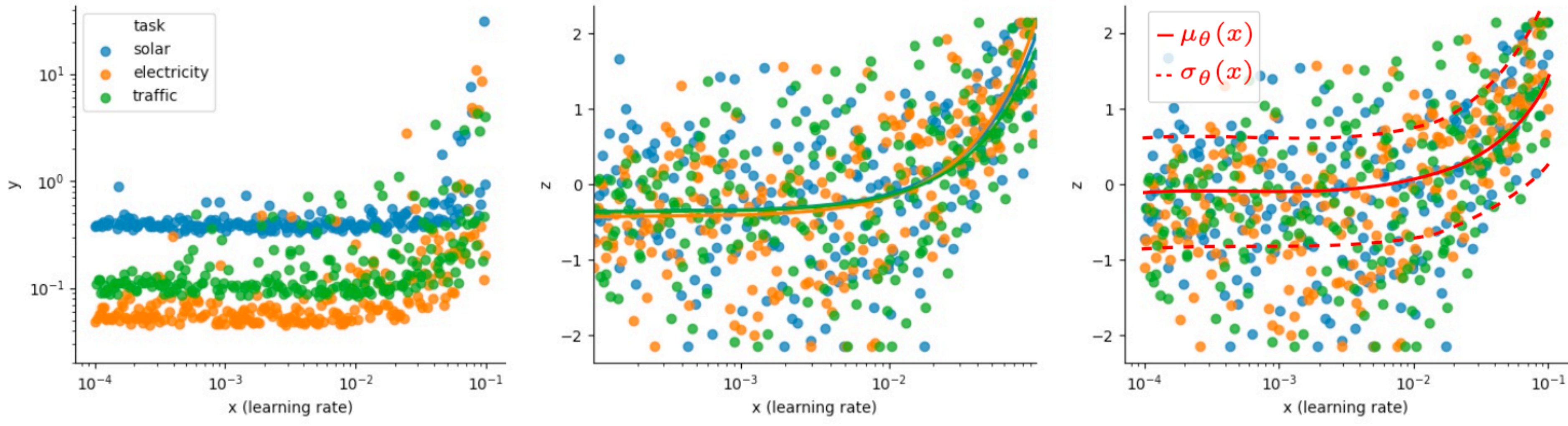


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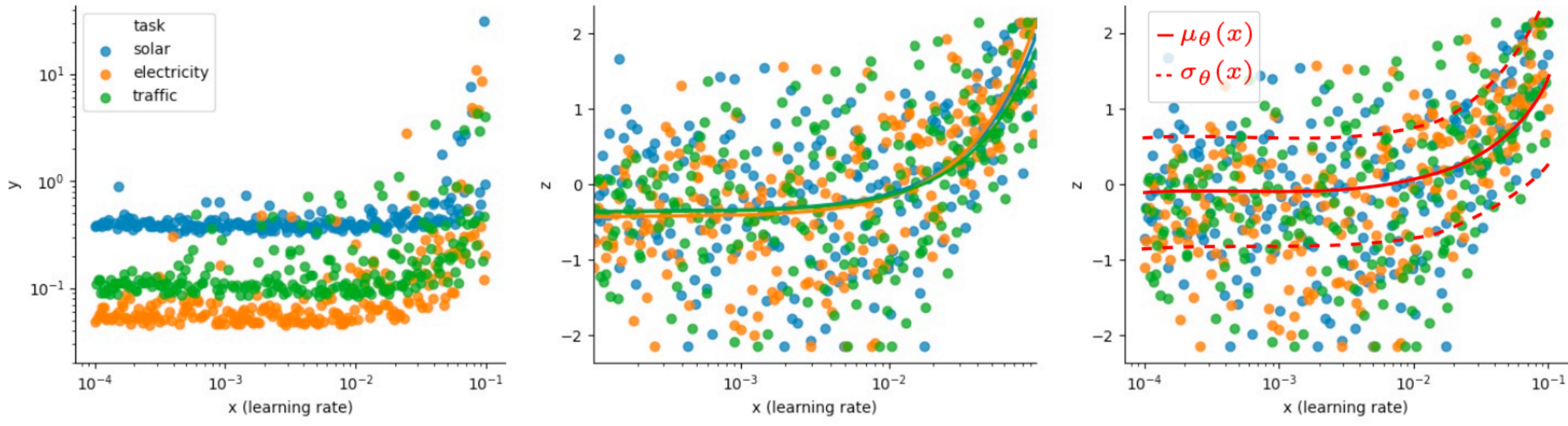


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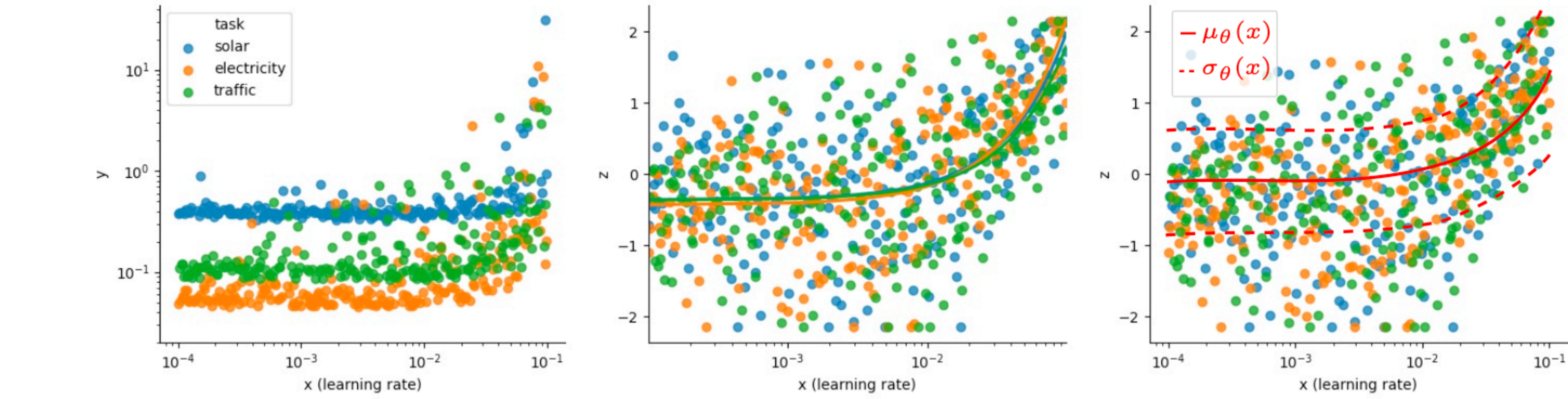


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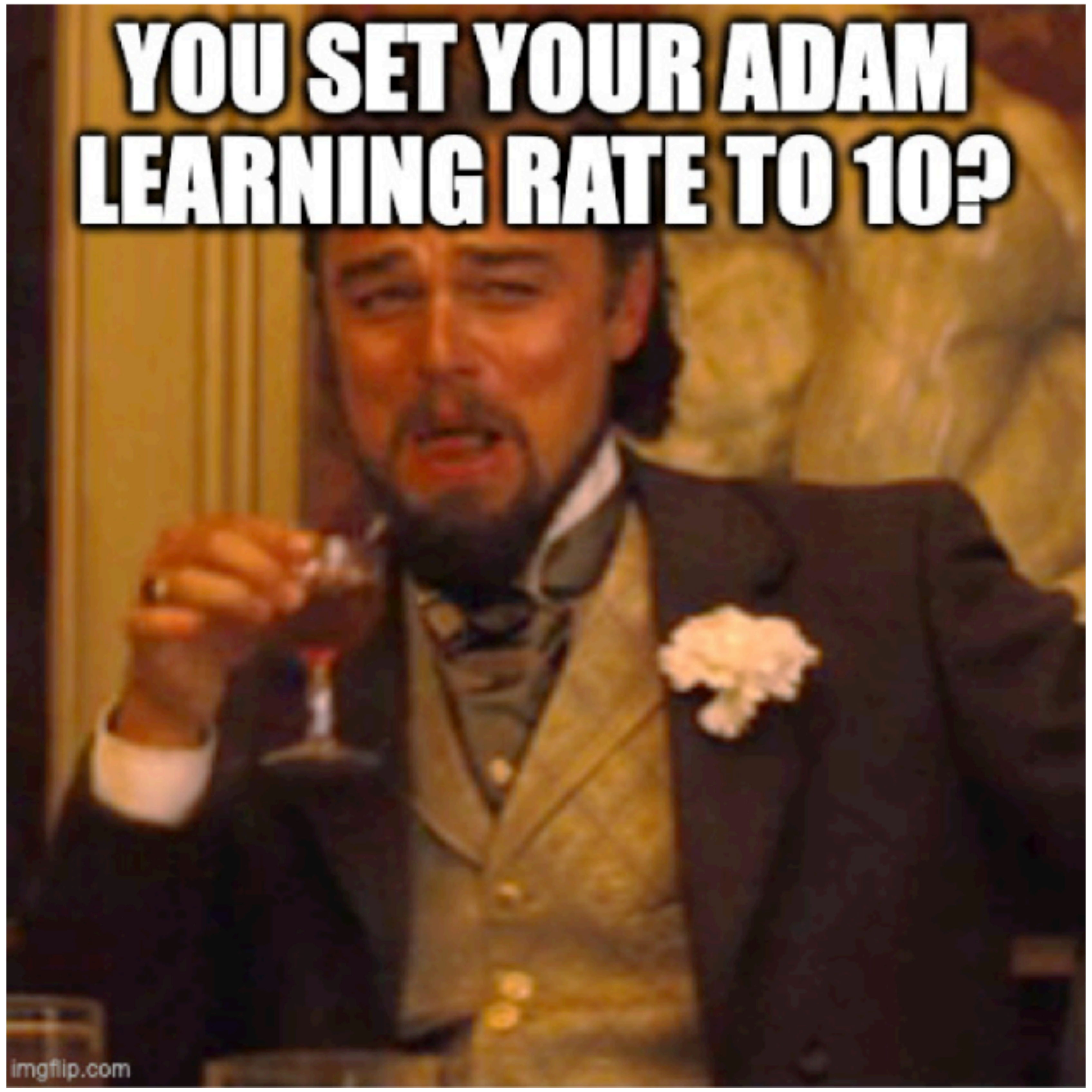

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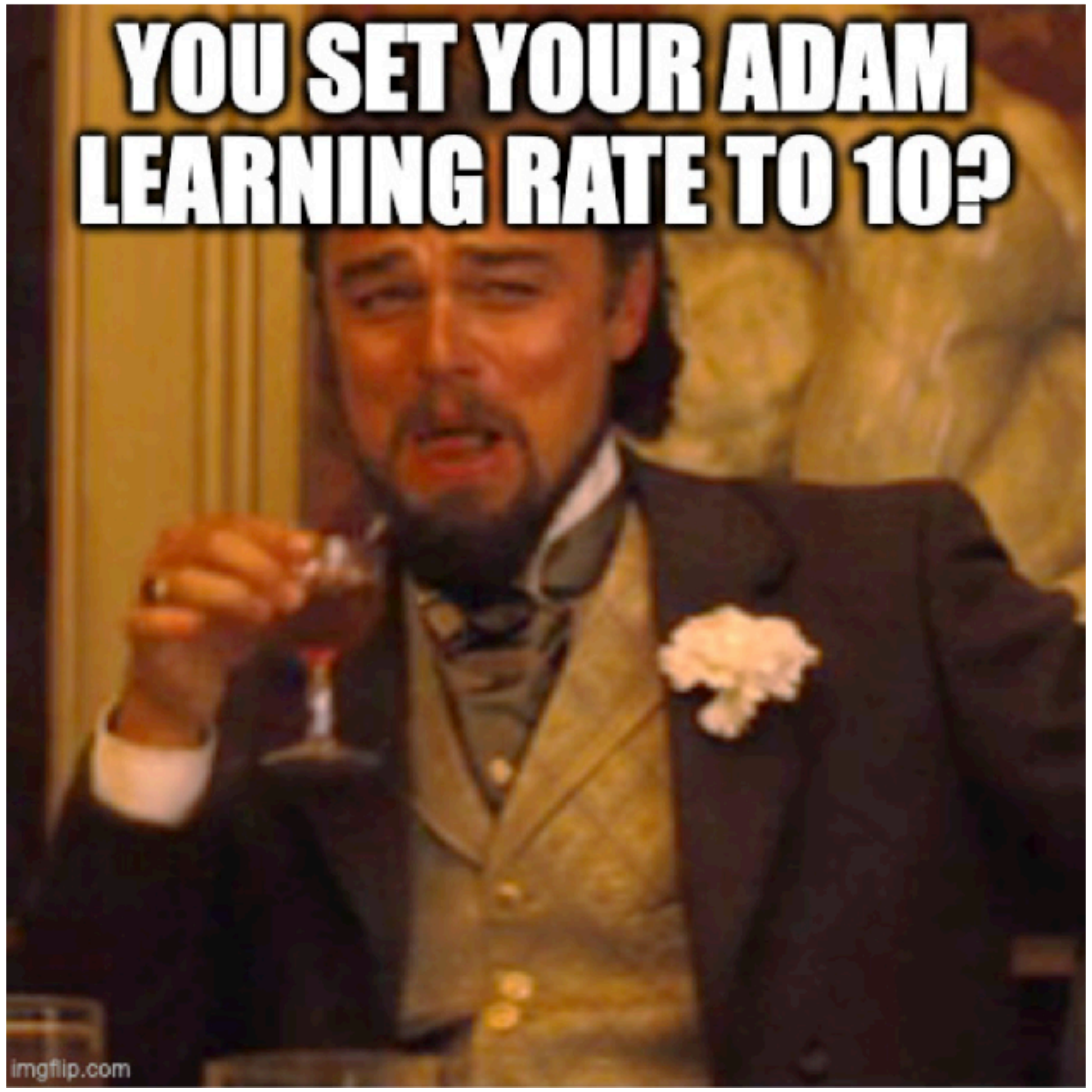

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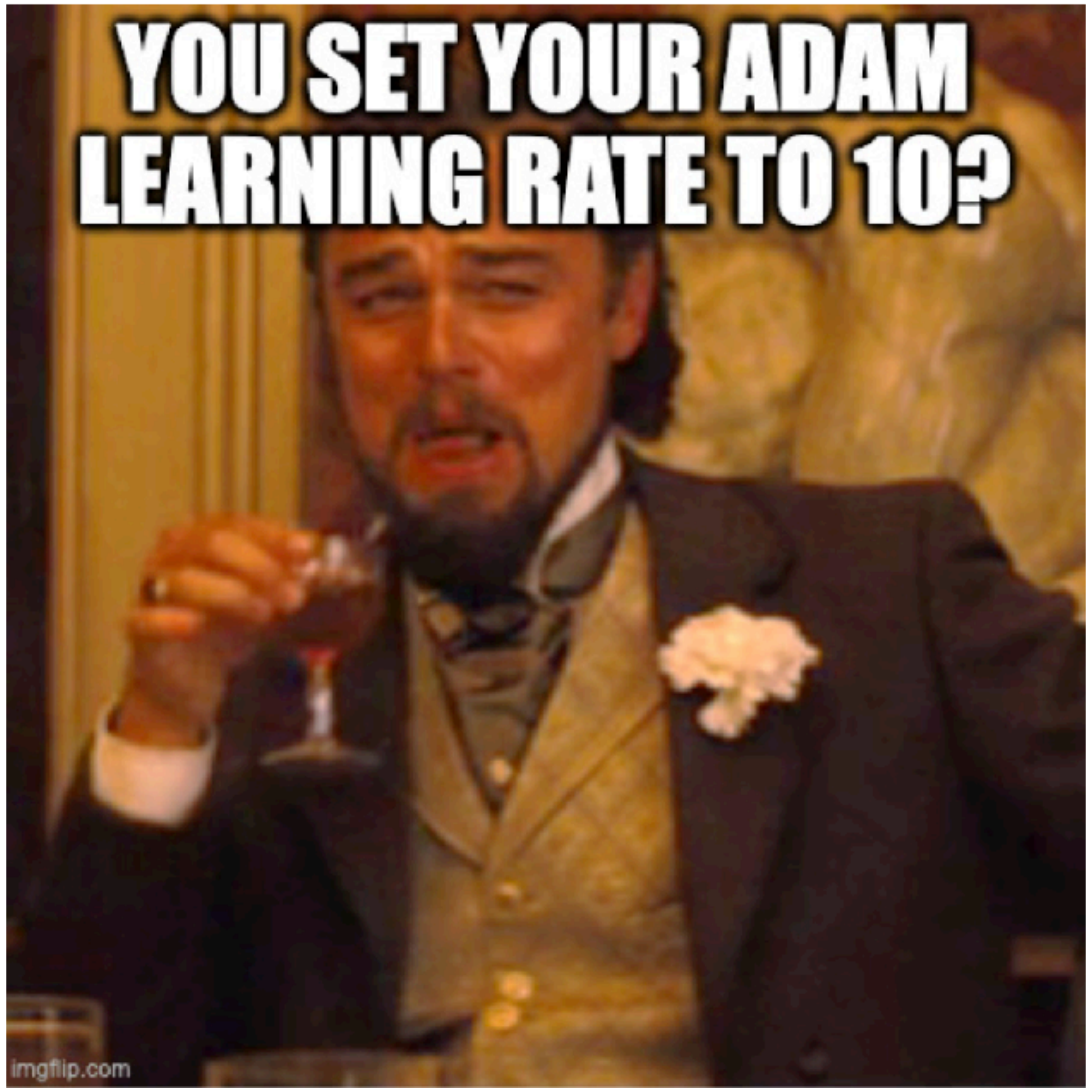

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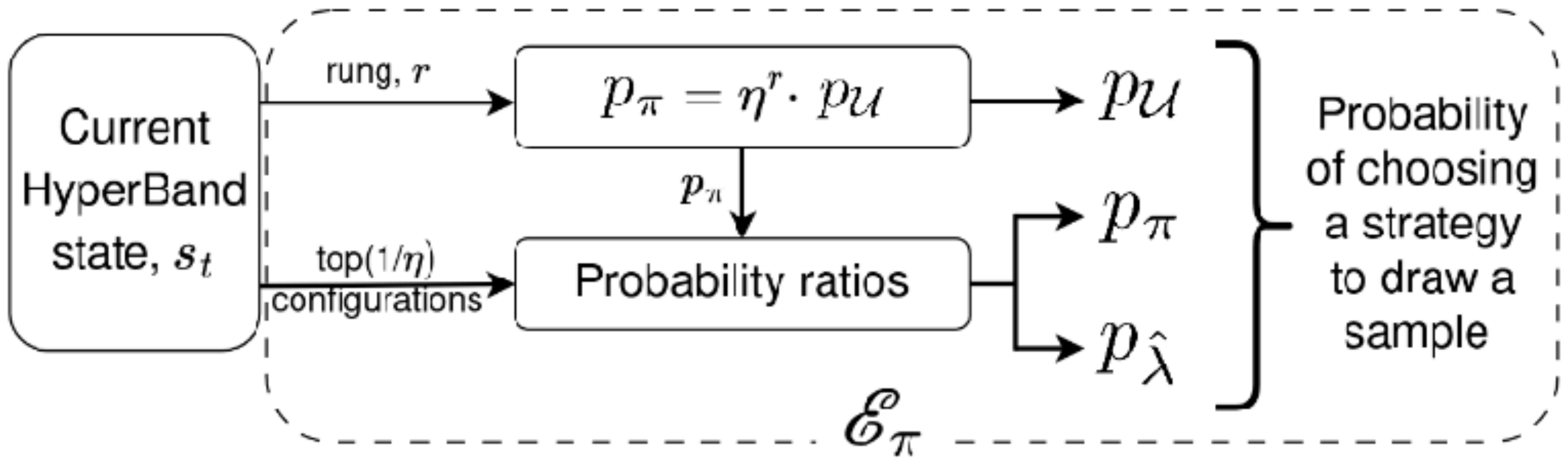


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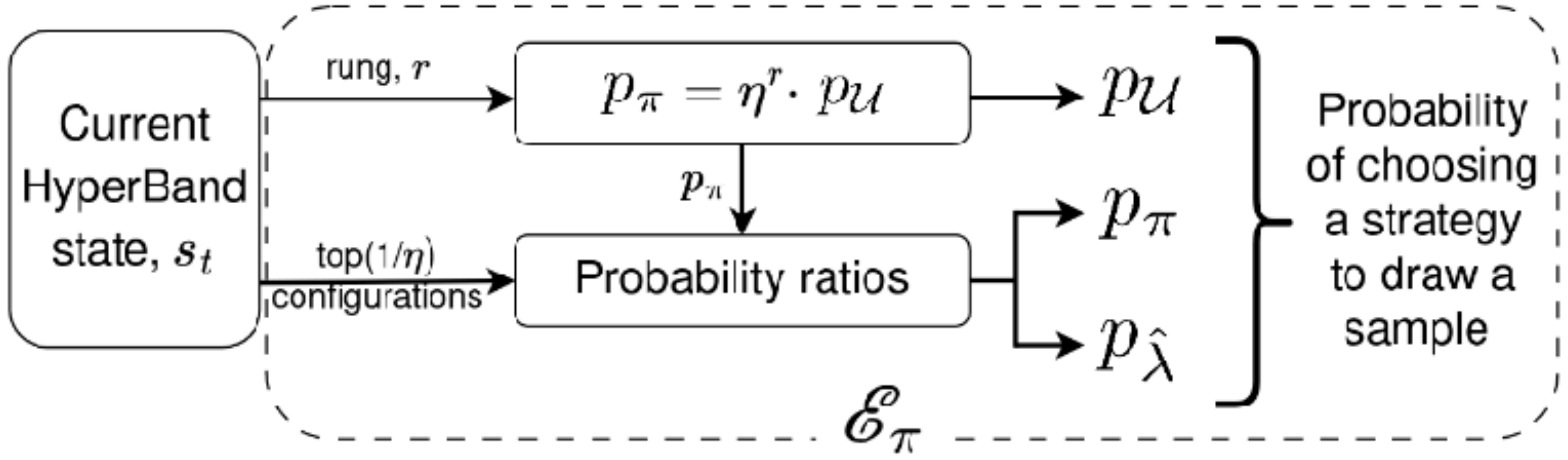


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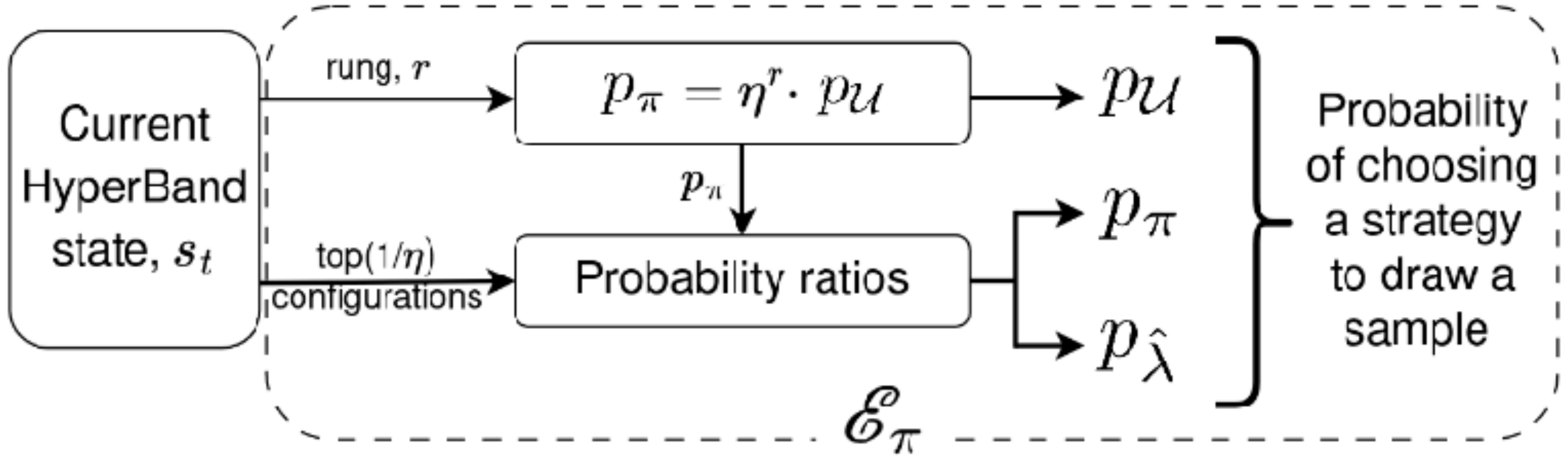


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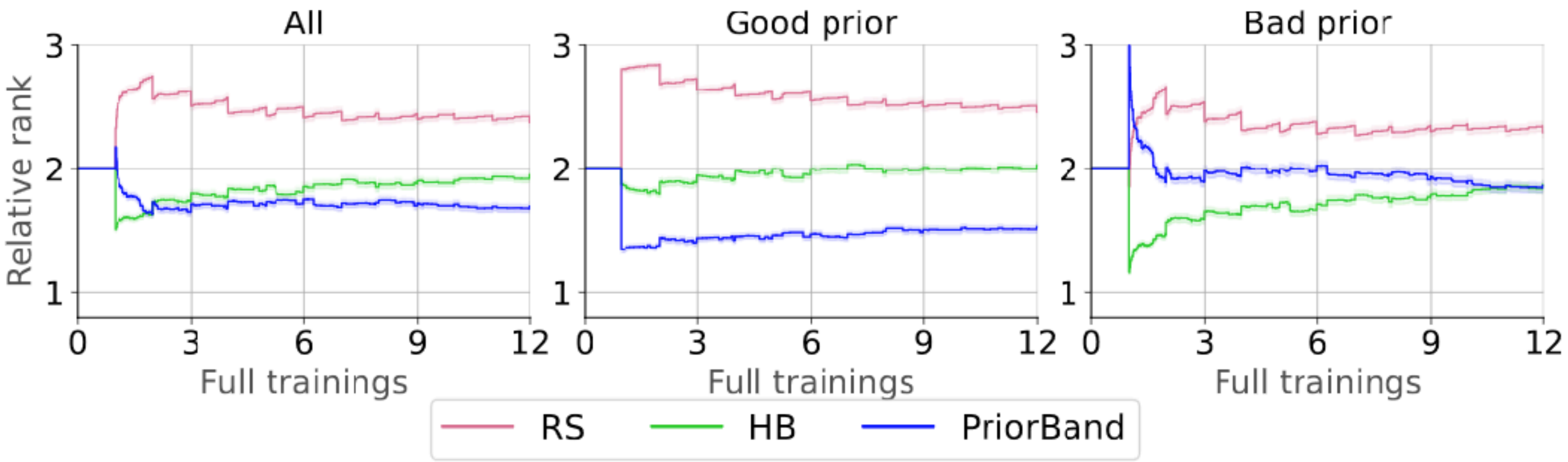


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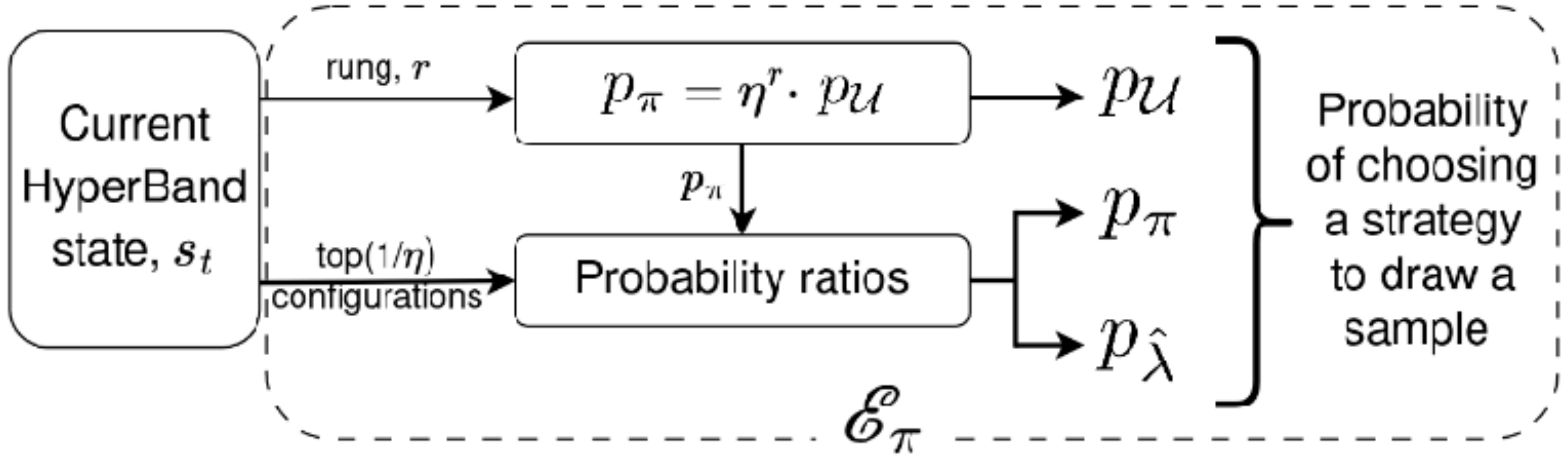


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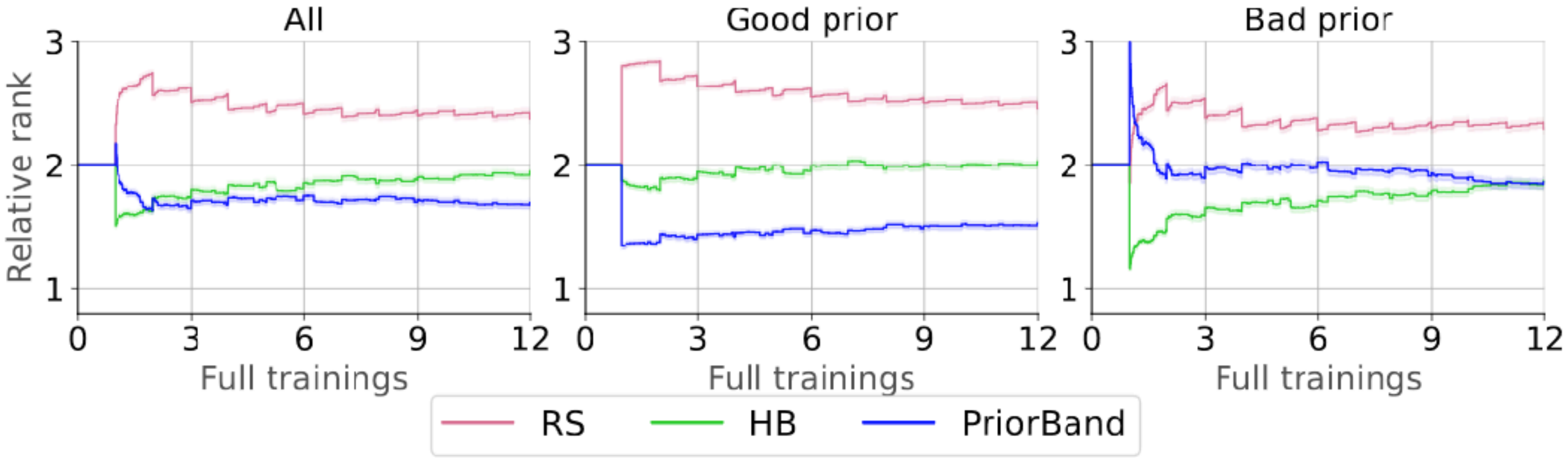


🥳 Learning which strategy is better allows failure in cases when user priors are bad

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# Methods

## Optformer

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Table 1: Example of a study $(m, \boldsymbol{h})$ with two parameters and two trials. Metadata $m$ appears in blue and history $\boldsymbol{h}$ in purple.


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"goal": "MAXIMIZE",
"algorithm": "random_search",
"parameter": {
"name":  "opt_kw.lr",
"type":  "DOUBLE",
"min_value":  1e-6,
"max_value":  1e-2,
"scale_type":  "LOG"
}
"parameter": {
"name":  "opt_type",
"type":  "CATEGORICAL",
"categories":  ["SGD", "Adam"],
}
"trial" {
"parameter":  {
"opt_kw.lr":  0.0021237573,
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"accuracy":  0.69482429,
}}
"trial" {
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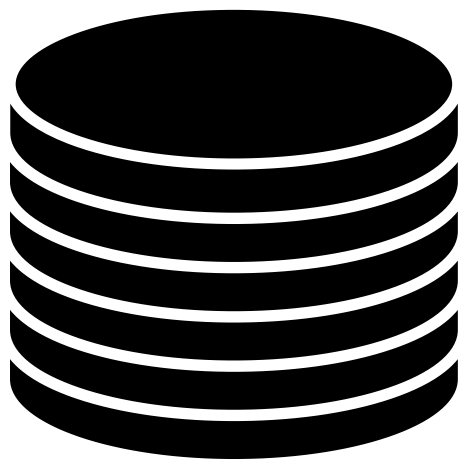

**Database of HPO runs containing**

- Metadata of problem studied (Convolution? Tabular?)
- Search space considered
- HPO method used
- List of hyperparameters evaluated and blackbox accuracy

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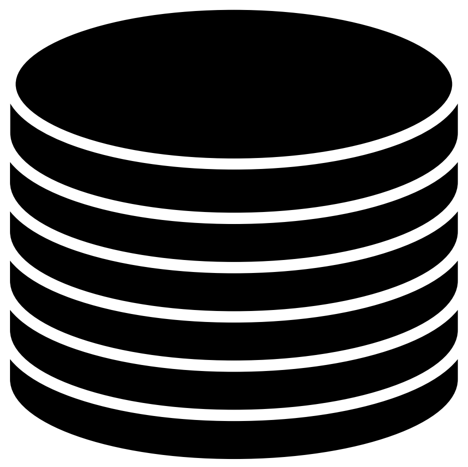

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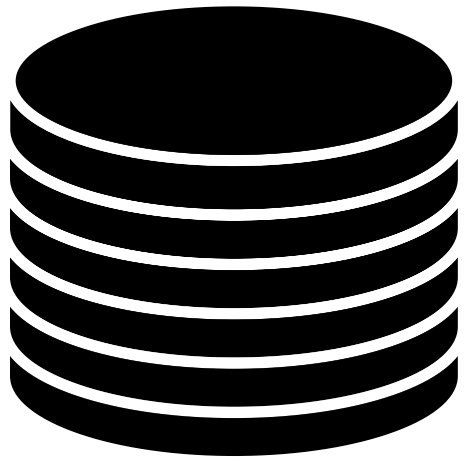

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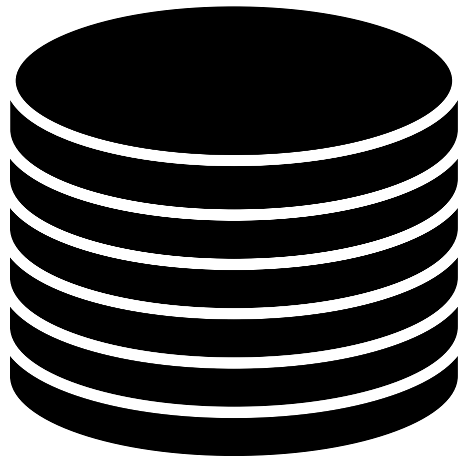

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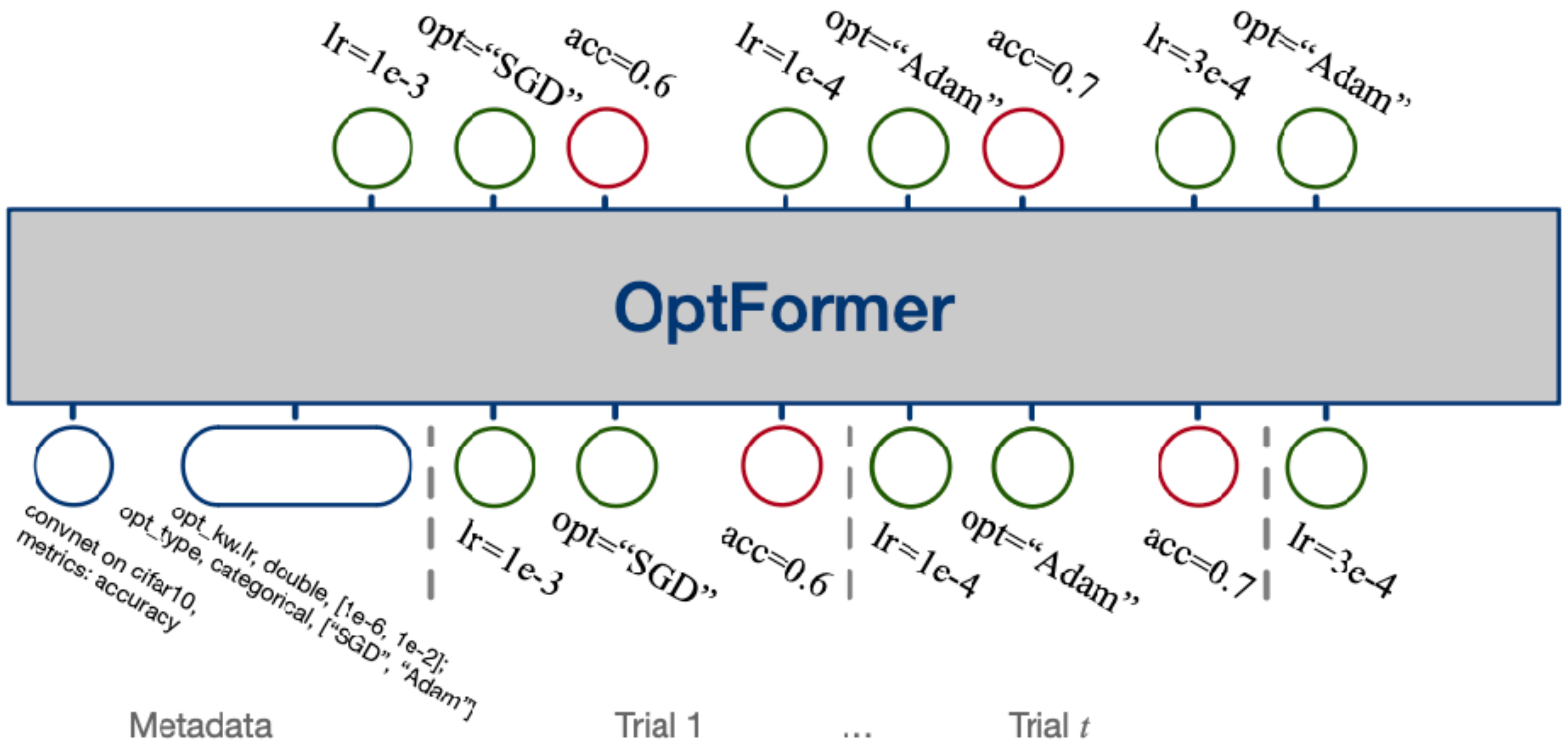


Figure 1: Illustration of the OptFormer model over a hyperparameter optimization trajectory. It is trained to predict both hyperparameter suggestions (in green) and response function values (in red).

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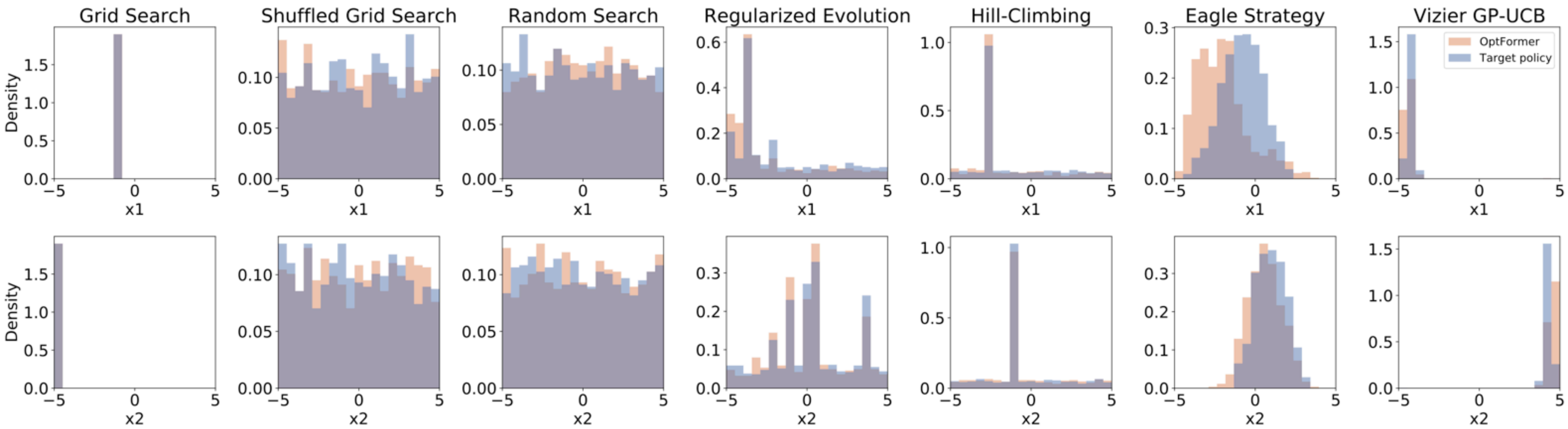

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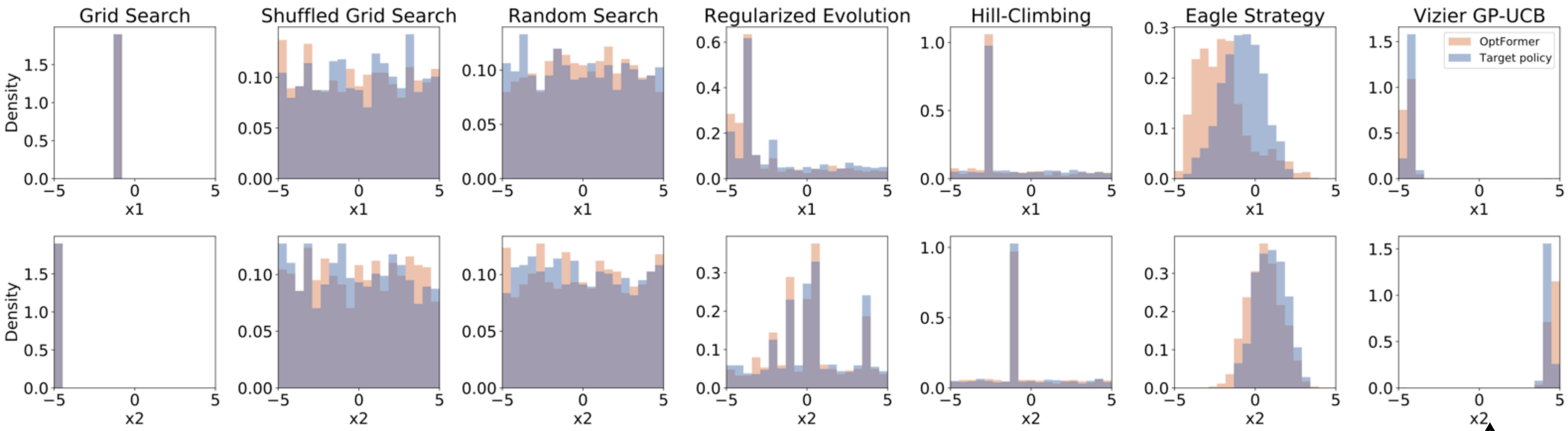


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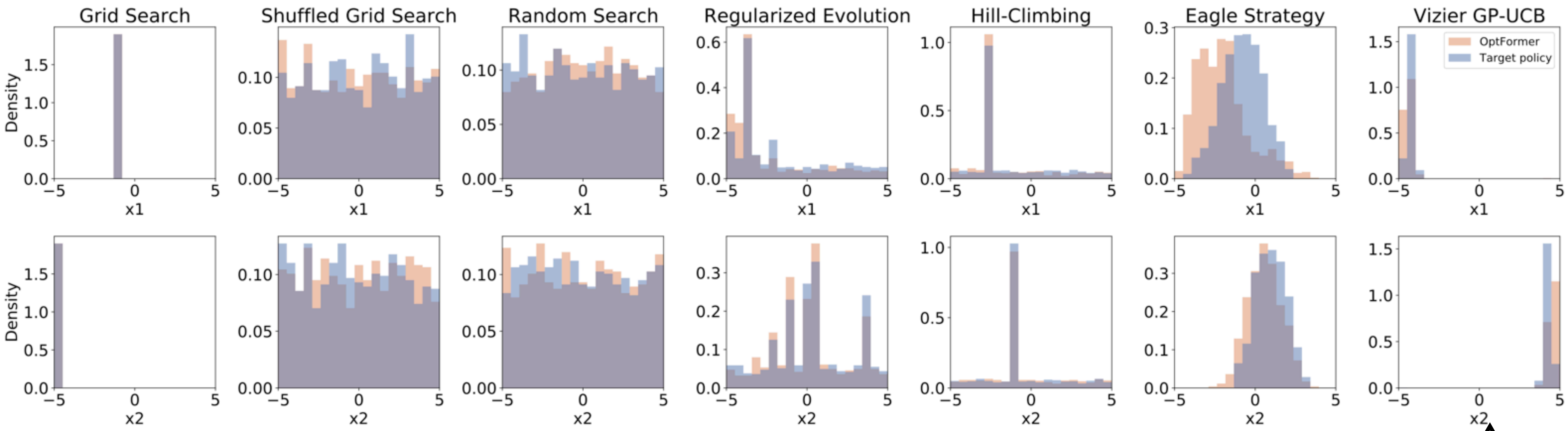


🤔 This is an impressive result! some methods are complex, for instance GP requires $\mathcal{O}(n^3)$ operations to select the next candidate given $n$ previous observations

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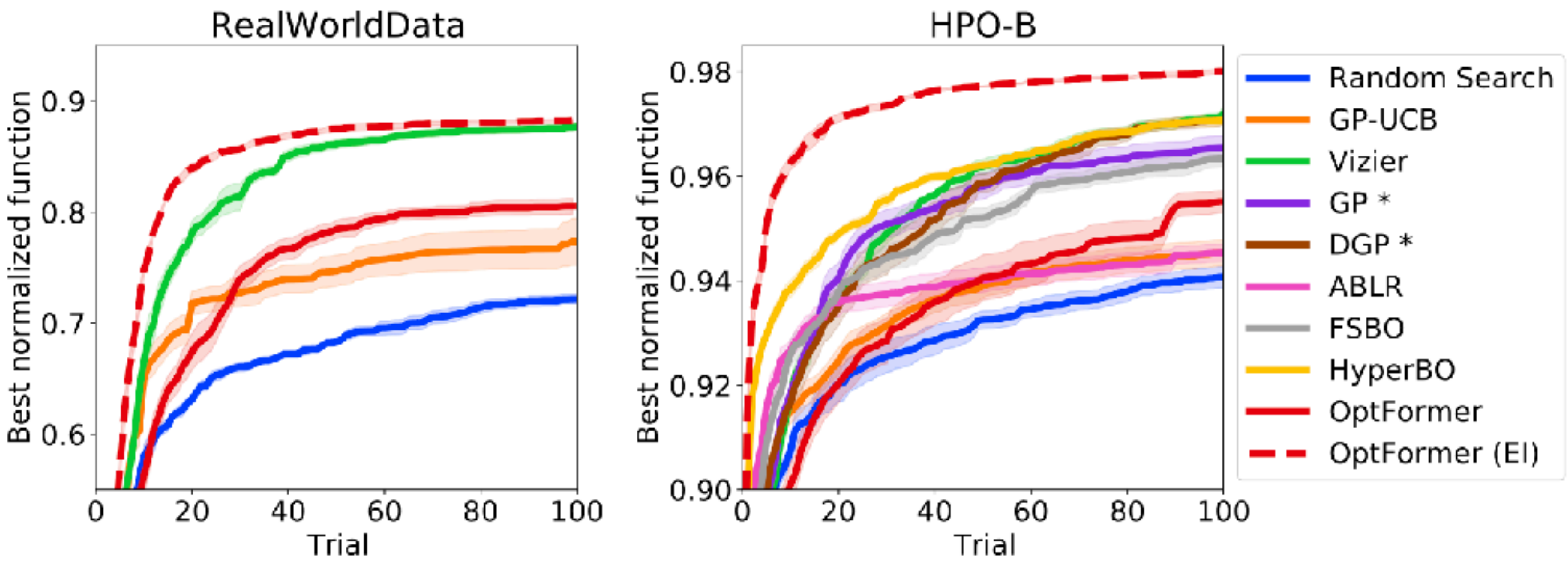


Figure 4: Higher is better. Best normalized function value averaged over 16 RealWorldData test functions (left) and over 86 HPO-B test functions (right) with 1-std confidence interval from 5 runs. GP* and DGP* results are provided by [5]. The transfer learning methods ABLR, FSBO and HyperBO cannot be applied to RealWorldData.

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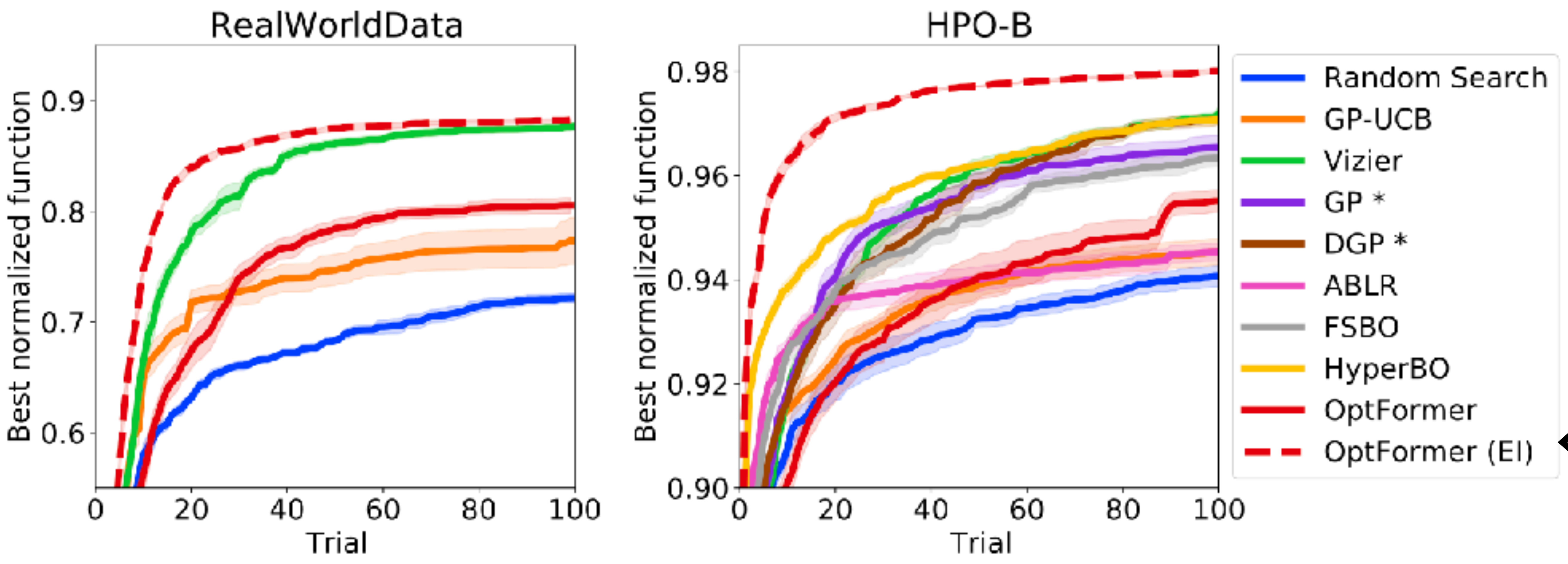


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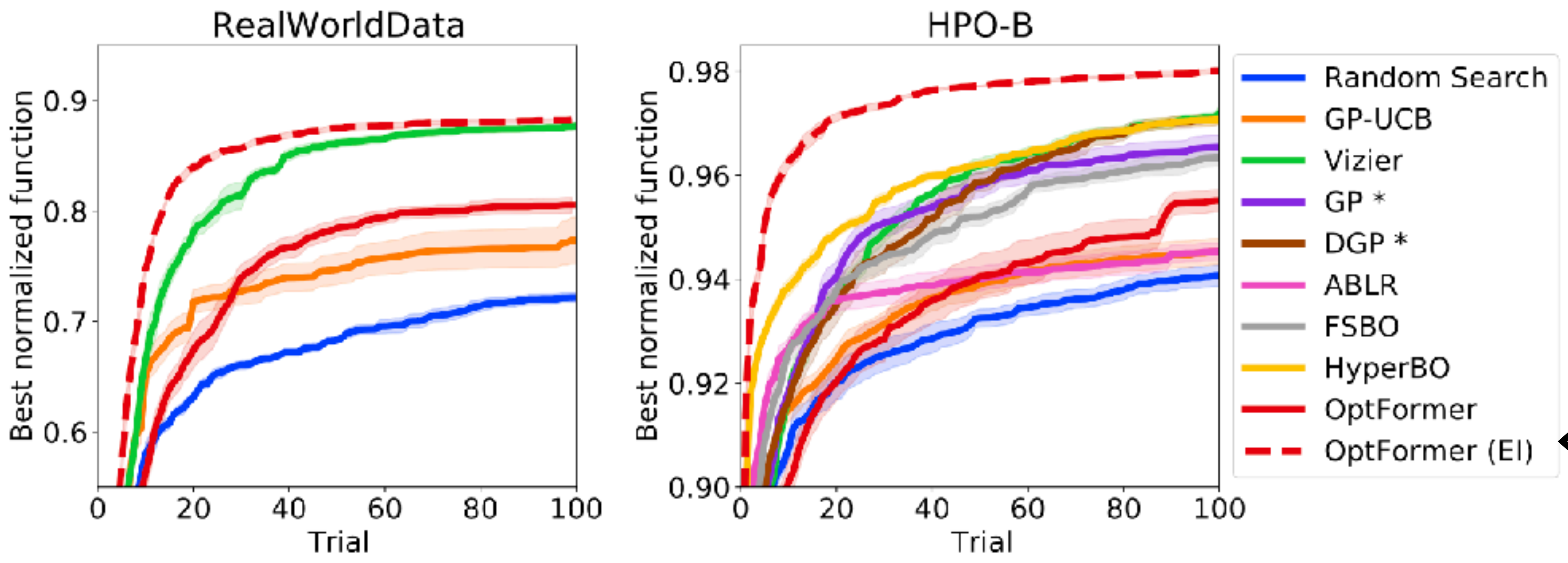


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✳ private model and evaluation code

# Application: Improving Tabular prediction with transfer learning

# Tabular prediction

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- Tabular prediction: problem definition

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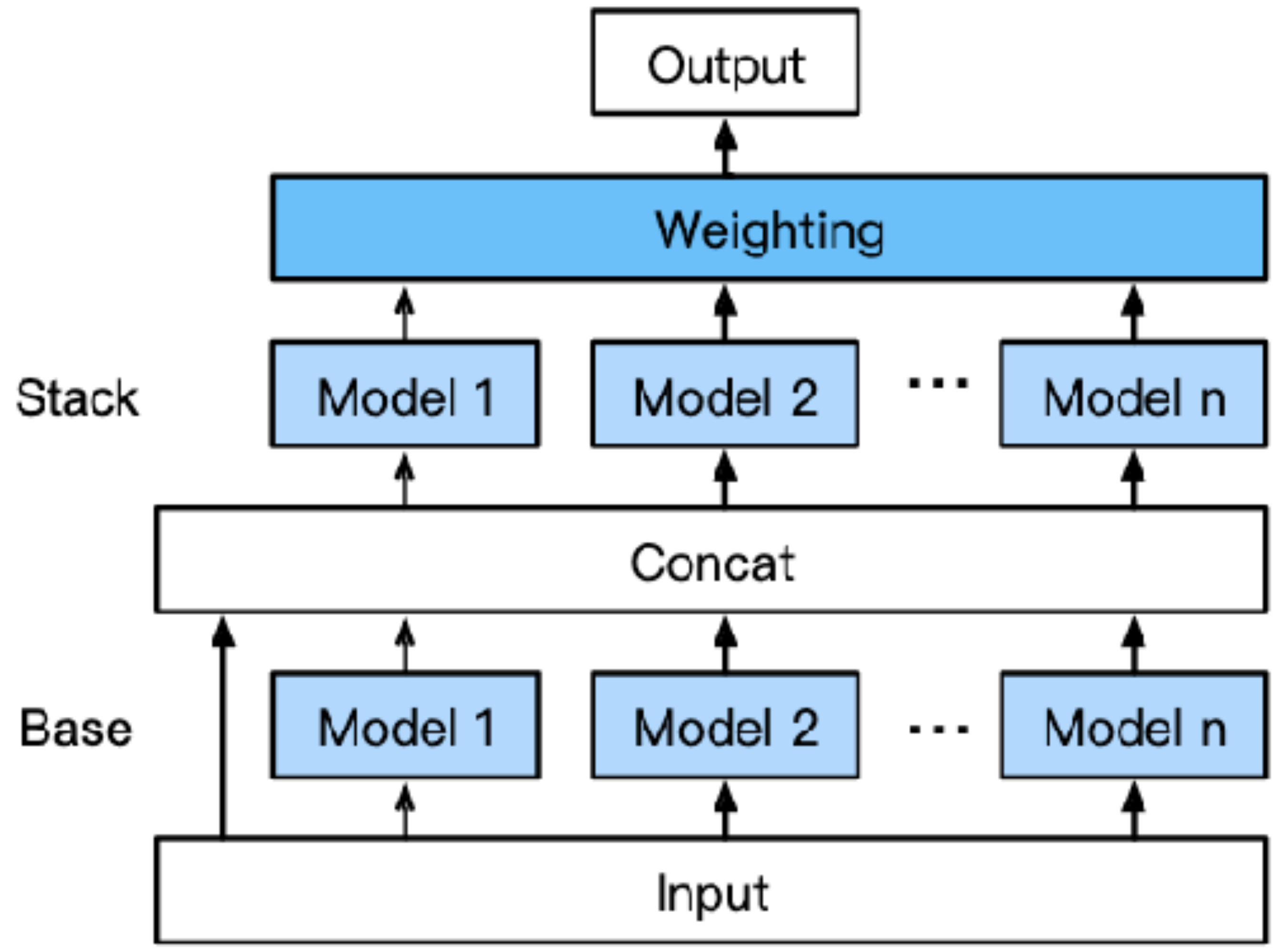


*Figure 2.* AutoGluon's multi-layer stacking strategy, shown here using two stacking layers and $n$ types of base learners.

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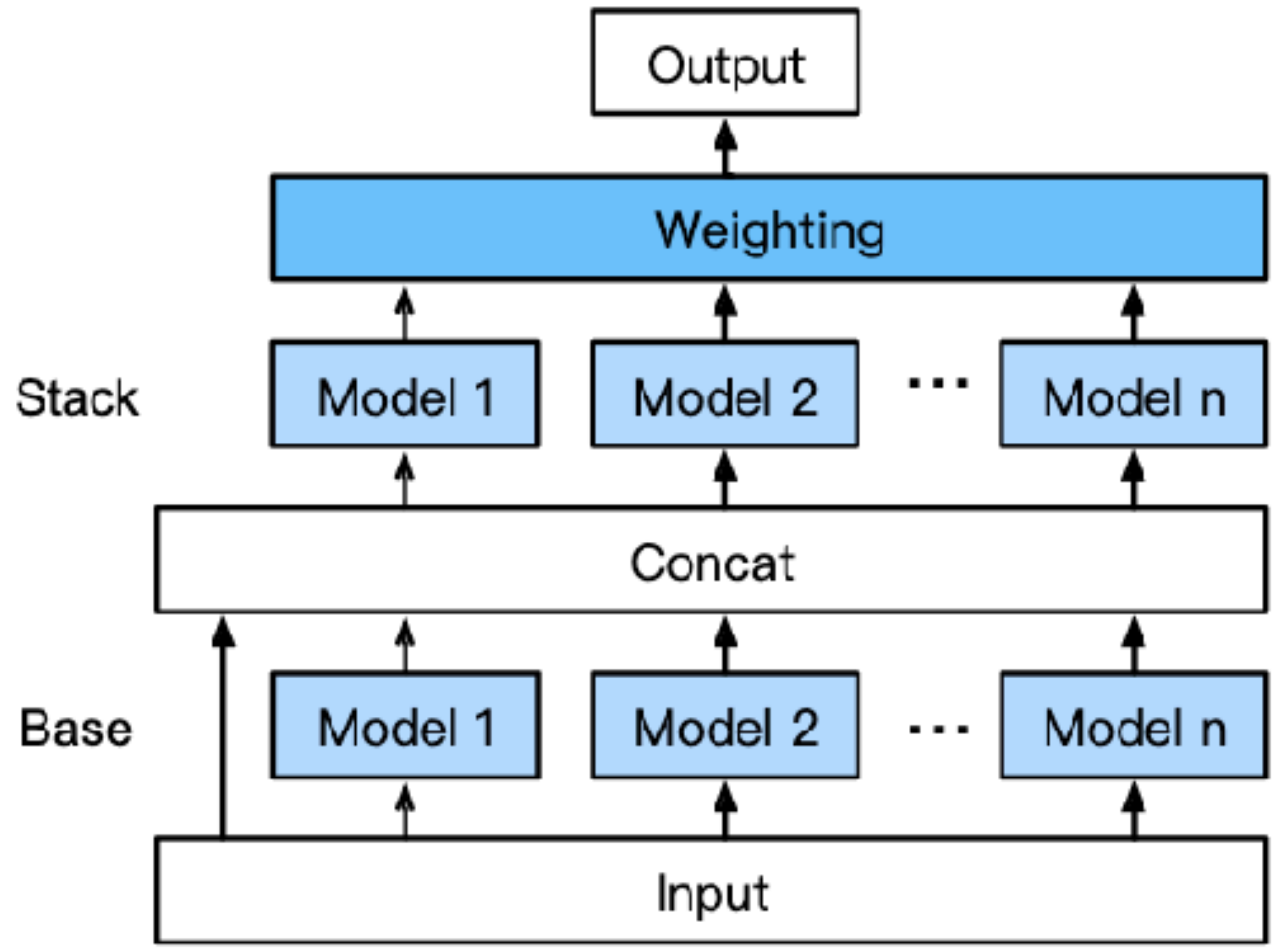


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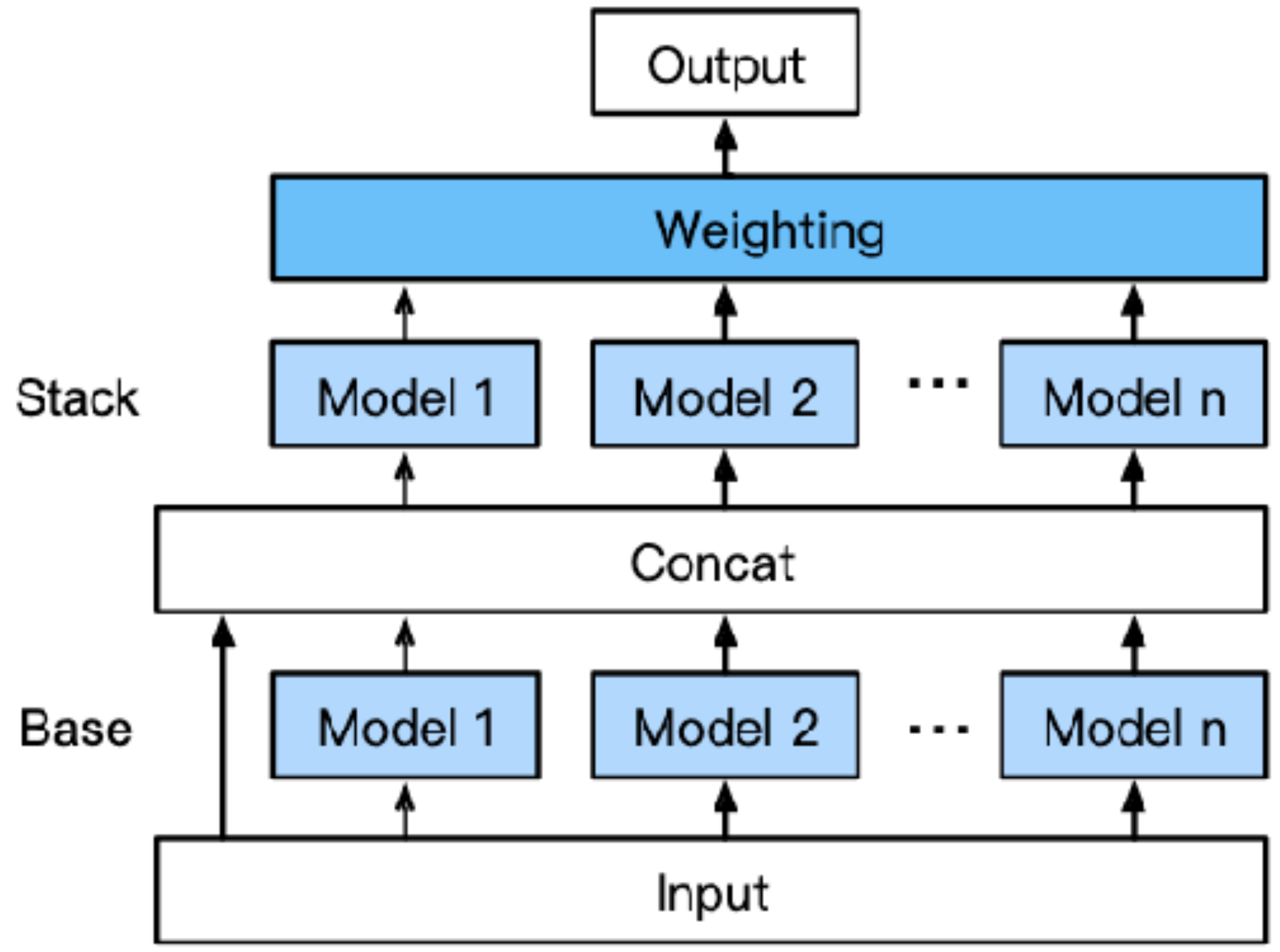


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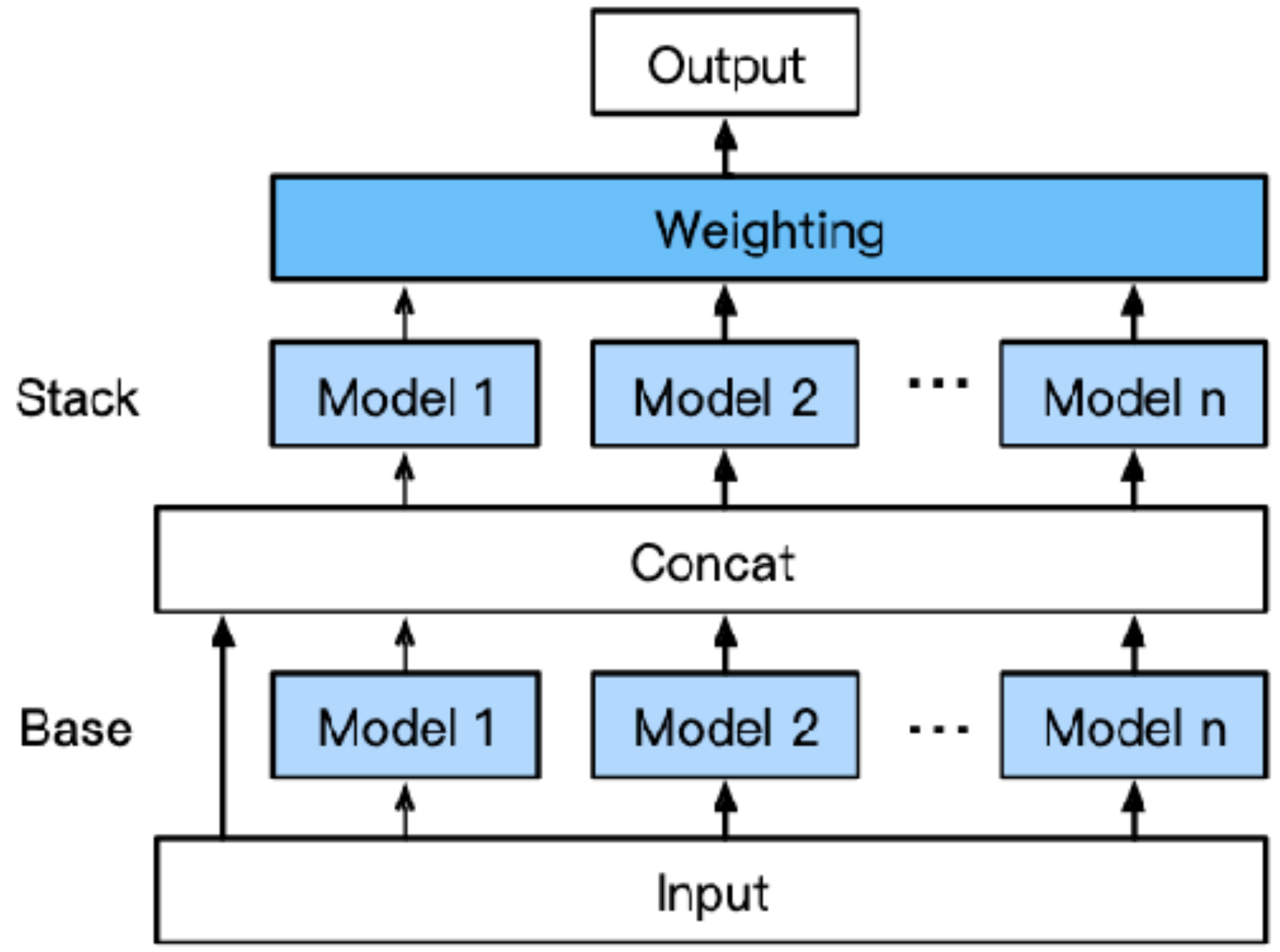


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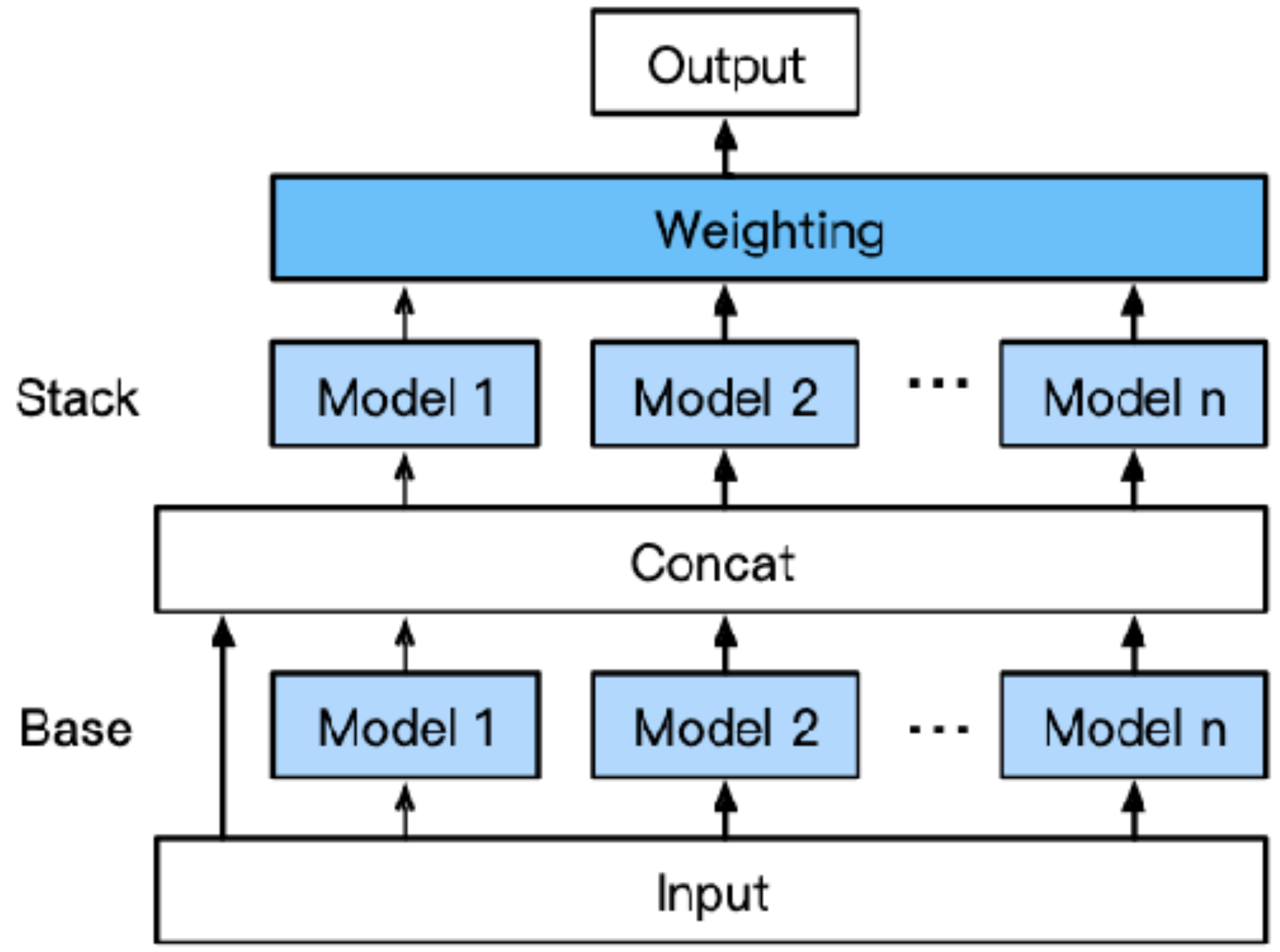


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Out of fold evaluation, image credit: data camp

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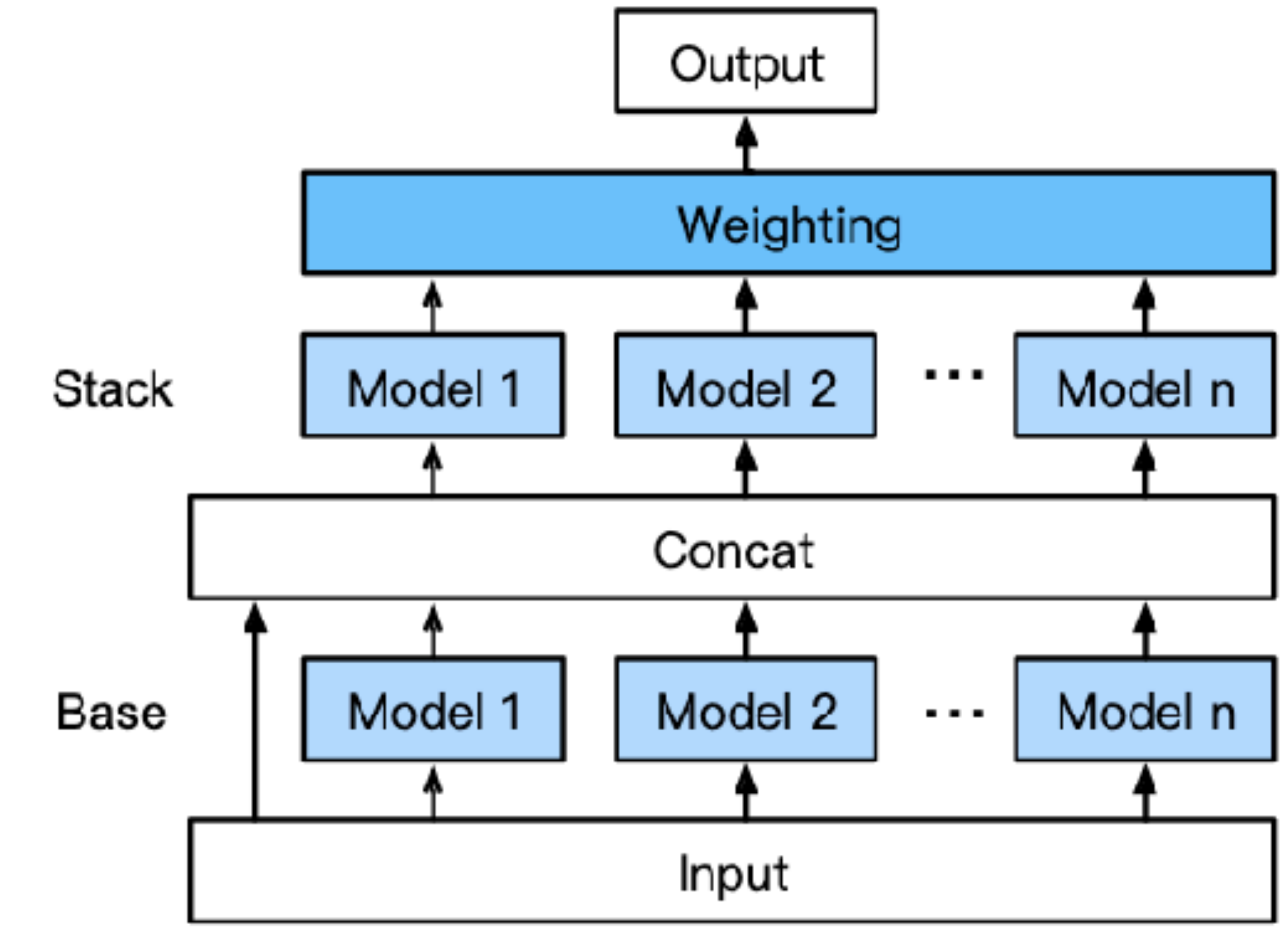


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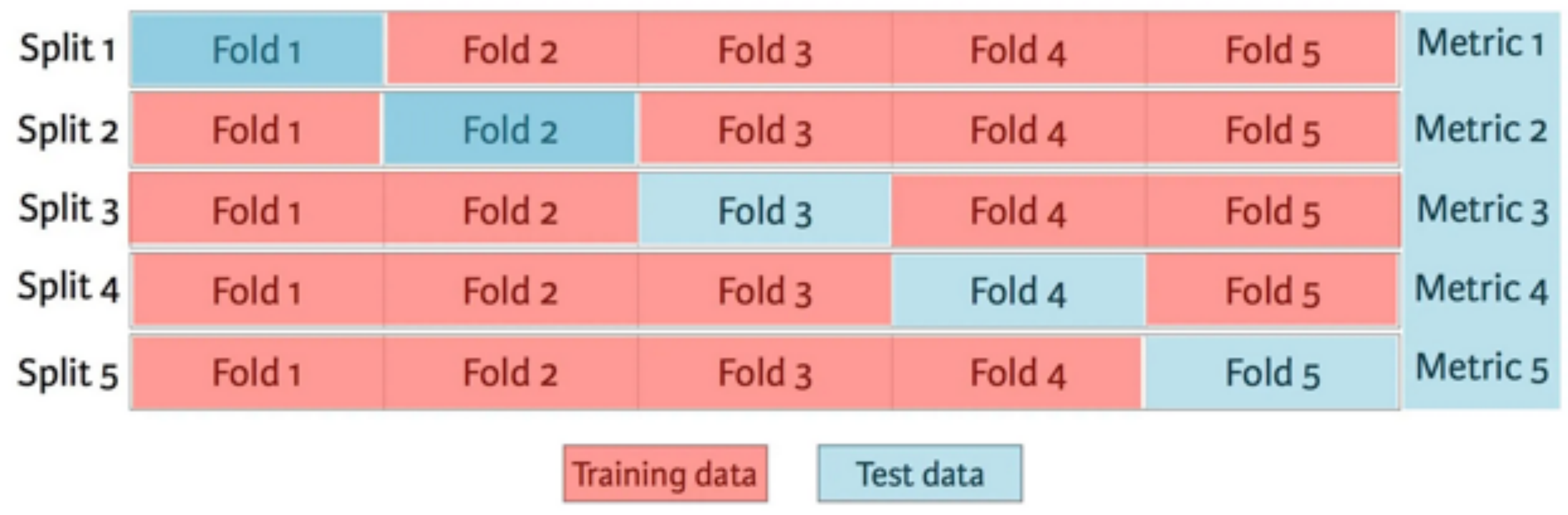


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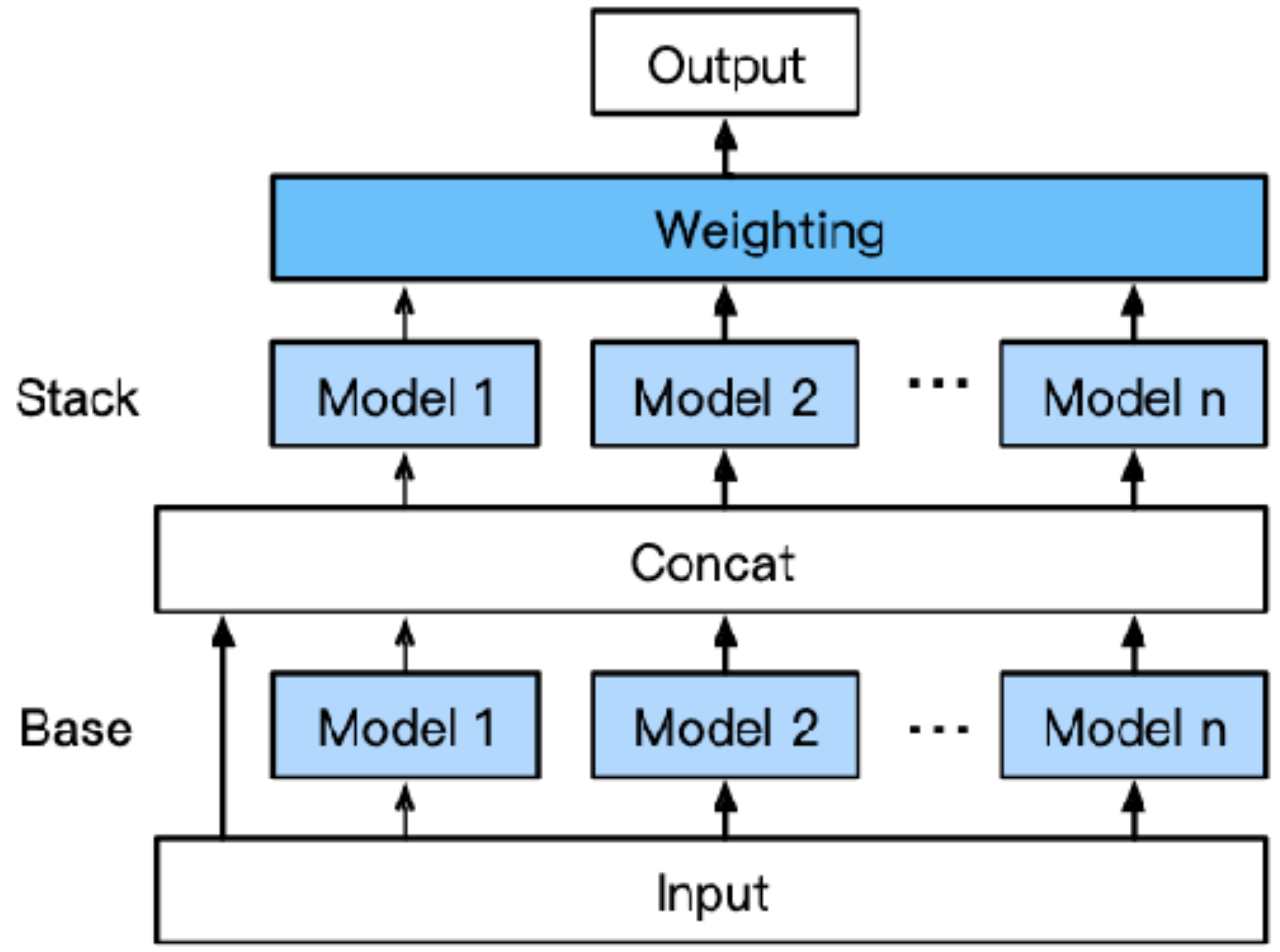


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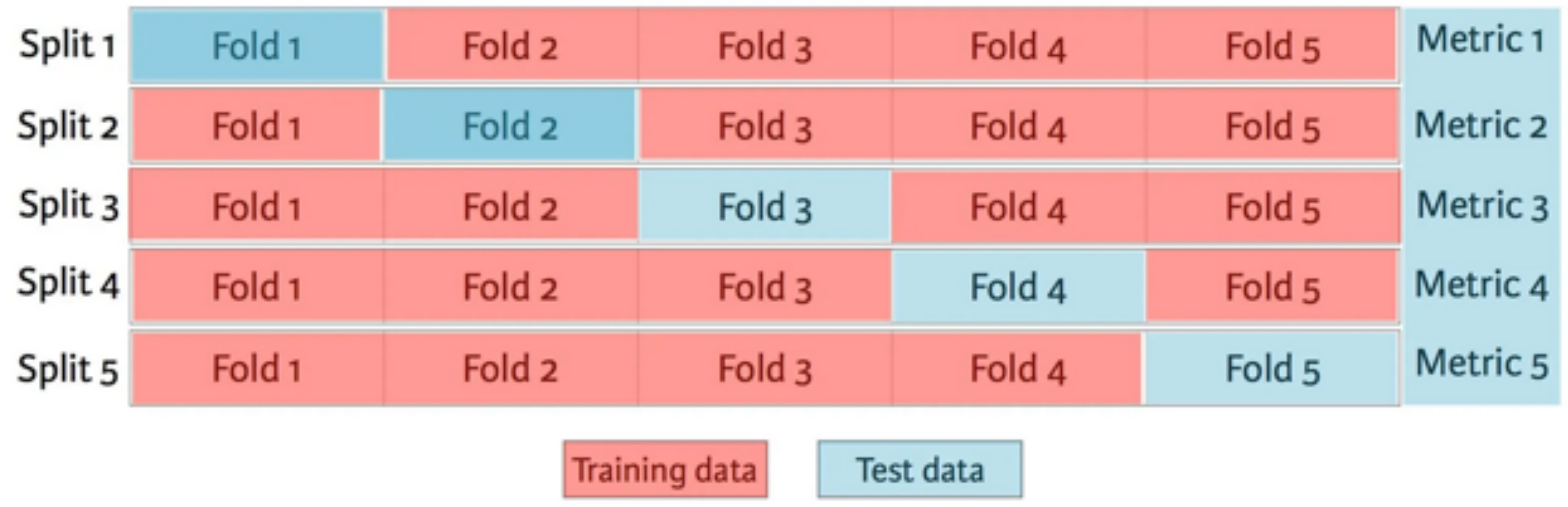


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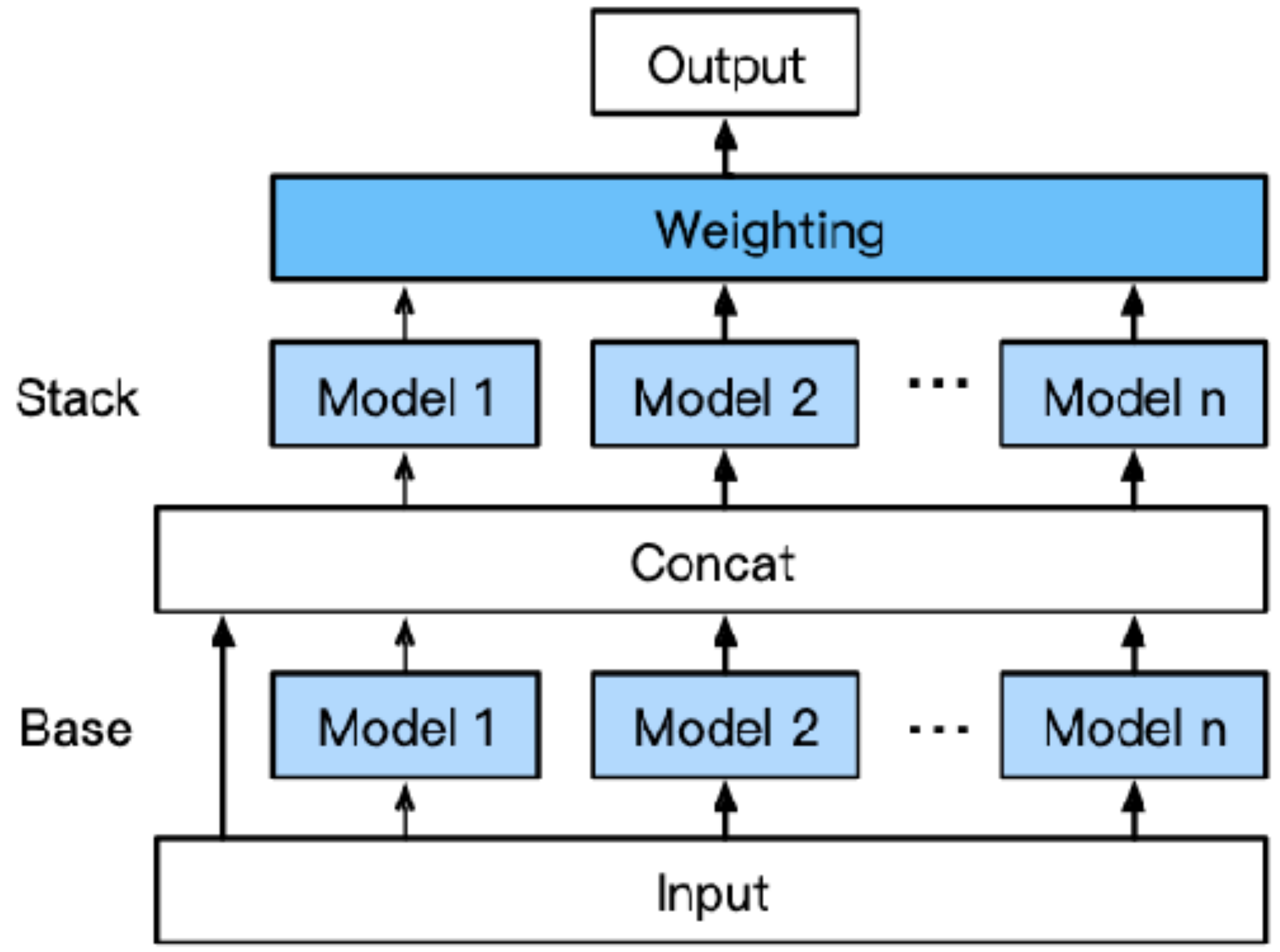


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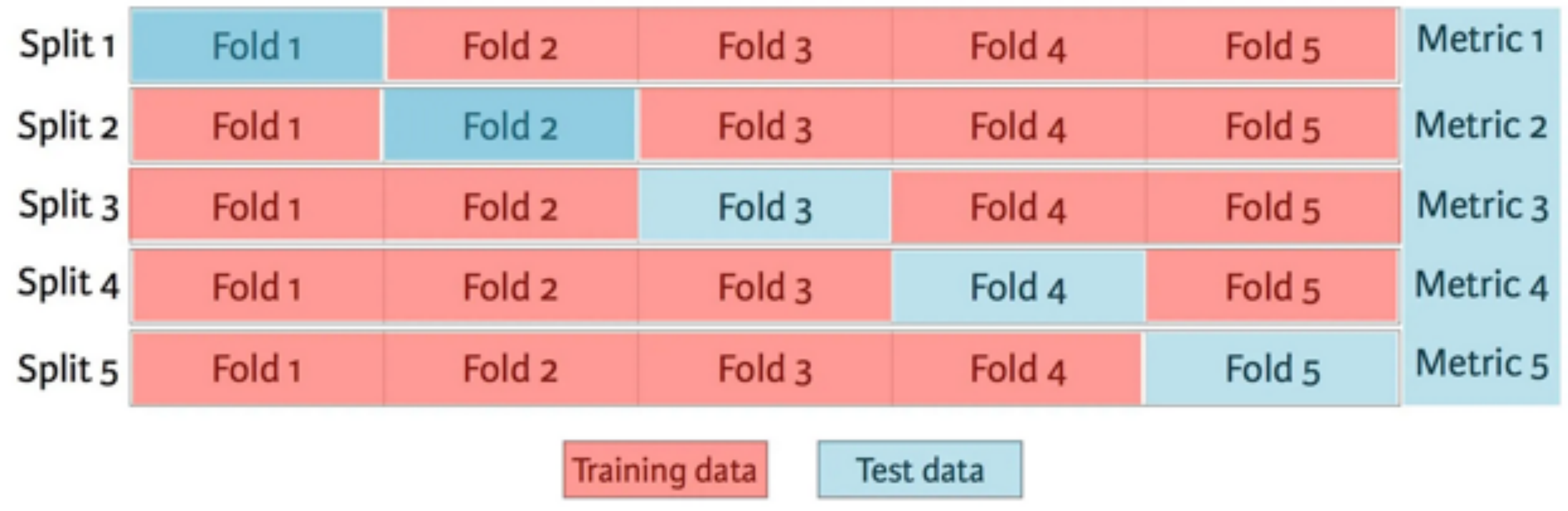


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  - Then perform ***stacking***: e.g. learn the models again while concatenating the predictions of the first *layer* with the original features
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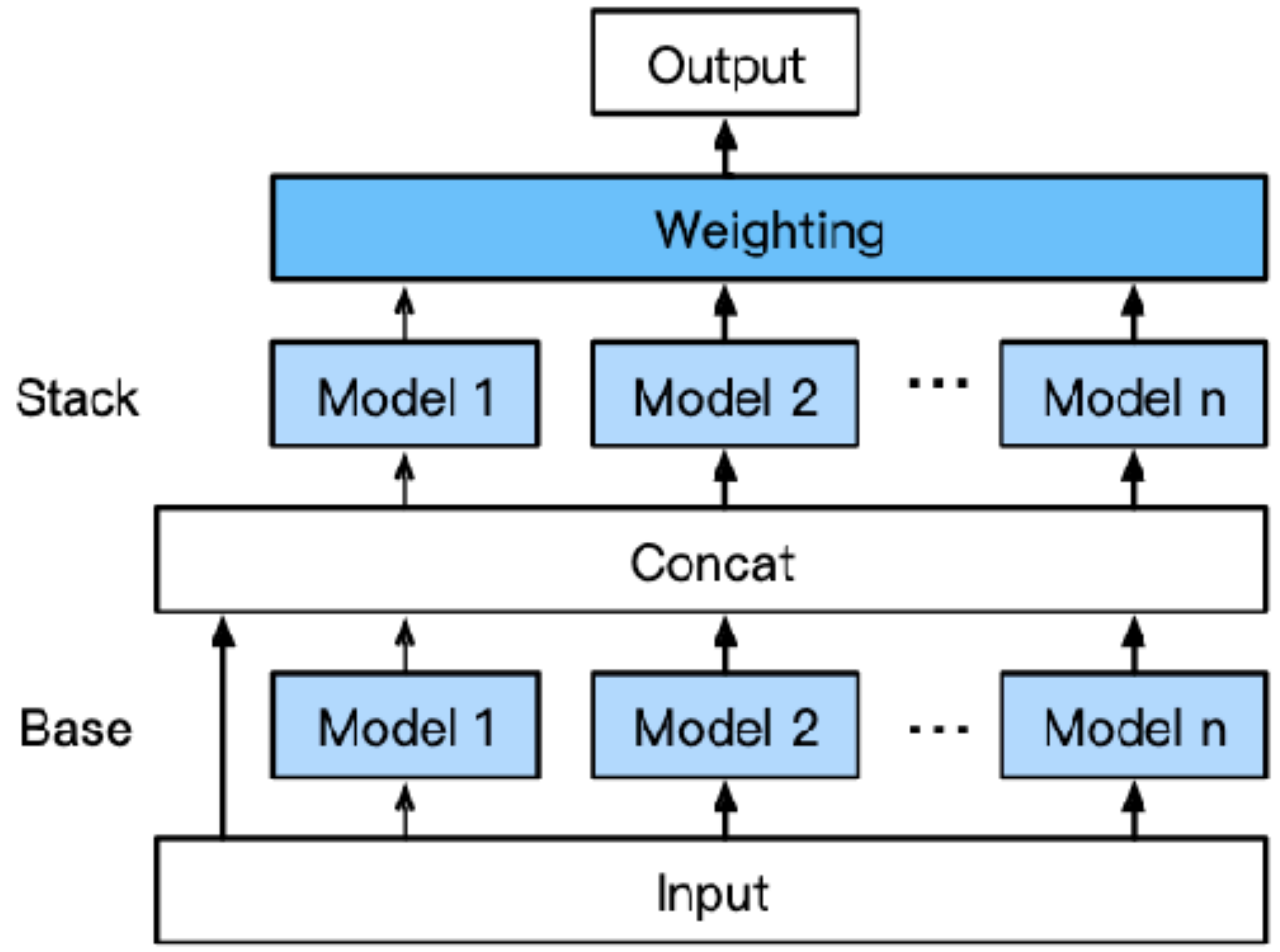
- Lets have a look at Autogluon now!

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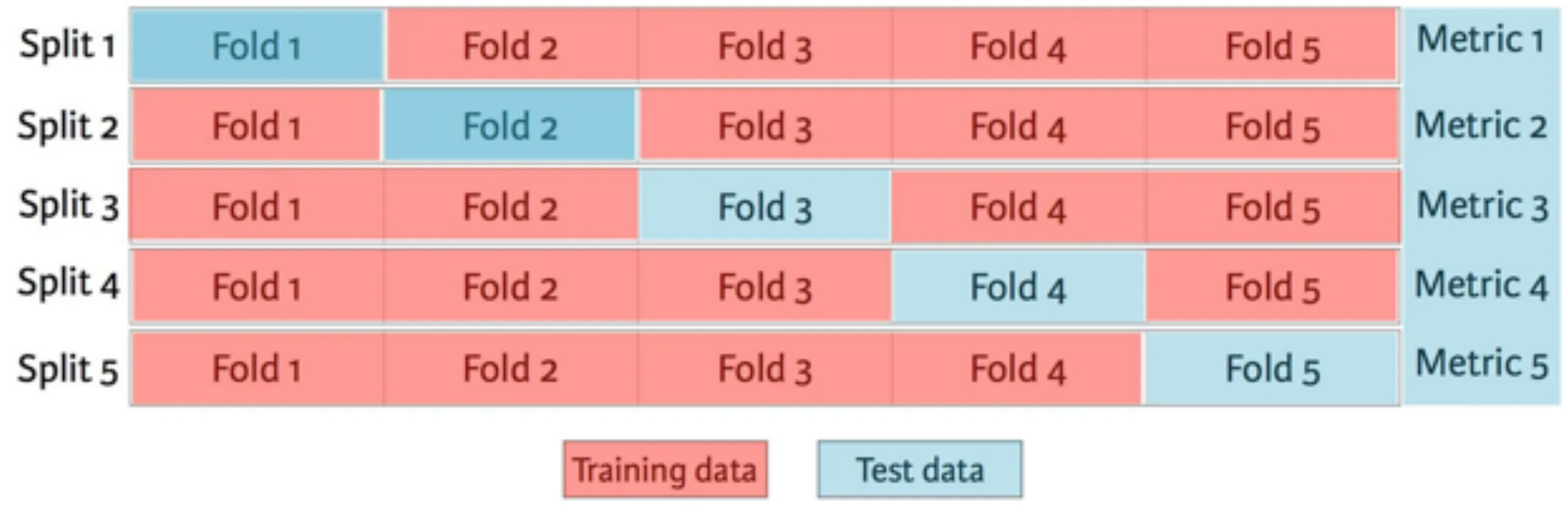


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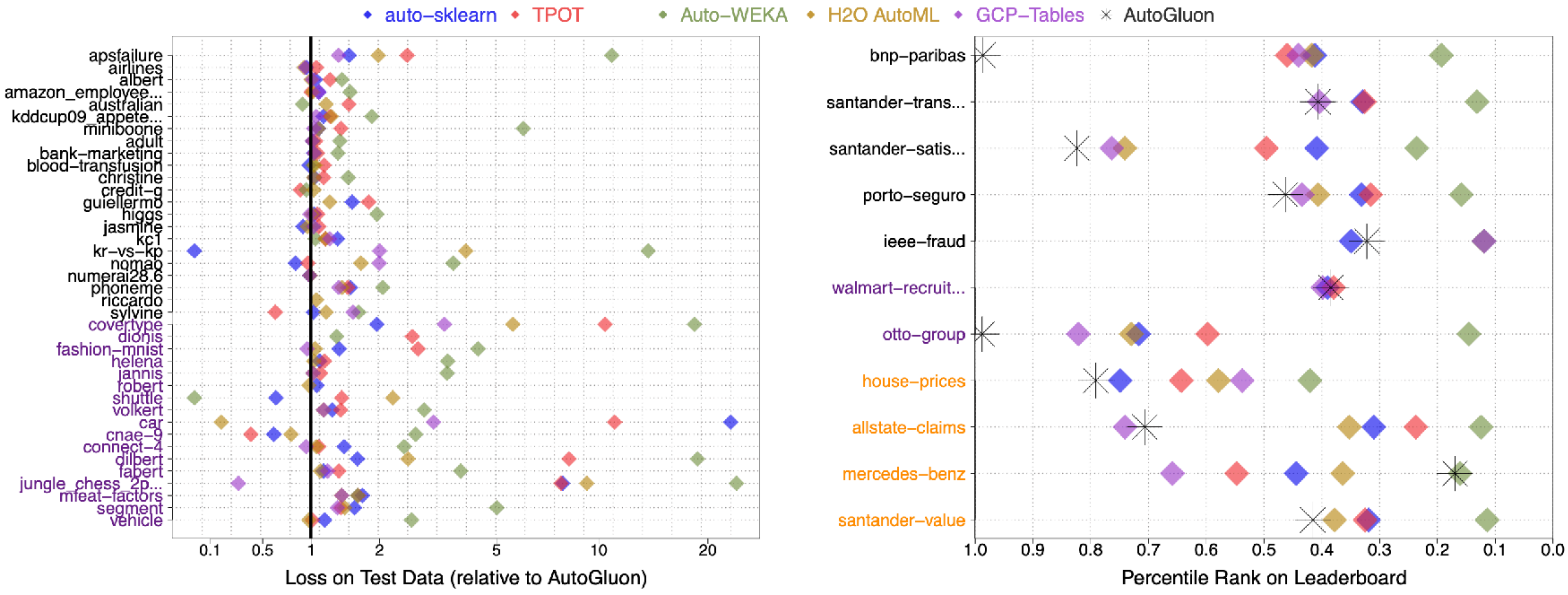


(A) AutoML Benchmark (1h)

(B) Kaggle Benchmark (4h)

Erickson & Mueller et al 2020

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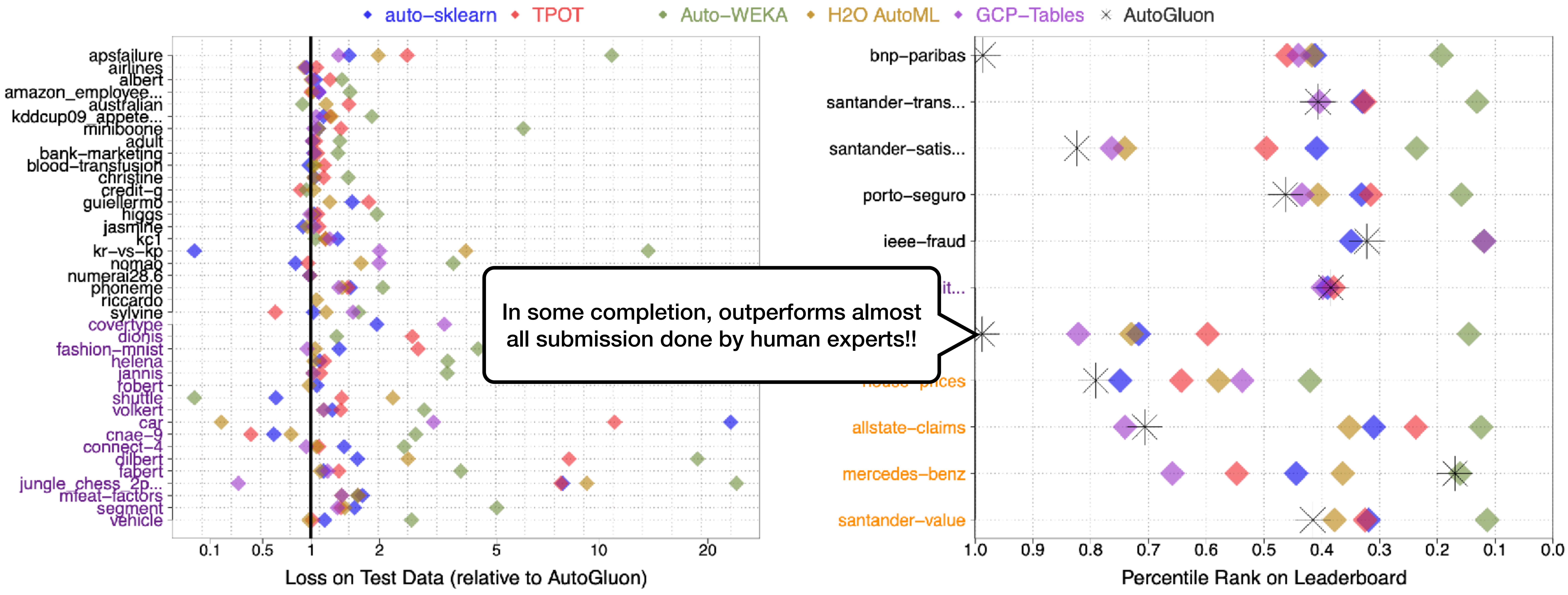


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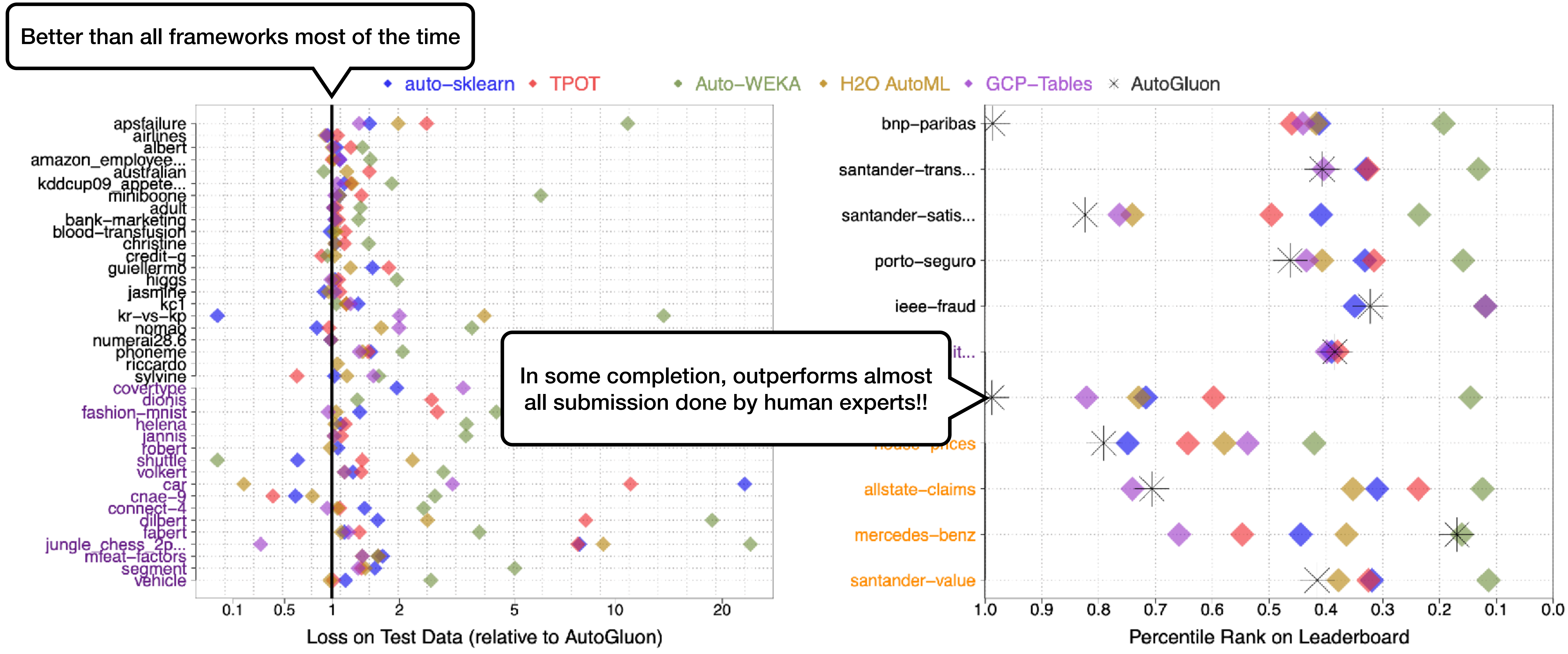


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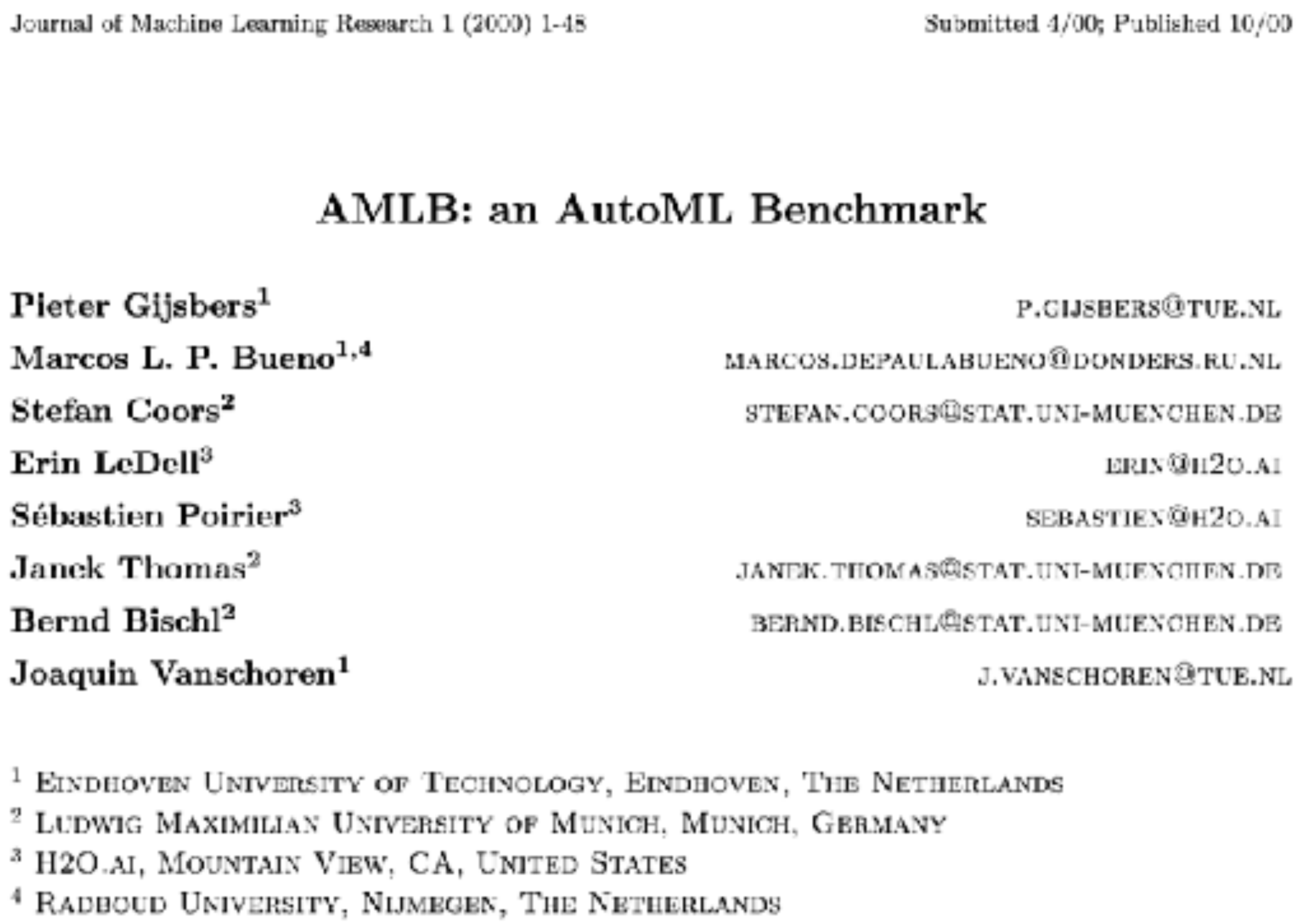
Journal of Machine Learning Research 1 (2000) 1-48 Submitted 4/00; Published 10/00

AMLB: an AutoML Benchmark

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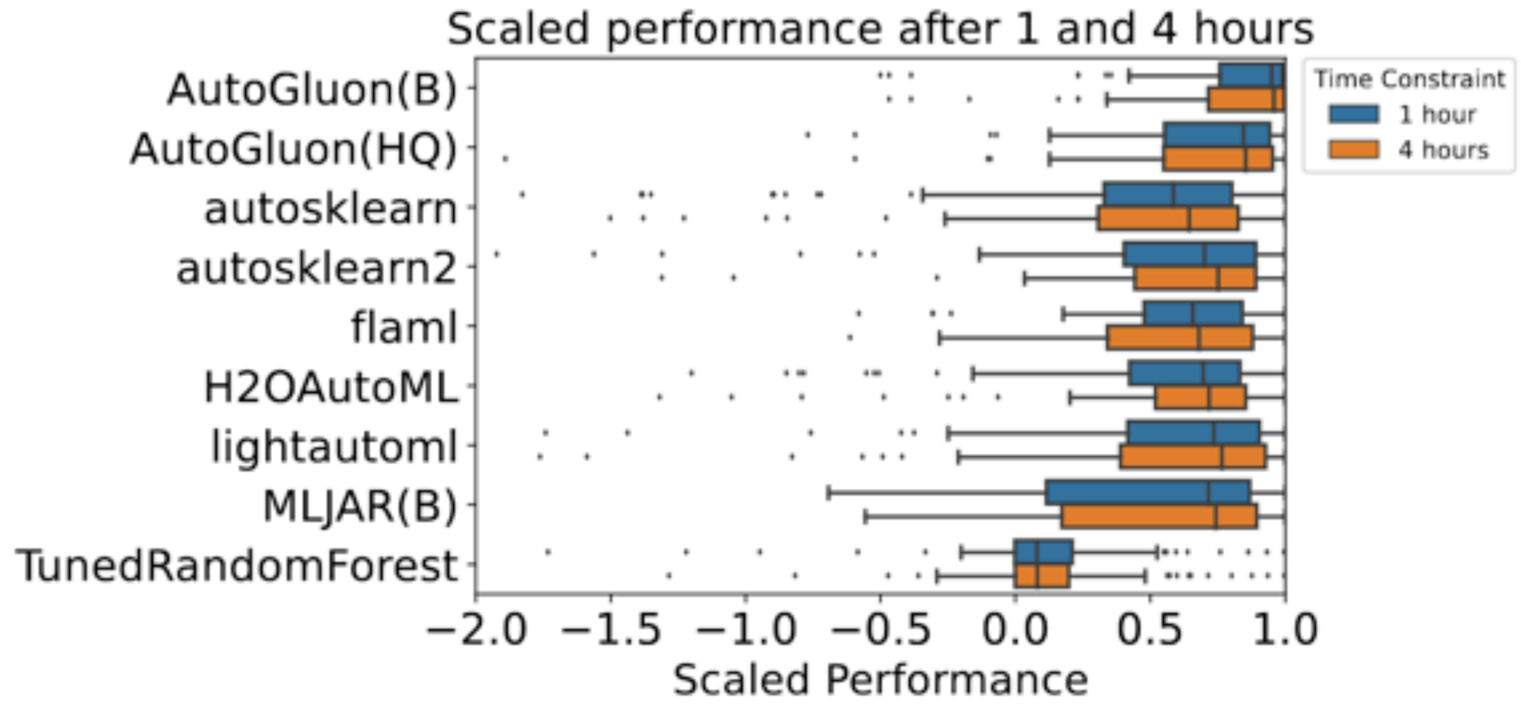


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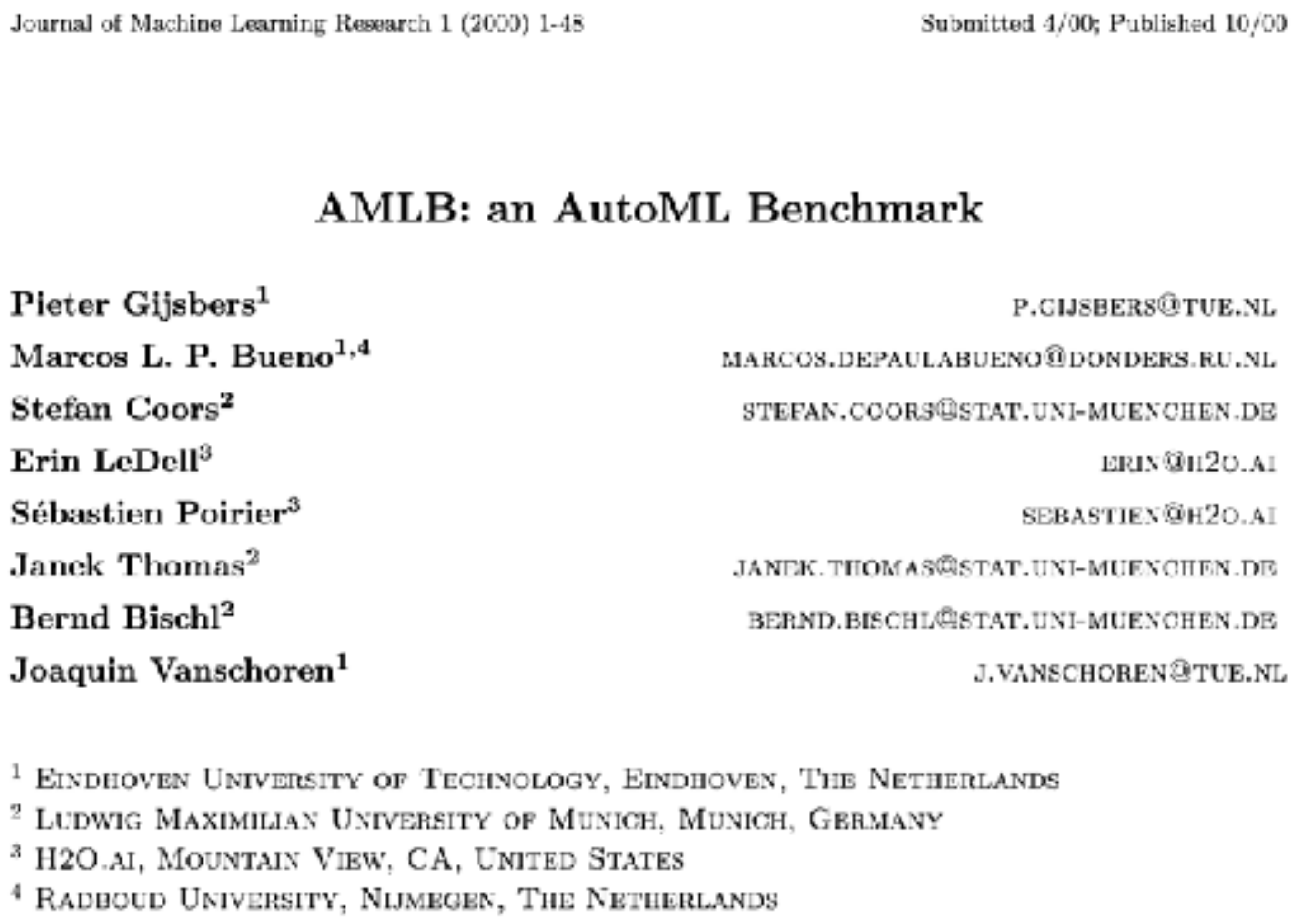
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AMLB: an AutoML Benchmark

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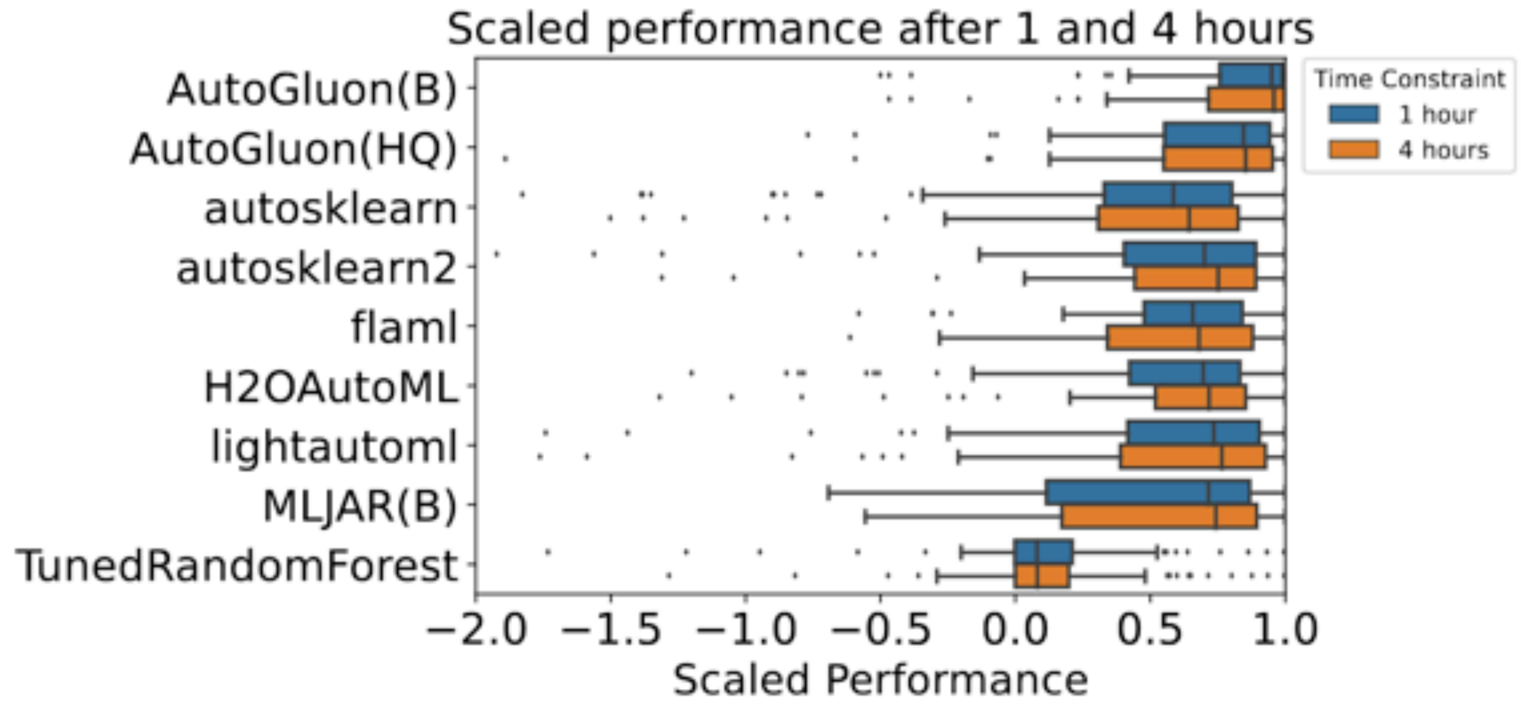


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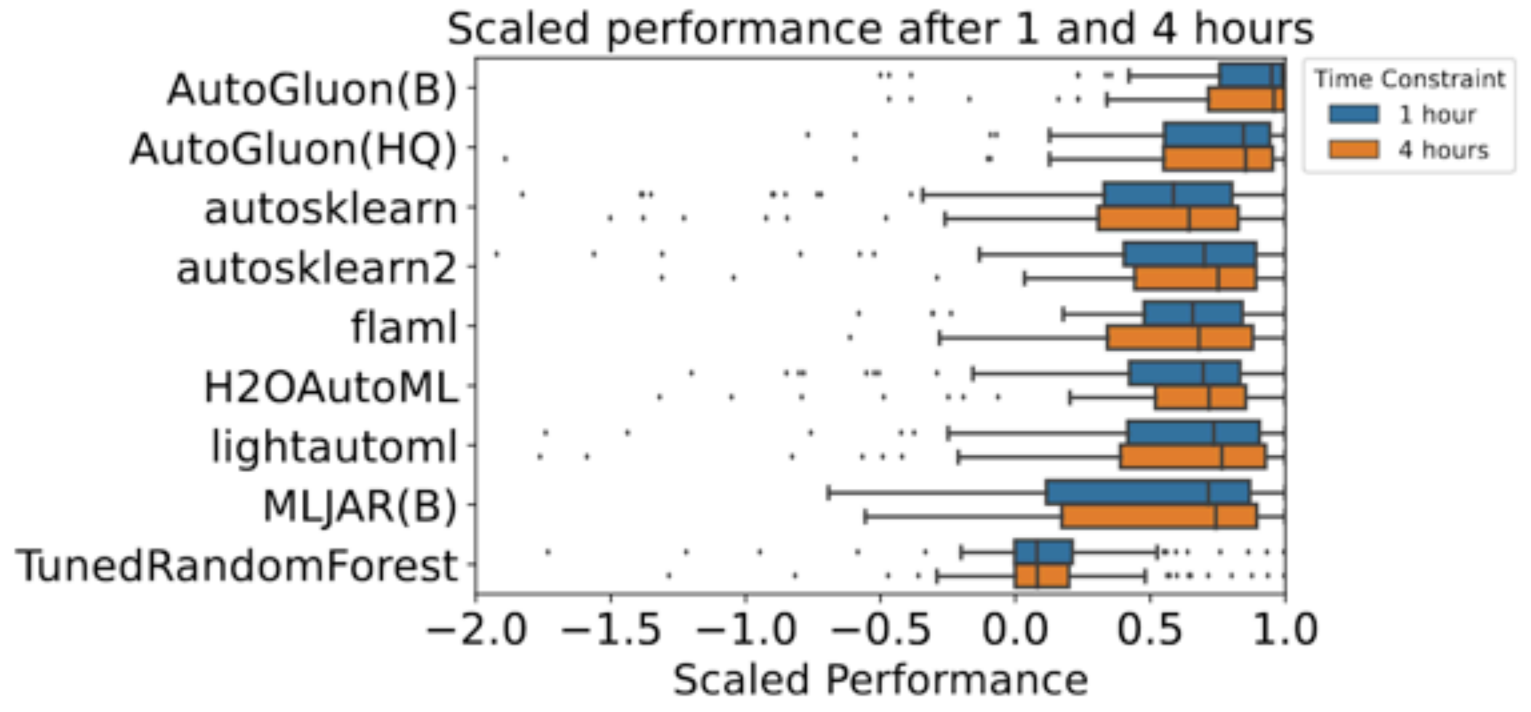


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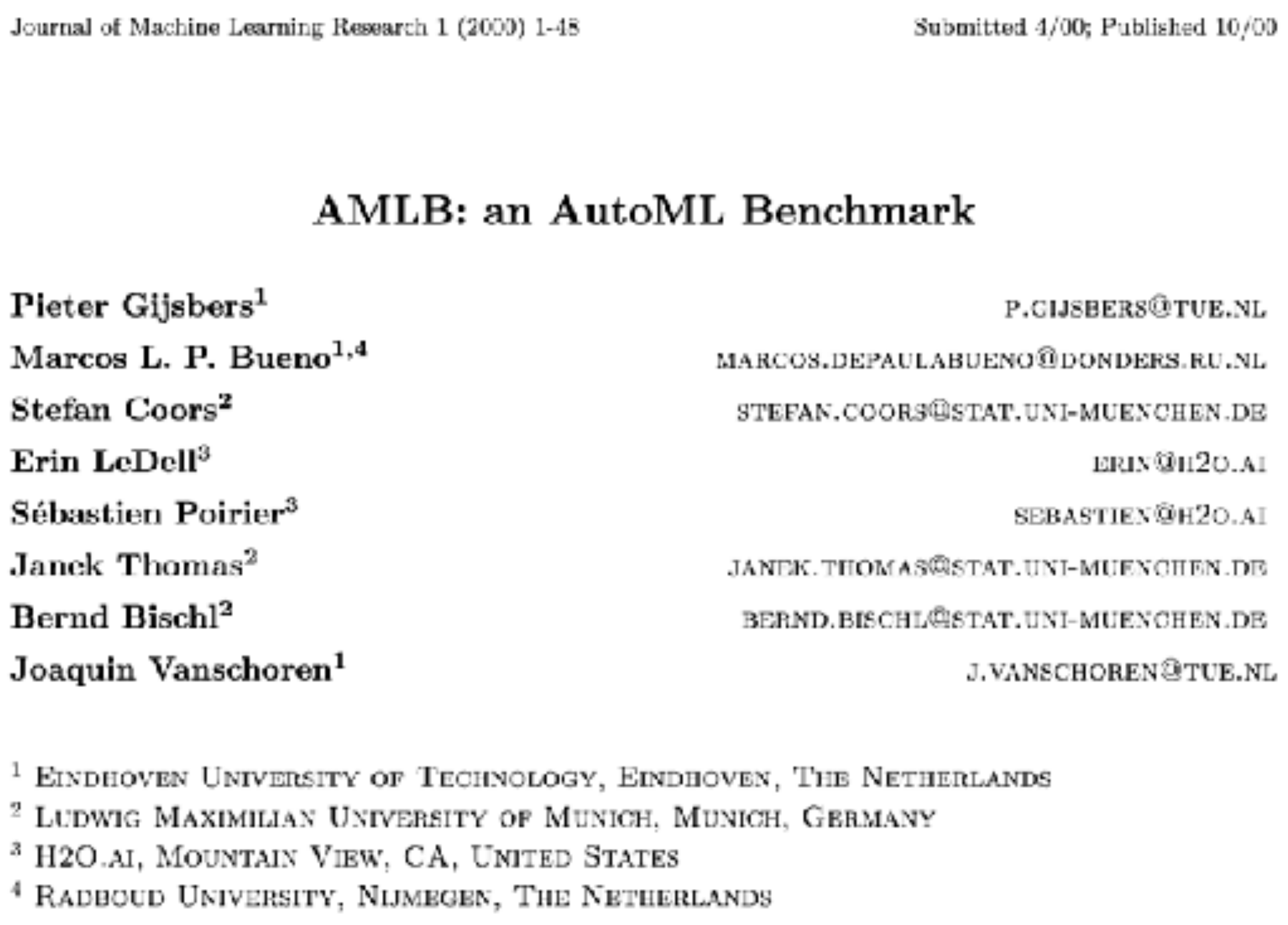

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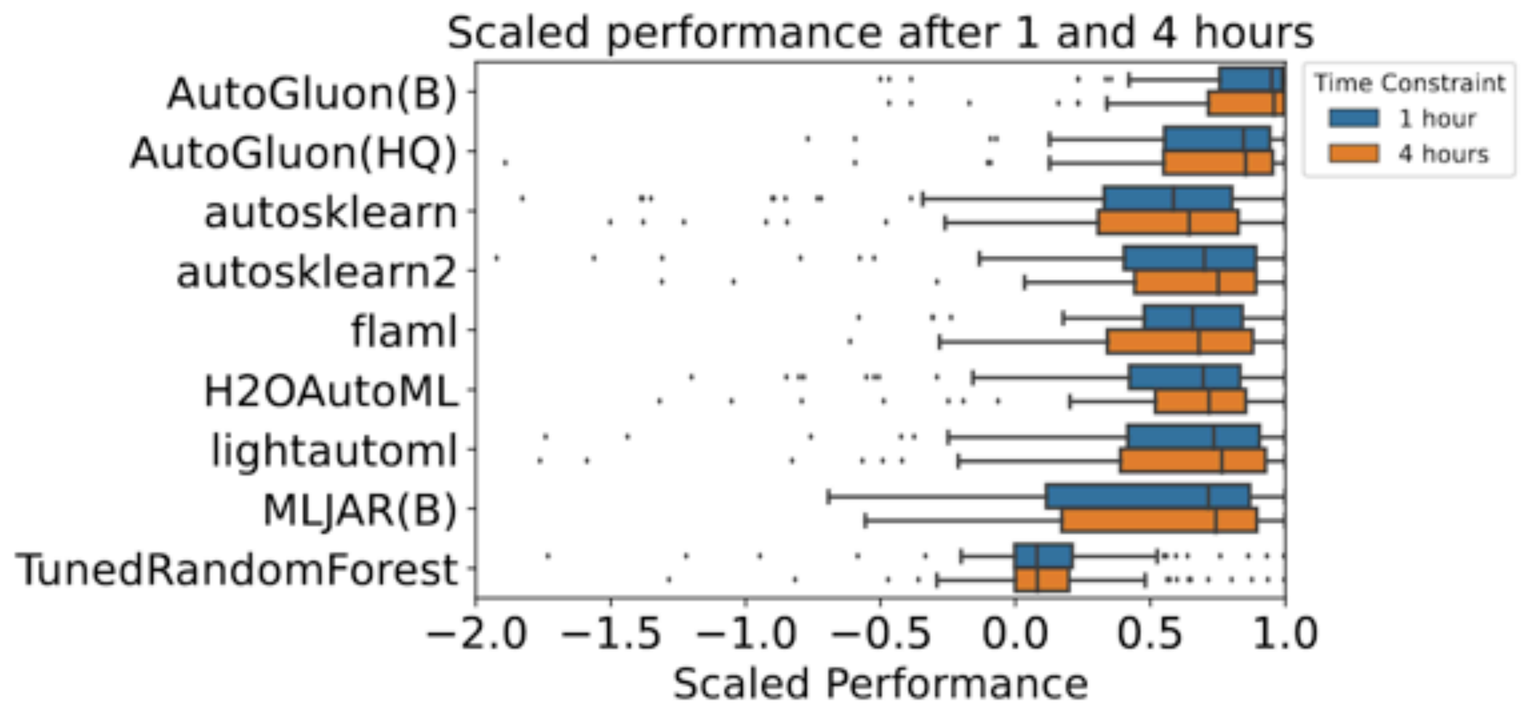


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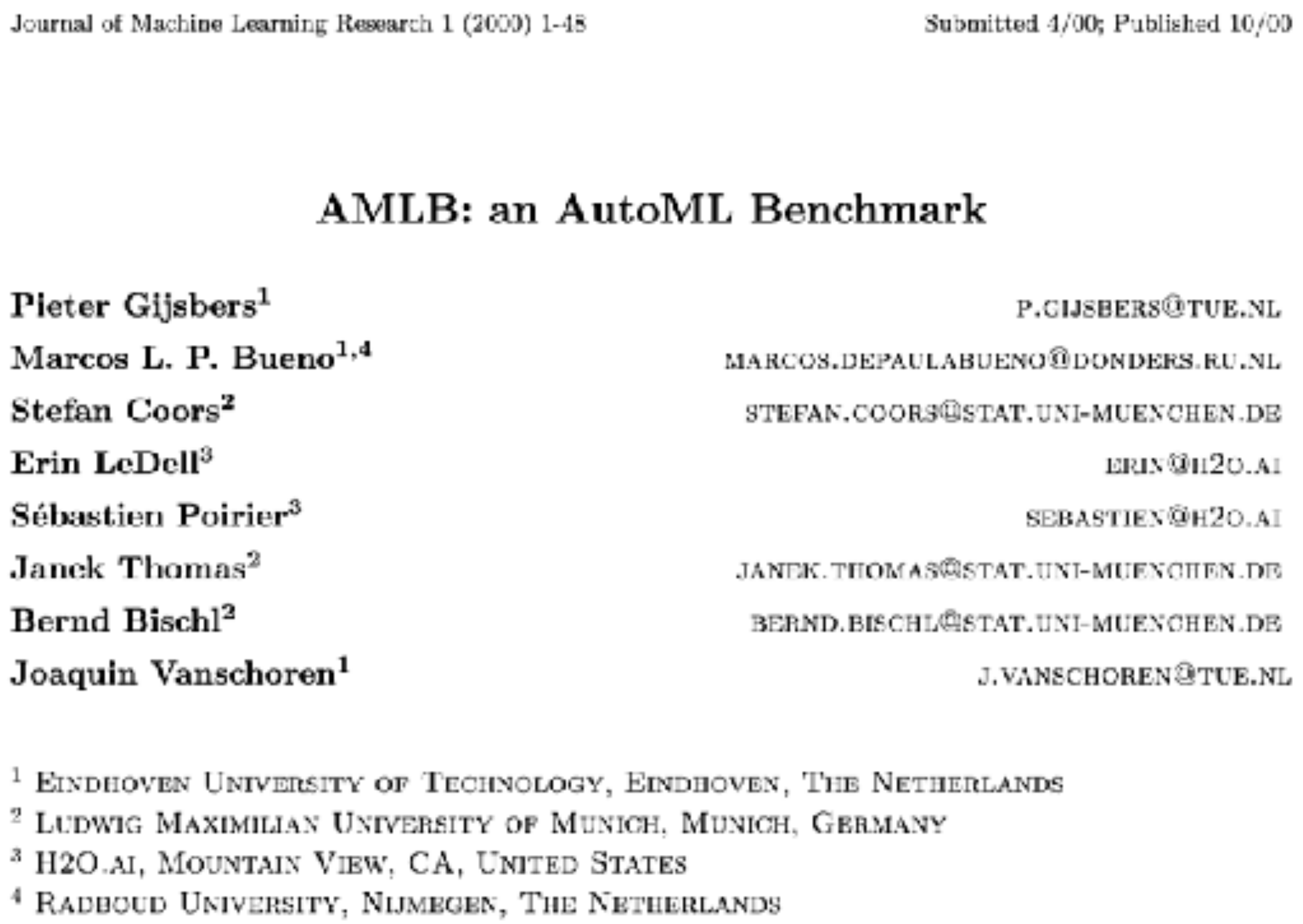

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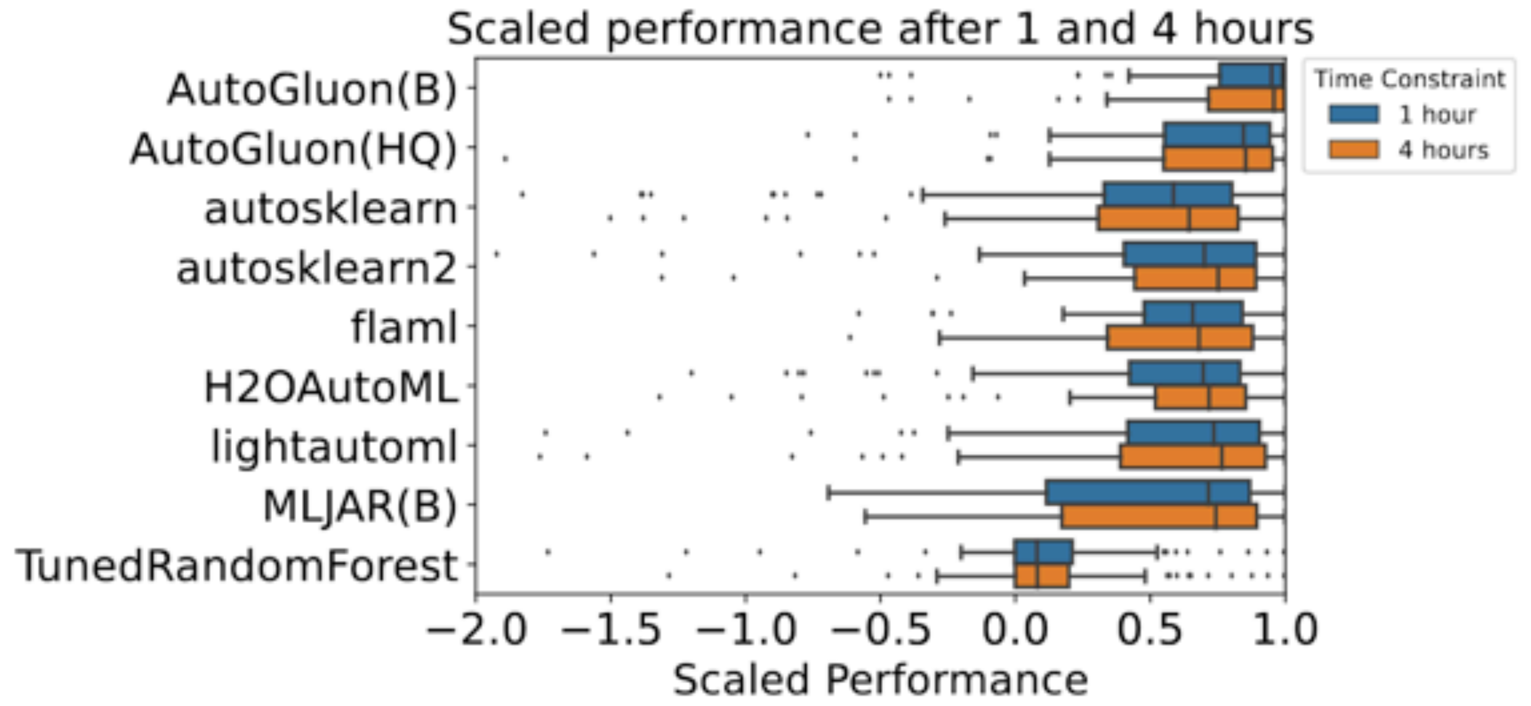


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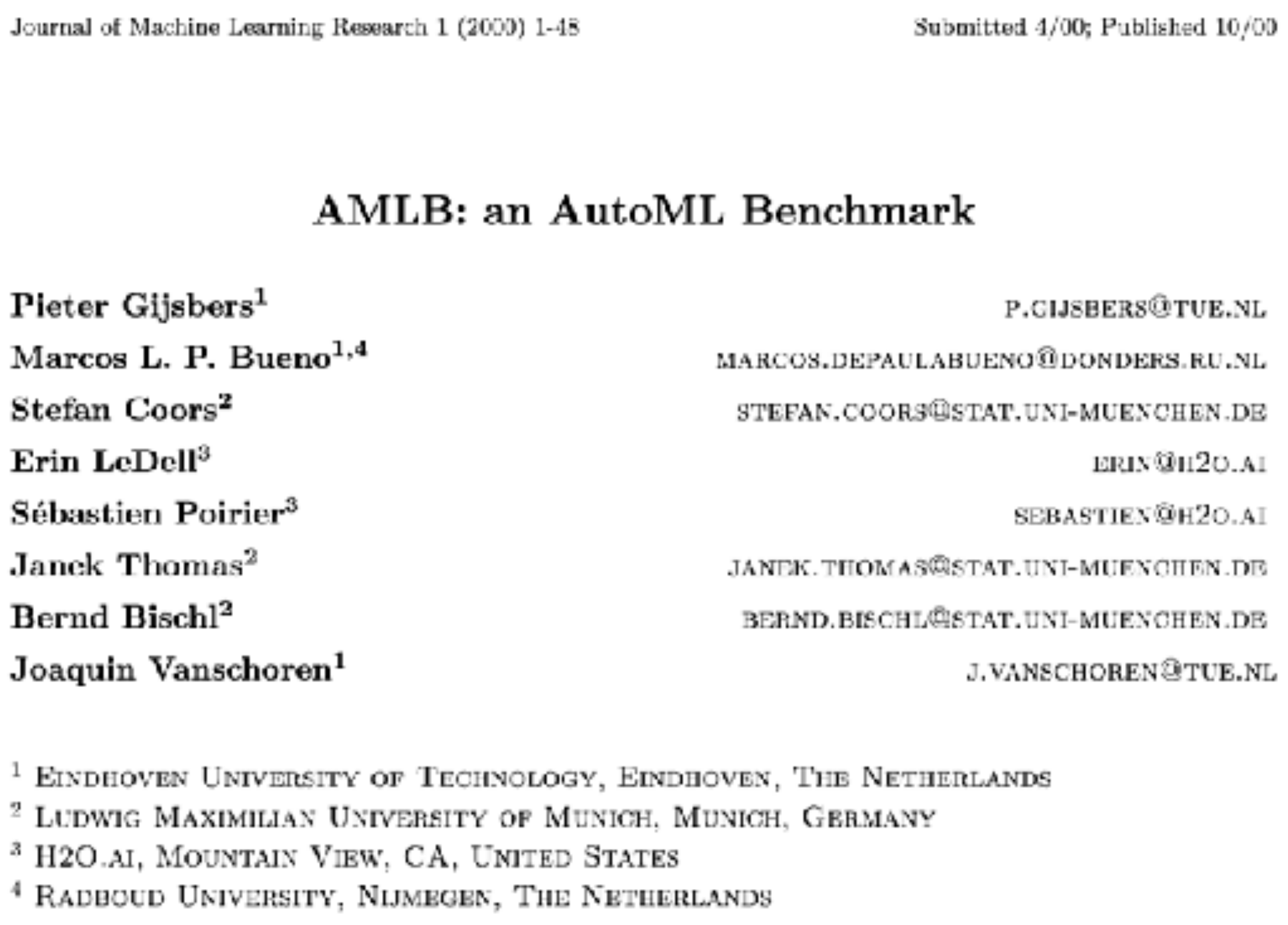

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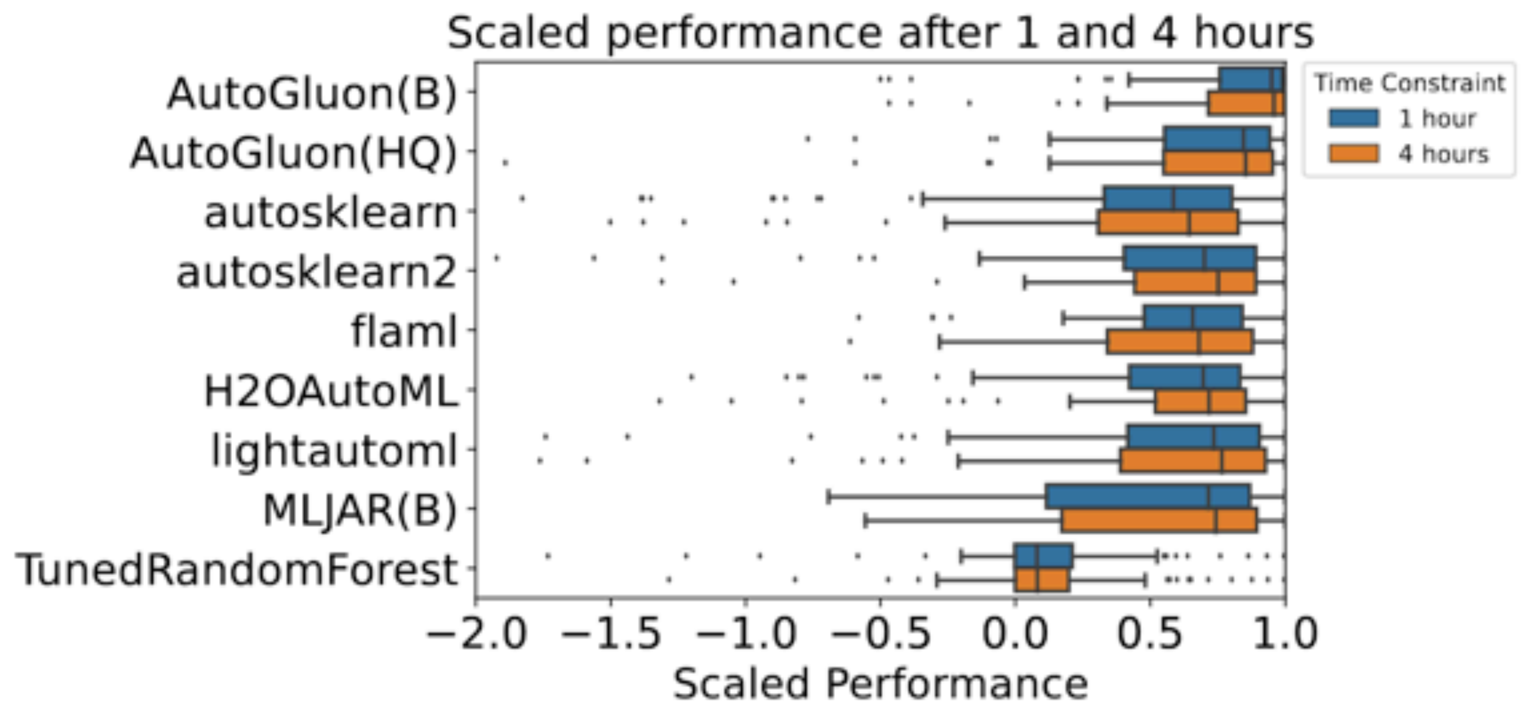


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🥳 The dataset combined with **portfolio learning** allows to outperform Autogluon!

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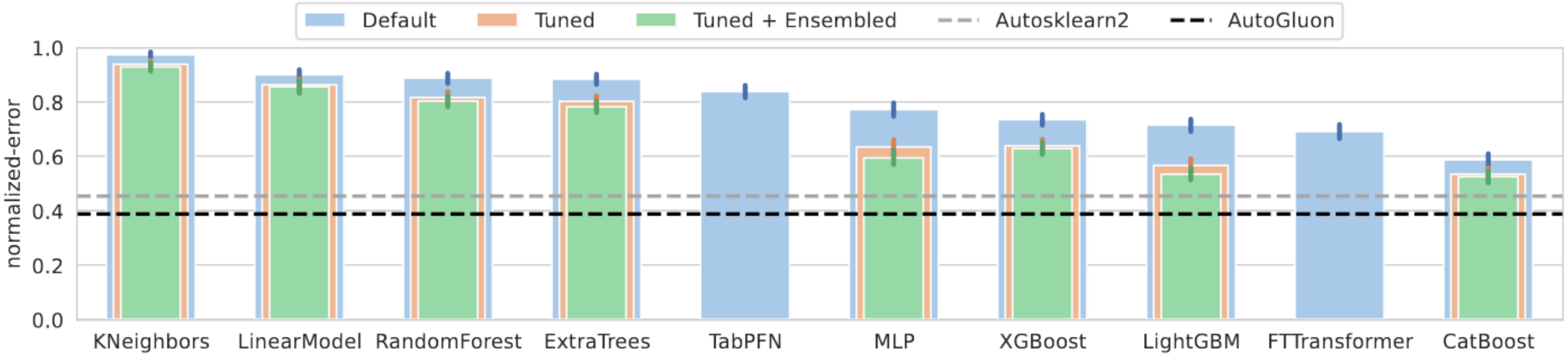


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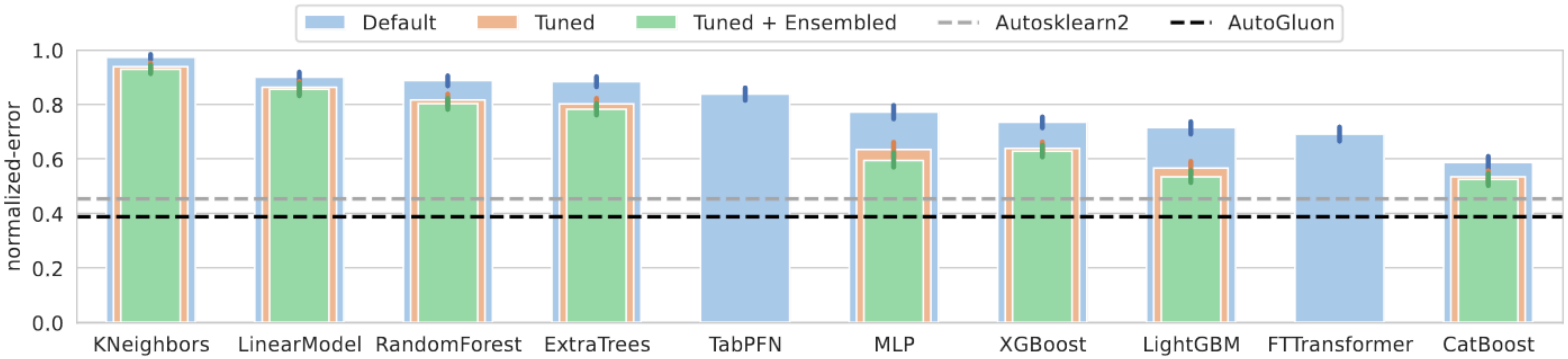


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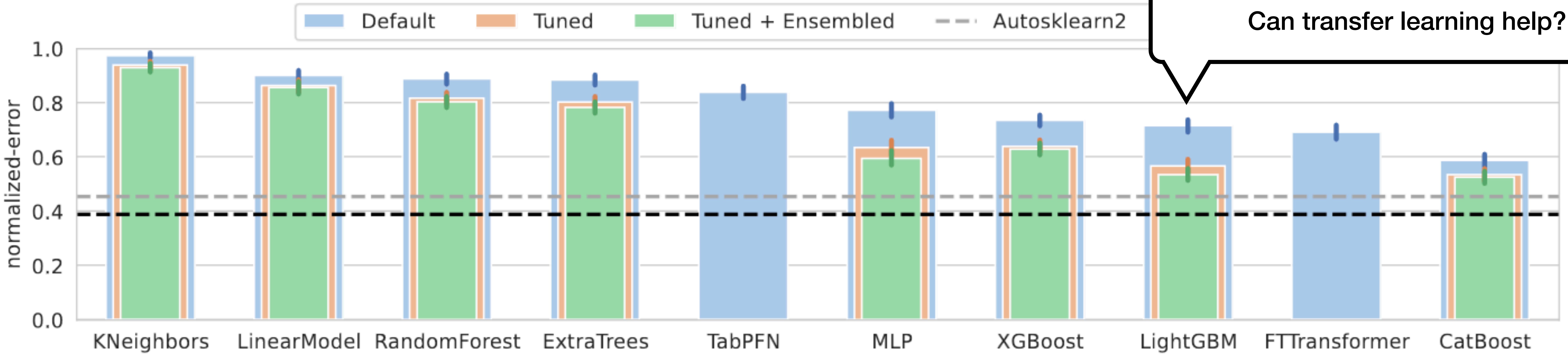


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... when using the best performing model on a given dataset

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**Benefits** 👍:
- Approximation guarantees from the original (sub-modular) problem
- Tractable
- Works extremely well in practice

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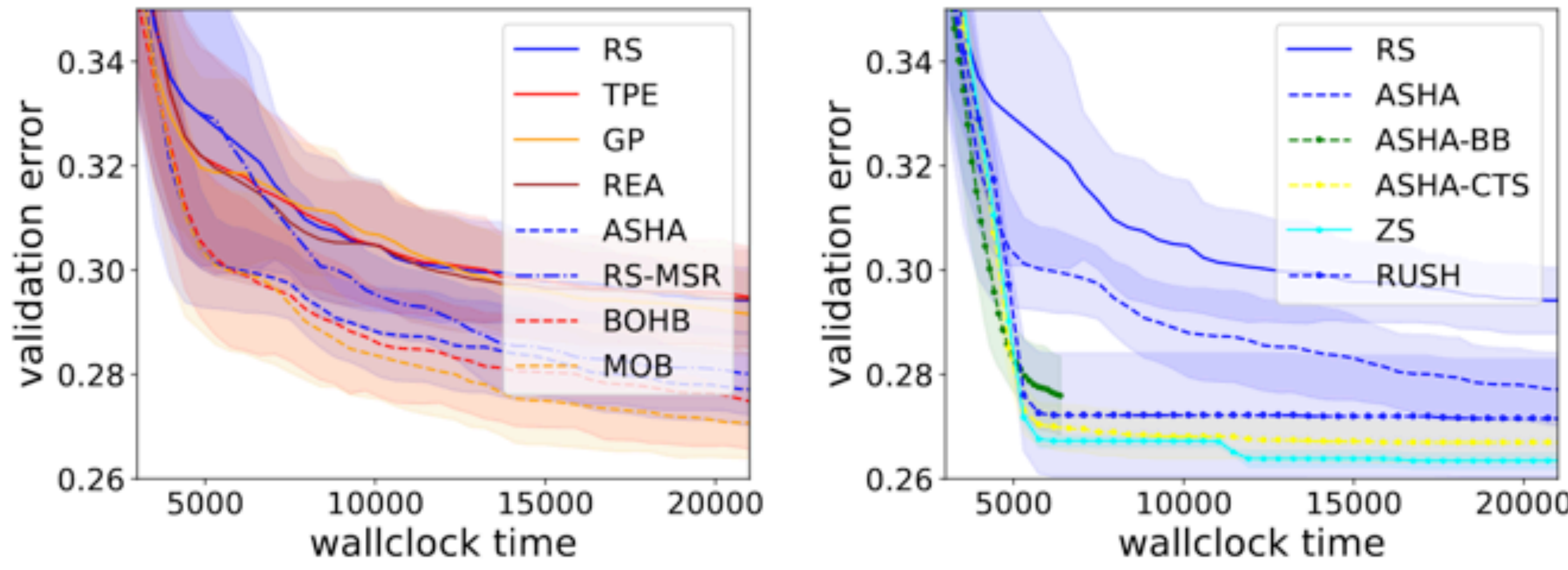


(b) NAS201: CIFAR-100.

Syne Tune: A Library for Large-Scale Hyperparameter Tuning and Reproducible Research [Salinas 2022]

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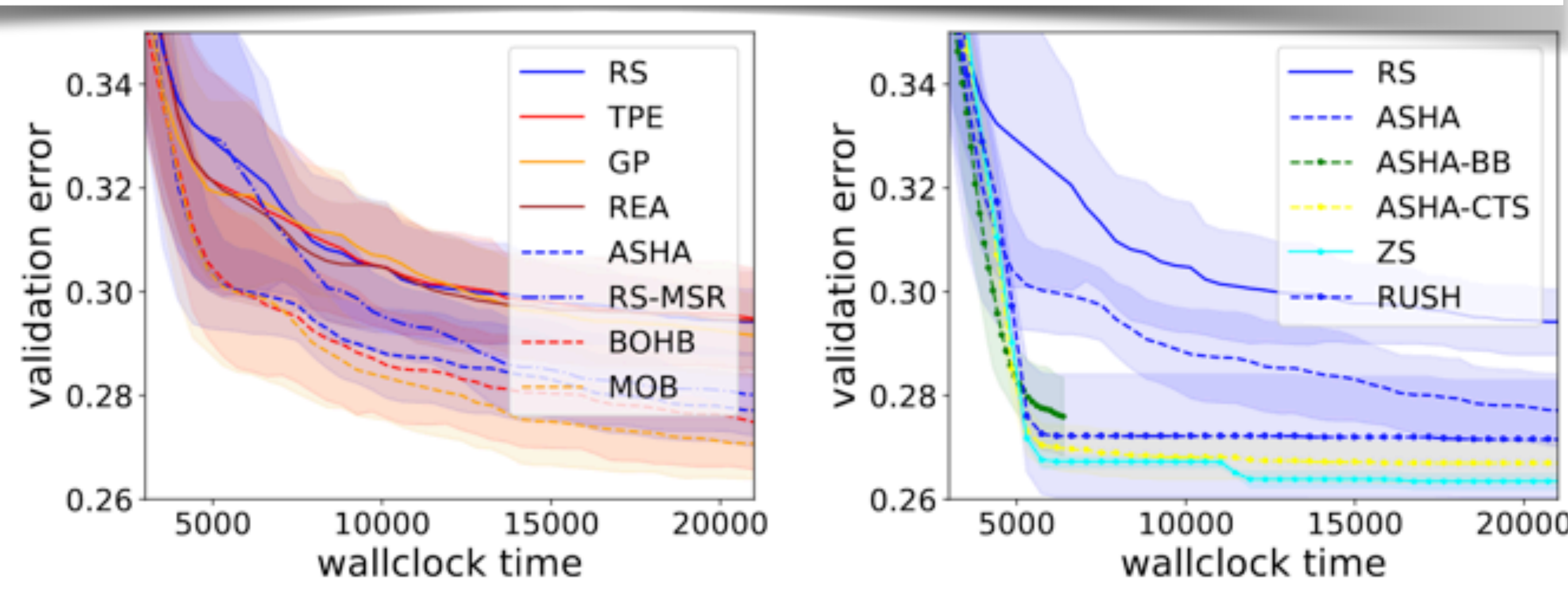


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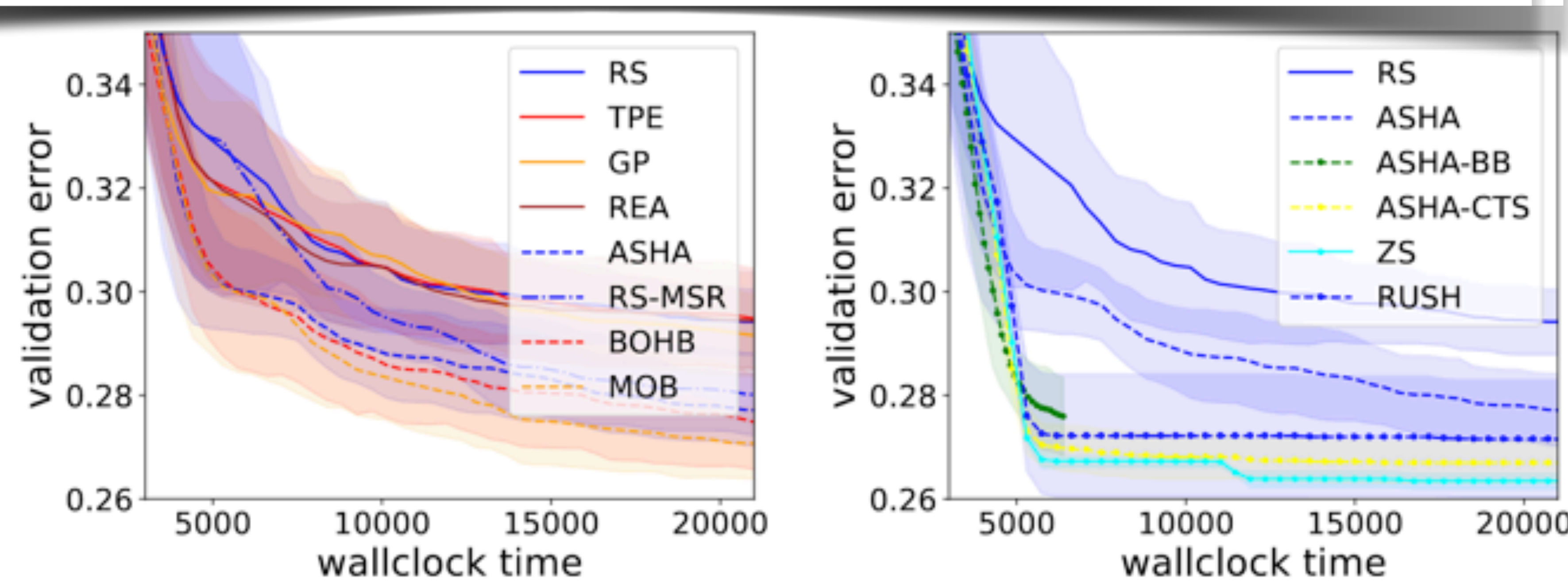
**My favourite transfer learning algorithm** ❤️ ❤️ ❤️

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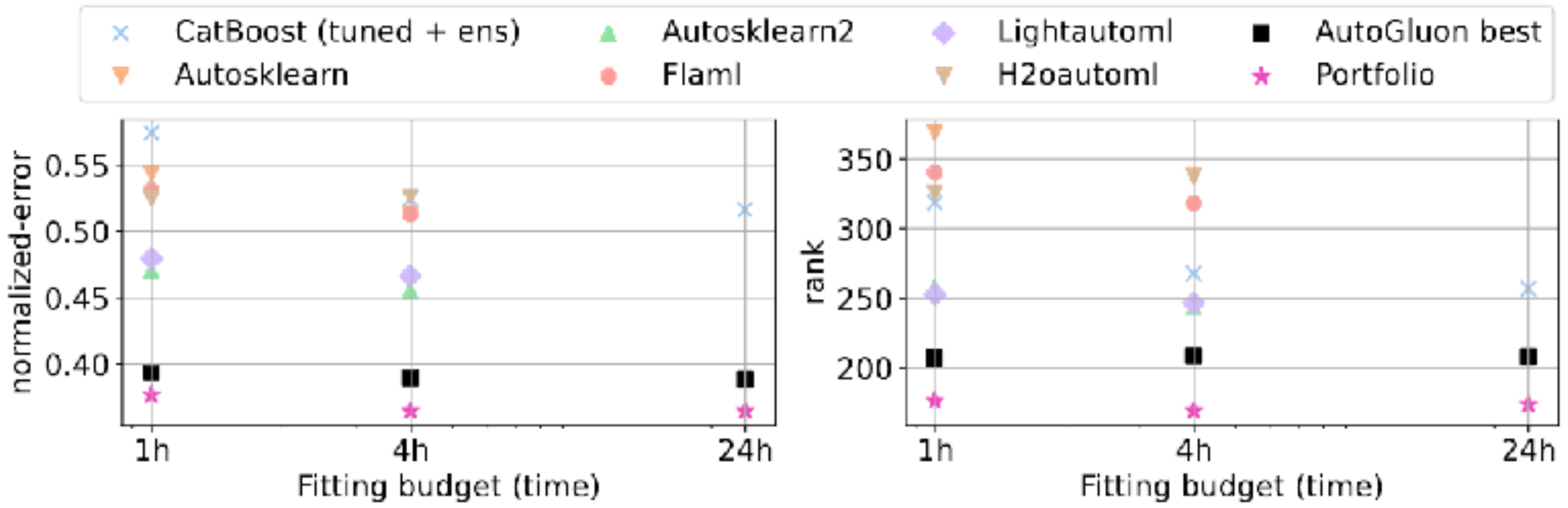

CatBoost (tuned + ens)
Autosklearn
Autosklearn2
Flaml
Lightautoml
H2oautoml
AutoGluon best
Portfolio
normalized-error
0.55
0.50
0.45
0.40
1h
4h
24h
Fitting budget (time)
rank
350
300
250
200
1h
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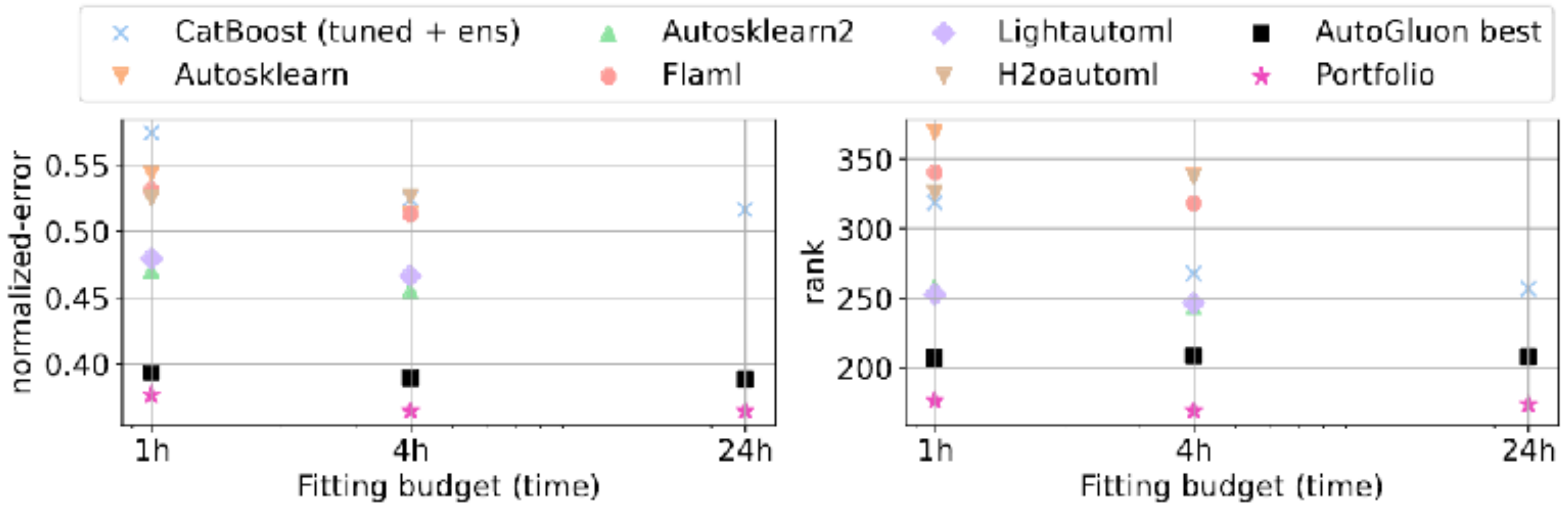

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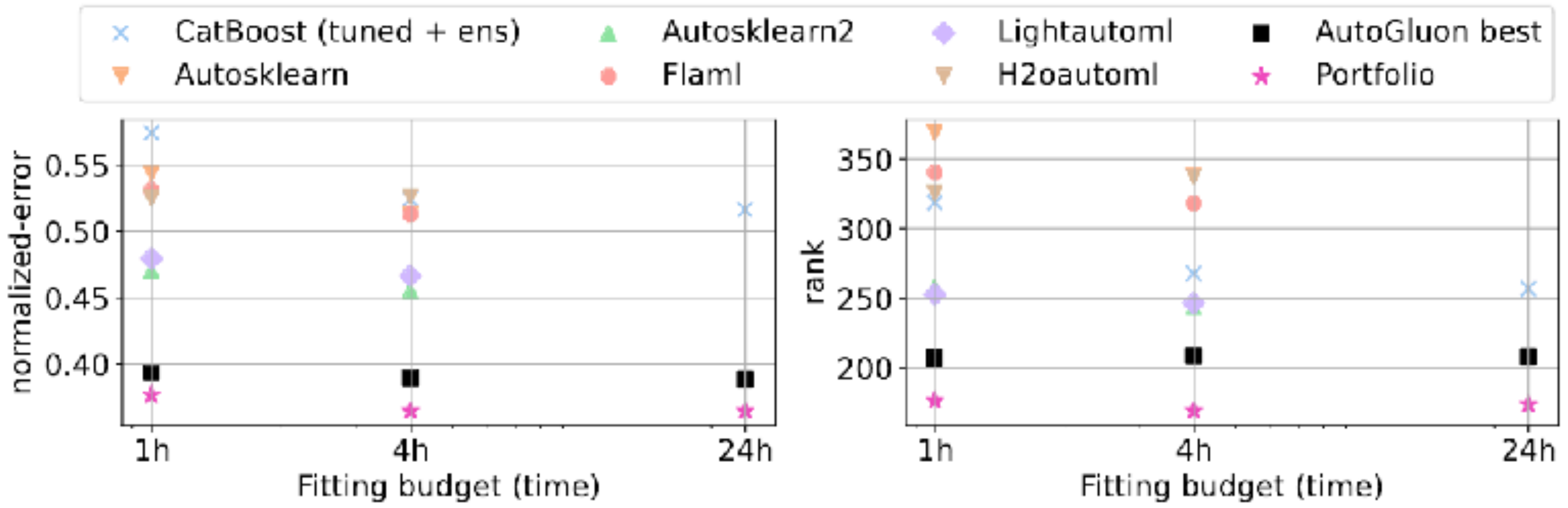

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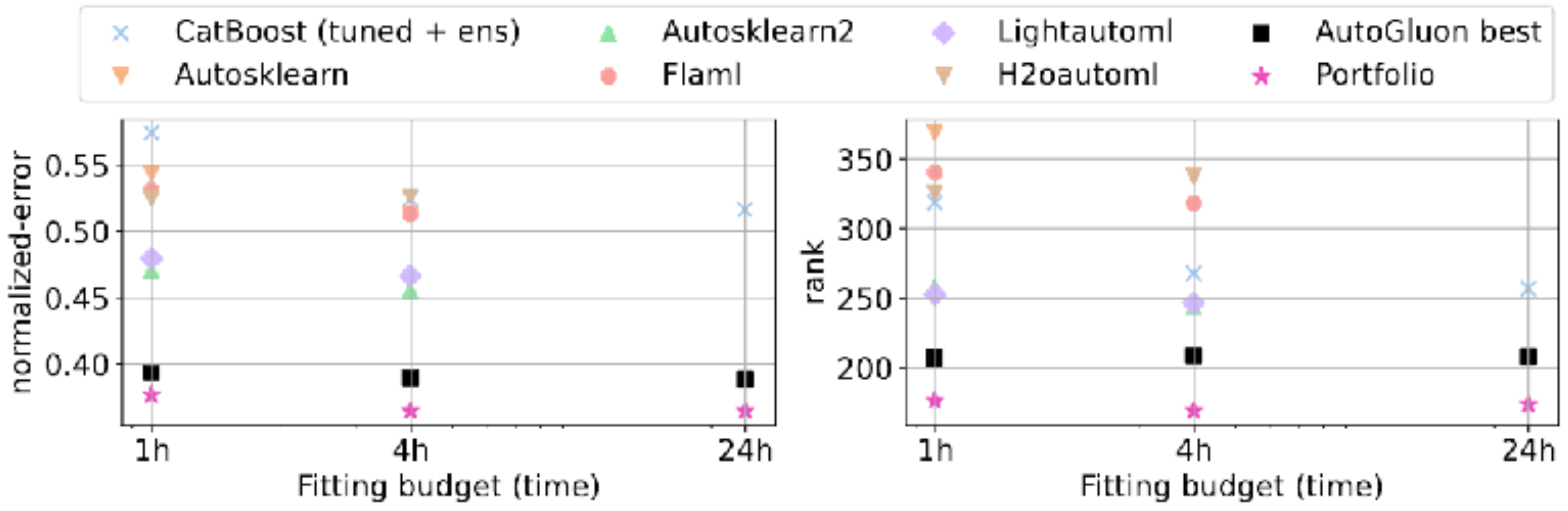


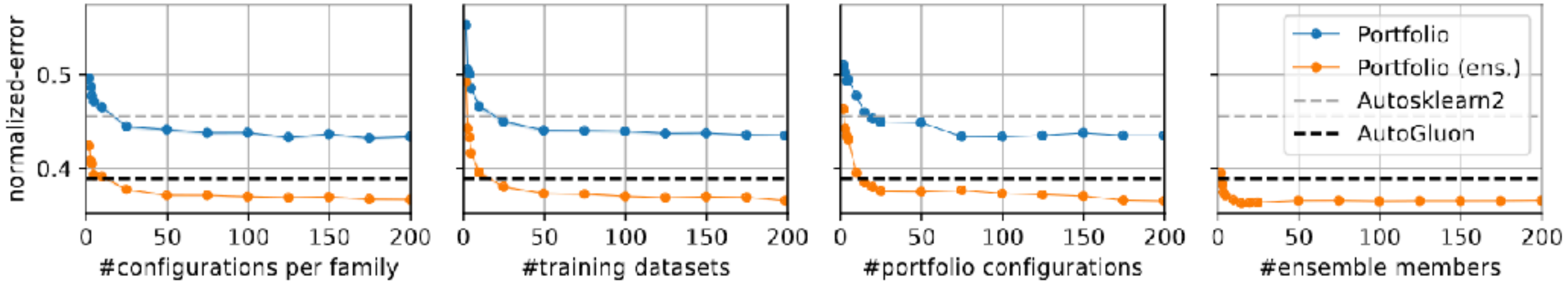


Figure 4: Impact on normalized error when varying the (a) number of configurations per family, (b) number of training datasets, (c) portfolio size and (d) number of ensemble members.

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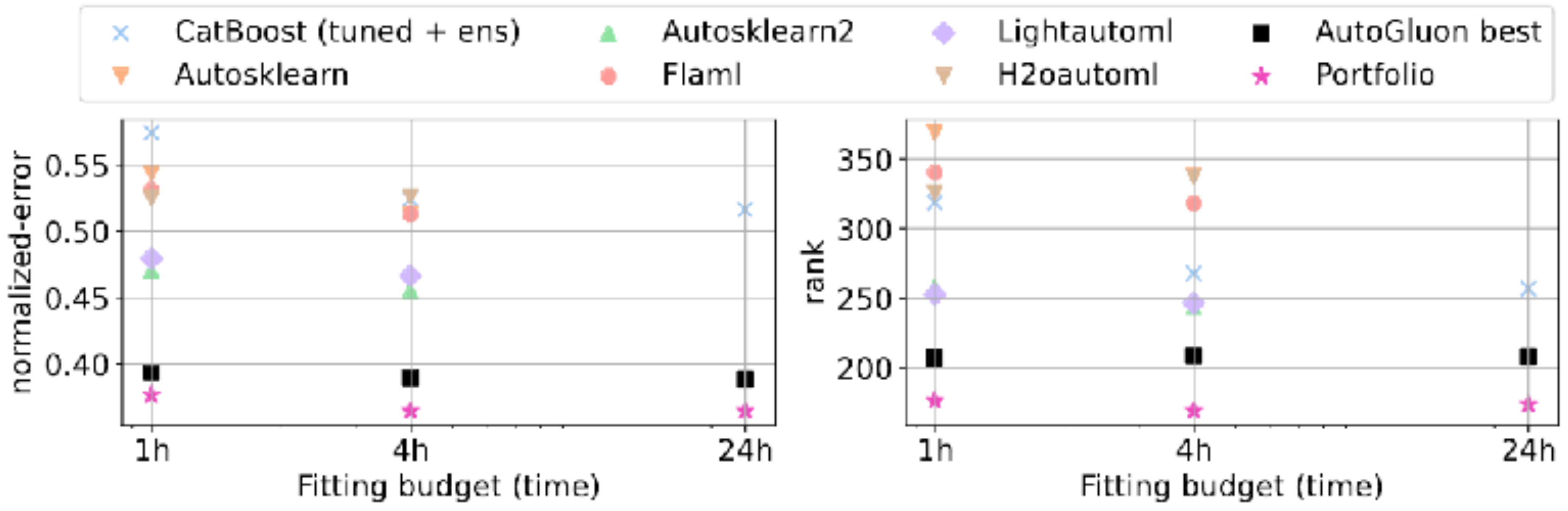


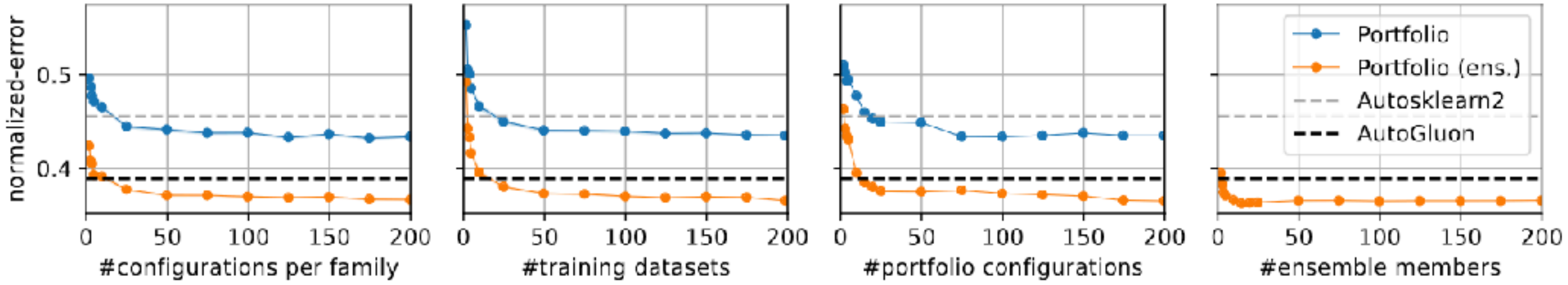


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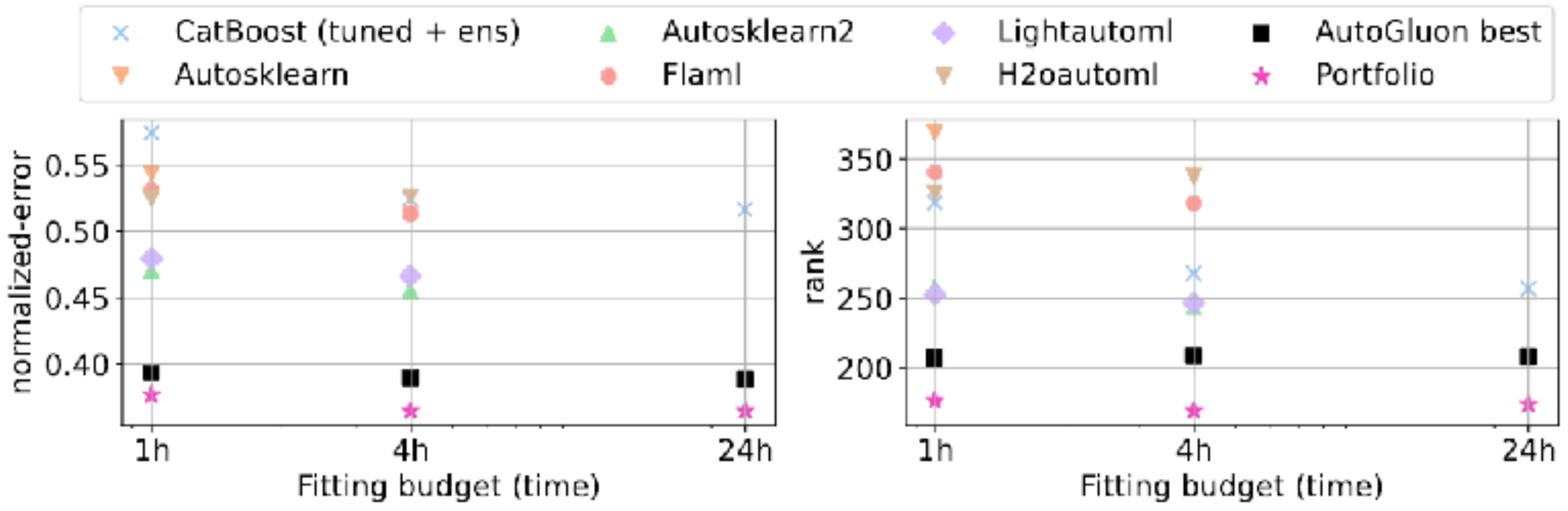
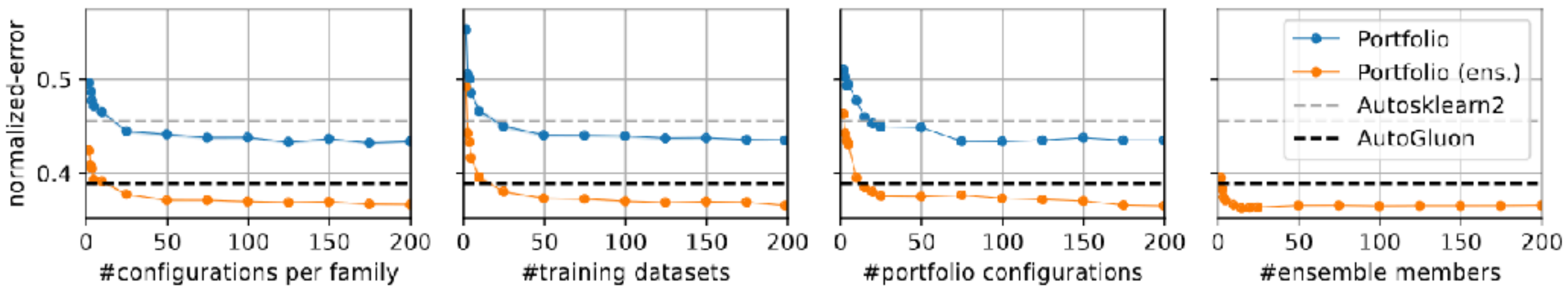



Table 2: Performance of AutoGluon combined with portfolios on AMLB.

| method | win-rate | loss reduc. |
|---|---|---|
| **AG + Portfolio (ours)** | - | 0% |
| AG | 67% | 2.8% |
| MLJAR | 81% | 22.5% |
| lightautoml | 83% | 11.7% |
| GAMA | 86% | 15.5% |
| FLAML | 87% | 16.3% |
| autosklearn | 89% | 11.8% |
| H2OAutoML | 92% | 10.3% |
| CatBoost | 94% | 18.1% |
| TunedRandomForest | 94% | 22.9% |
| RandomForest | 97% | 25.0% |
| XGBoost | 98% | 20.9% |
| LightGBM | 98% | 23.6% |

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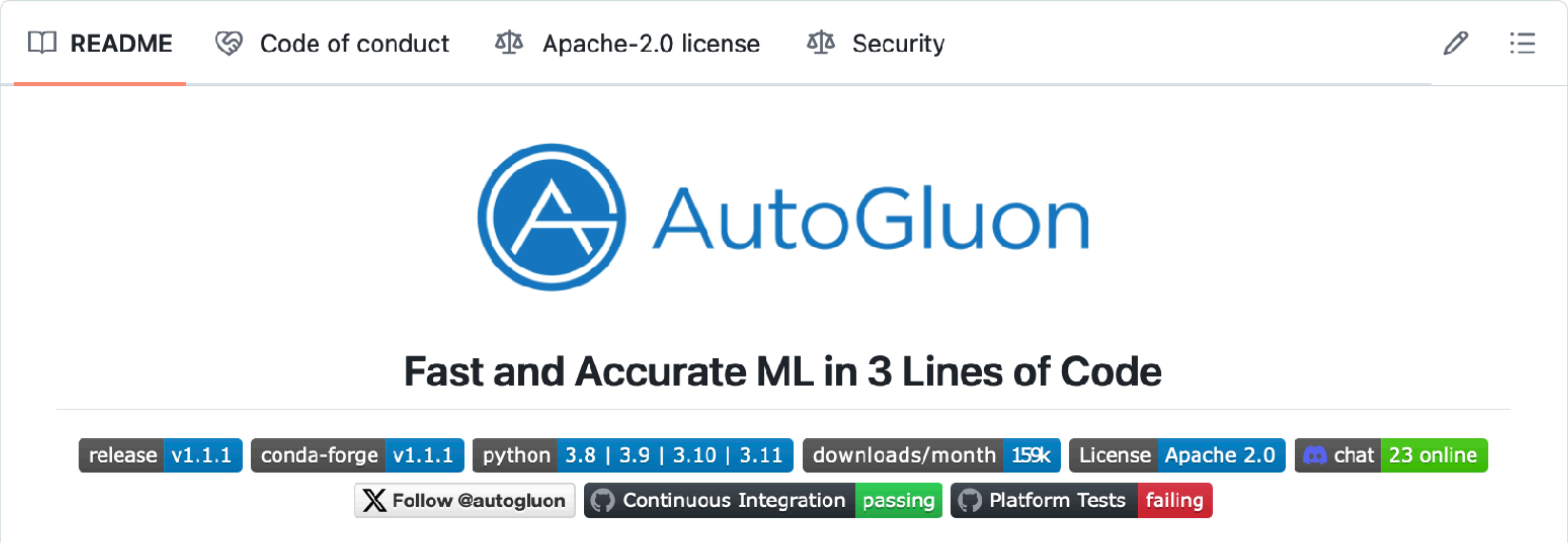


https://github.com/autogluon/autogluon

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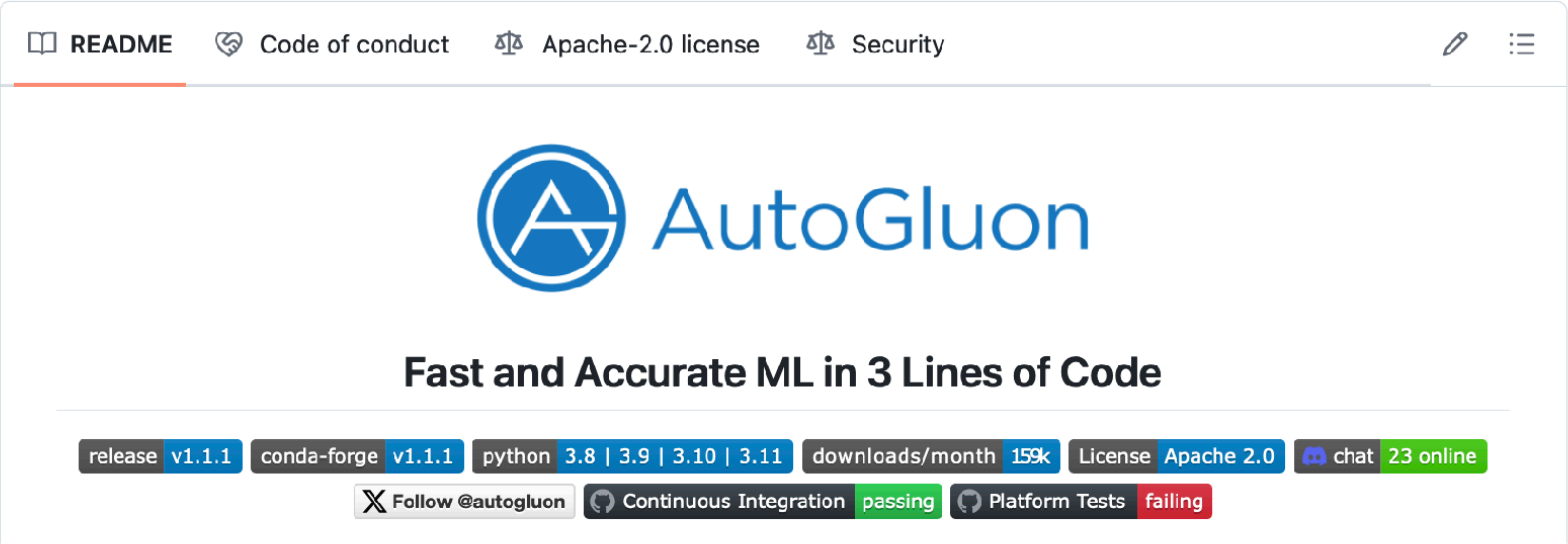
- State of the art for tabular prediction and time series forecasting

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# Code and libraries

# Code

## HPO Libraries that support transfer learning

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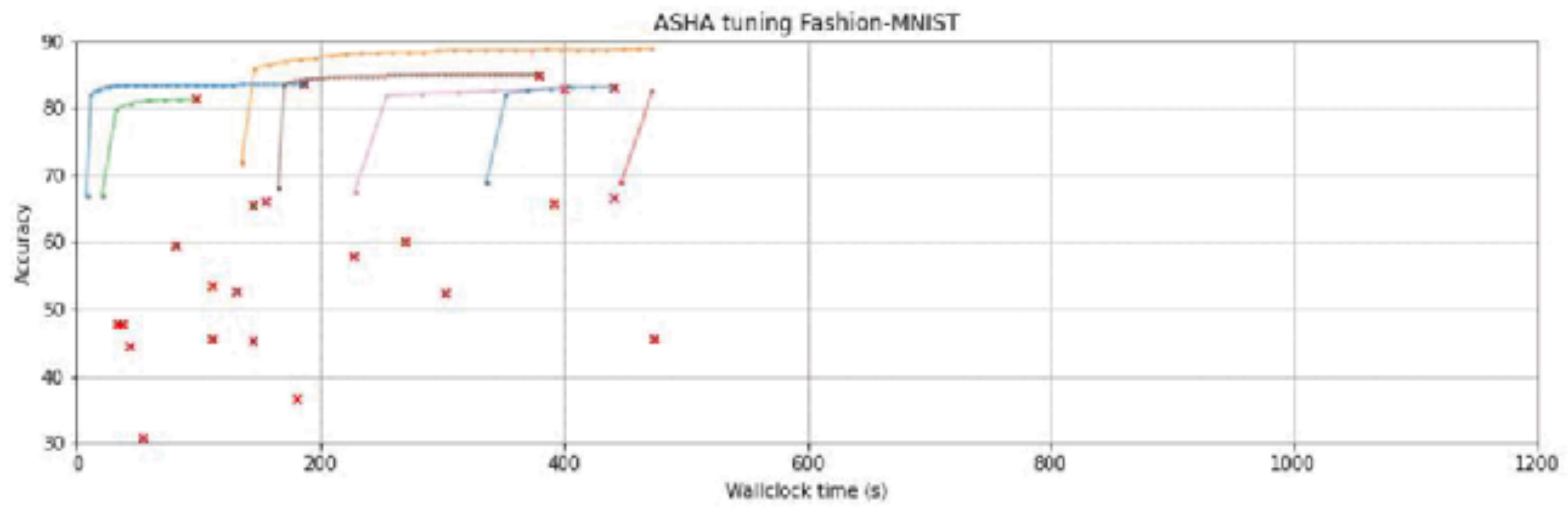
README | Code of conduct | Apache-2.0 license | License | Security

### Syne Tune: Large-Scale and Reproducible Hyperparameter Optimization

release v0.13.0 | license Apache 2.0 | downloads/month 44k | docs passing | python 3.7 | 3.8 | 3.9 | codecov 64%




Documentation | Tutorials | API Reference | PyPI | Latest Blog Post

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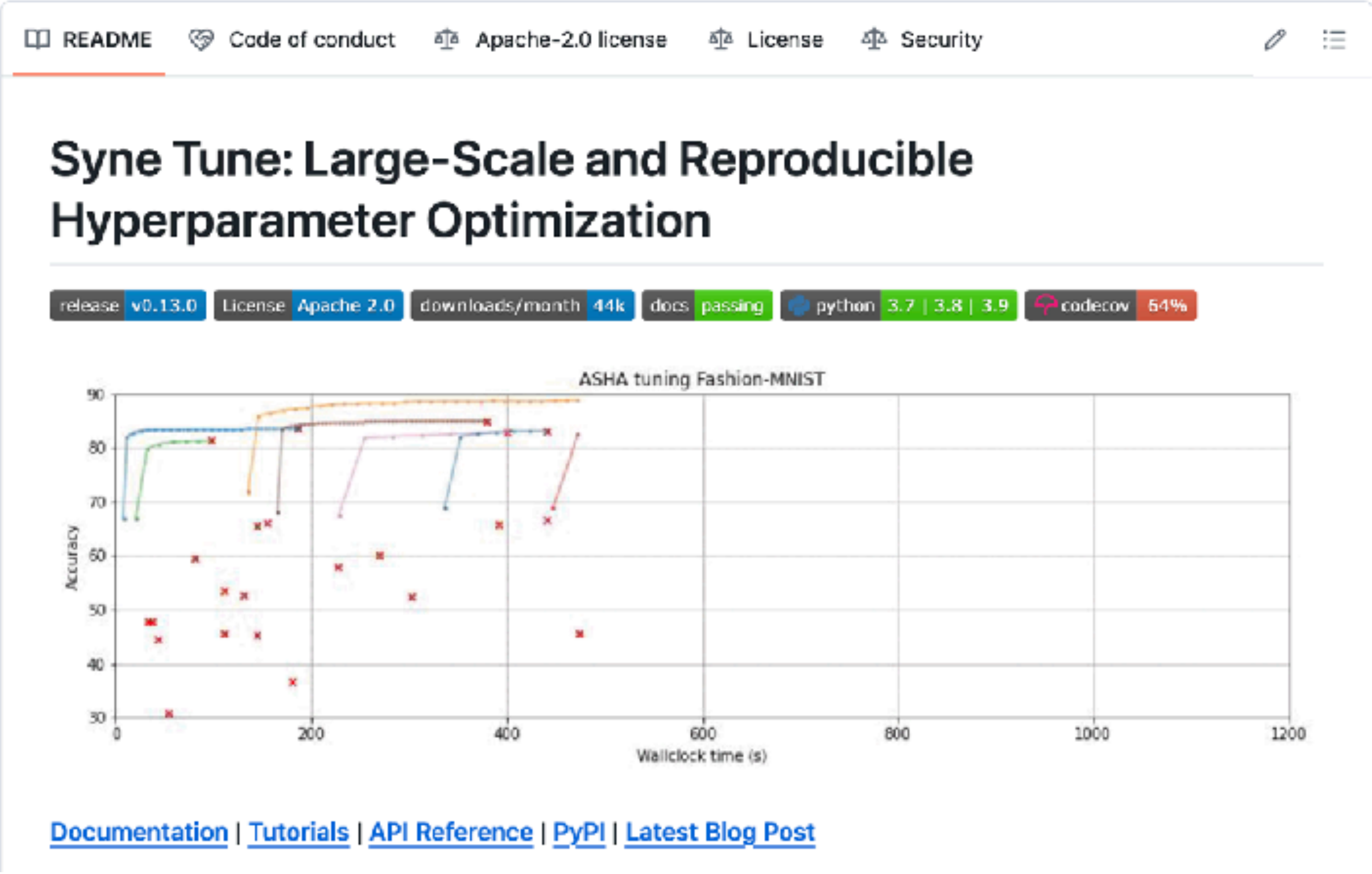

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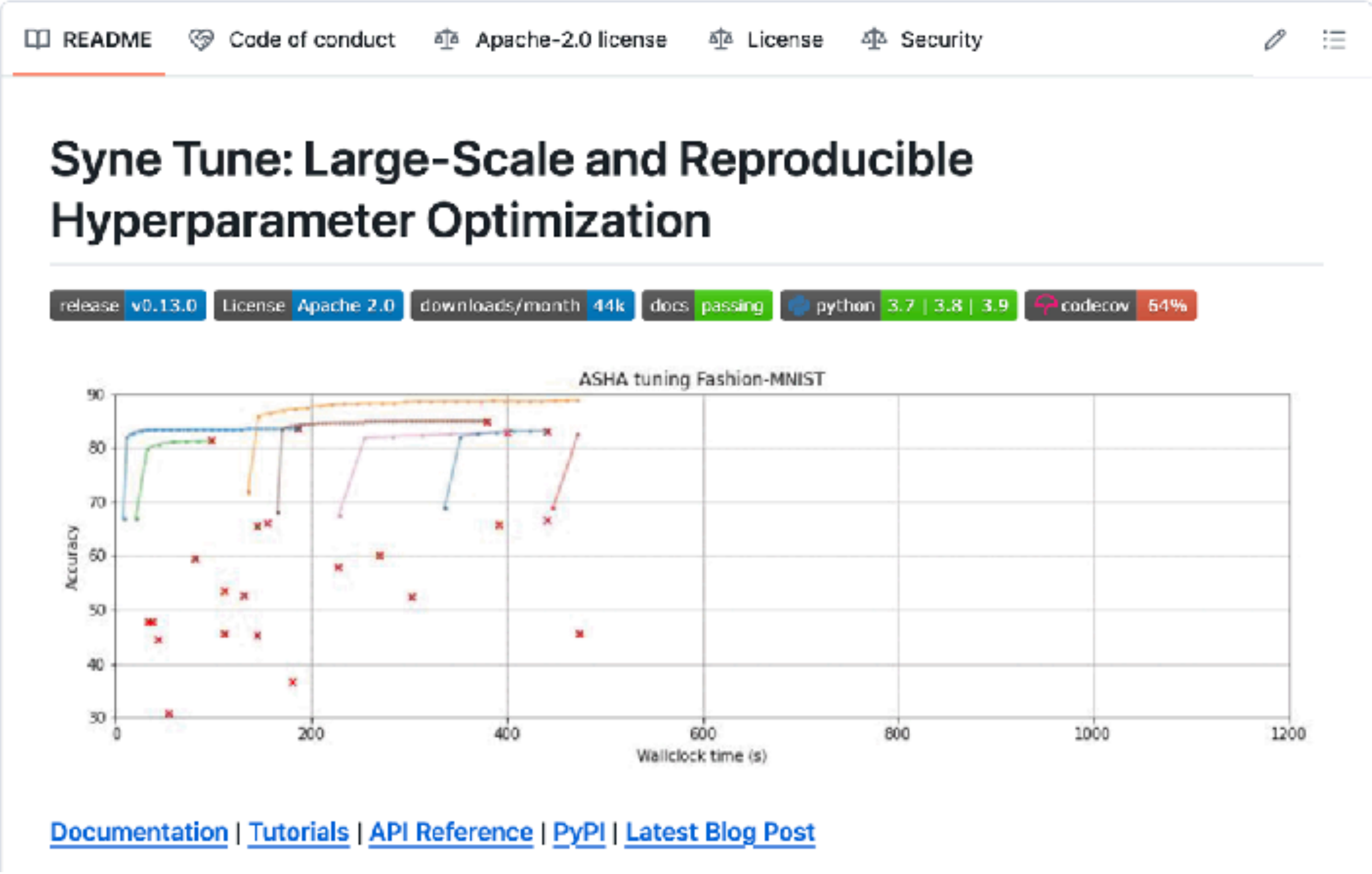

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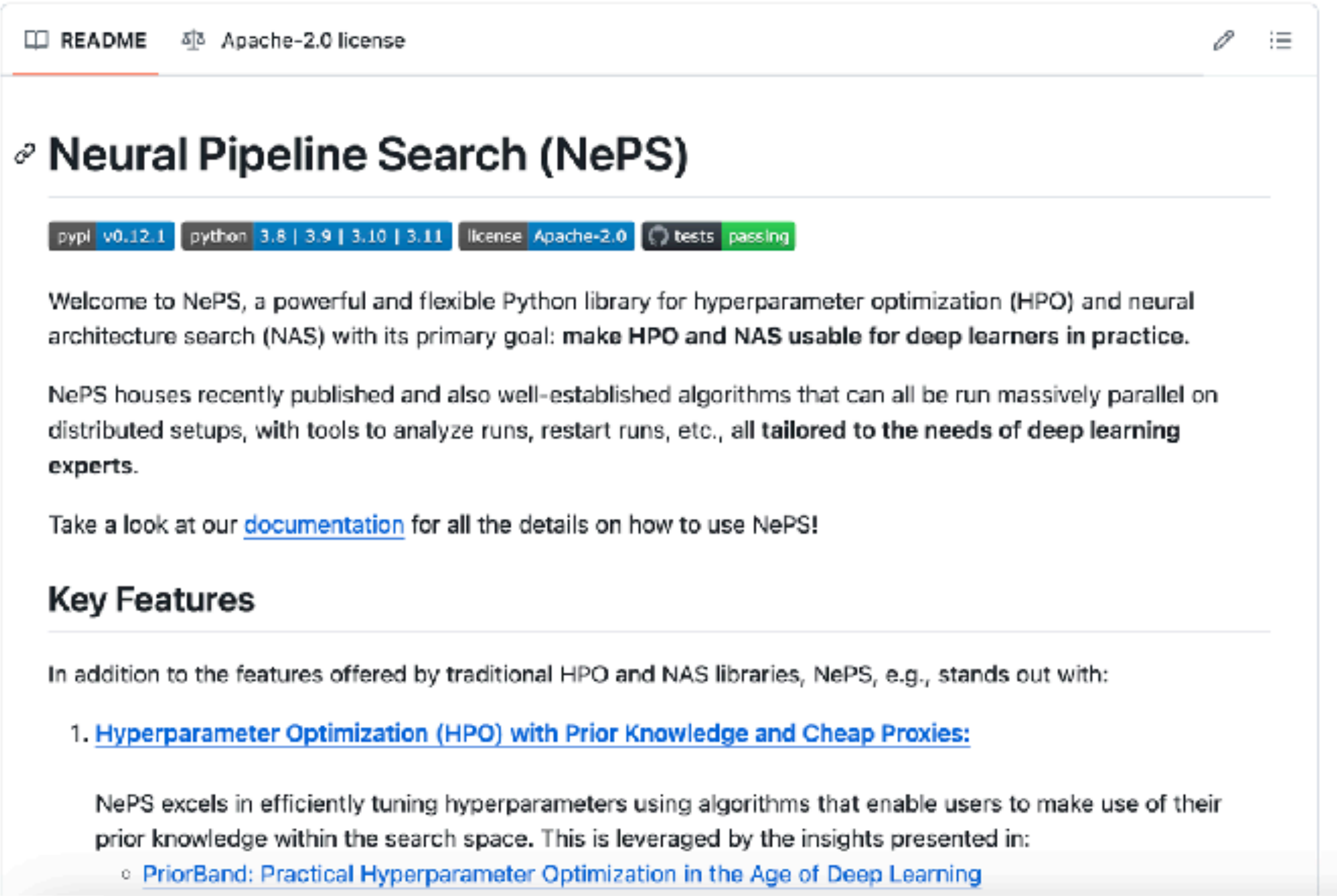

README | Apache-2.0 license

### Neural Pipeline Search (NePS)

pypi v0.12.1 | python 3.8 | 3.9 | 3.10 | 3.11 | license Apache-2.0 | tests passing

Welcome to NePS, a powerful and flexible Python library for hyperparameter optimization (HPO) and neural architecture search (NAS) with its primary goal: **make HPO and NAS usable for deep learners in practice.**

NePS houses recently published and also well-established algorithms that can all be run massively parallel on distributed setups, with tools to analyze runs, restart runs, etc., all **tailored to the needs of deep learning experts.**

Take a look at our documentation for all the details on how to use NePS!

#### Key Features

In addition to the features offered by traditional HPO and NAS libraries, NePS, e.g., stands out with:

1. **Hyperparameter Optimization (HPO) with Prior Knowledge and Cheap Proxies:**

   NePS excels in efficiently tuning hyperparameters using algorithms that enable users to make use of their prior knowledge within the search space. This is leveraged by the insights presented in:
   - PriorBand: Practical Hyperparameter Optimization in the Age of Deep Learning

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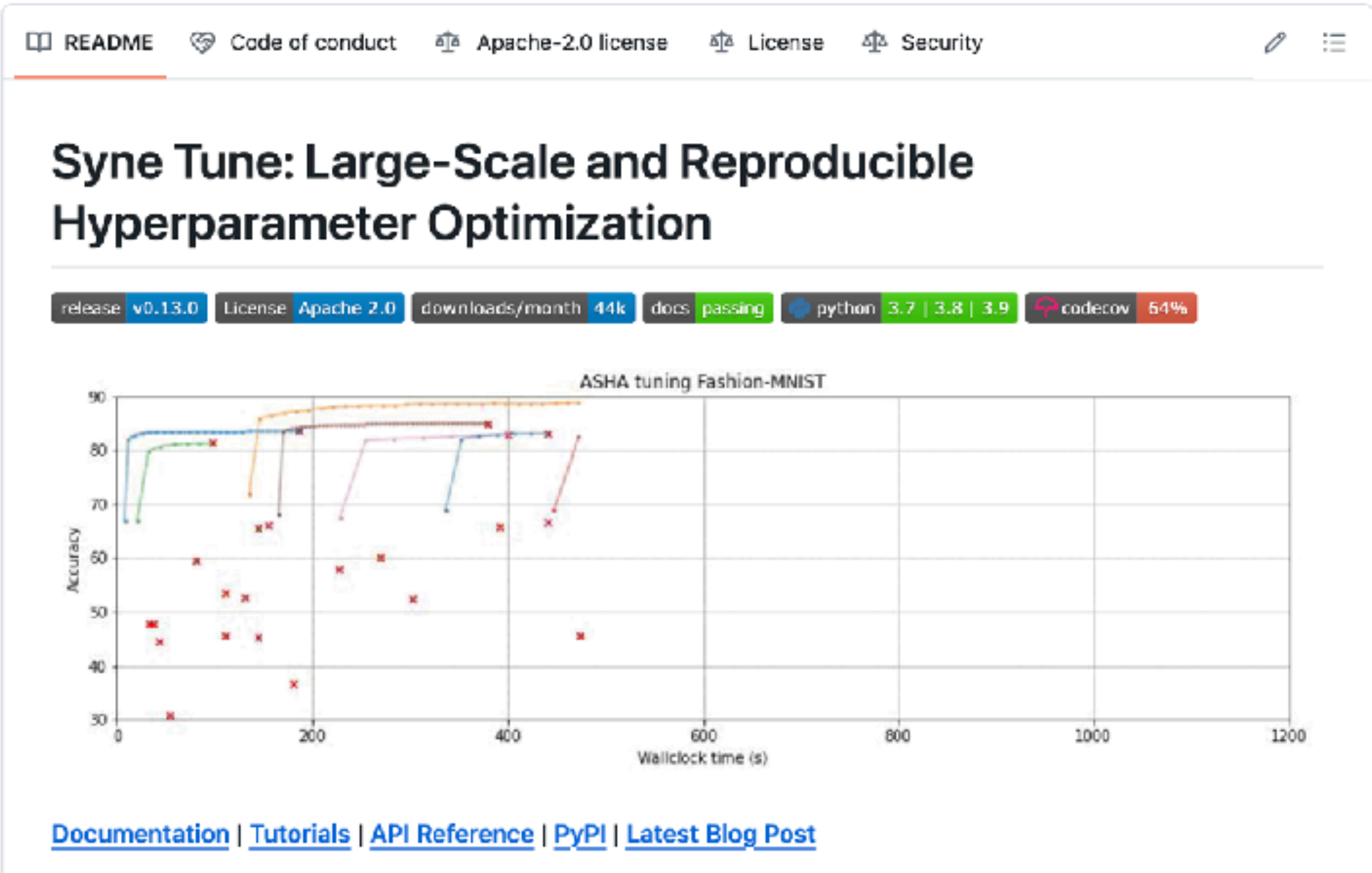
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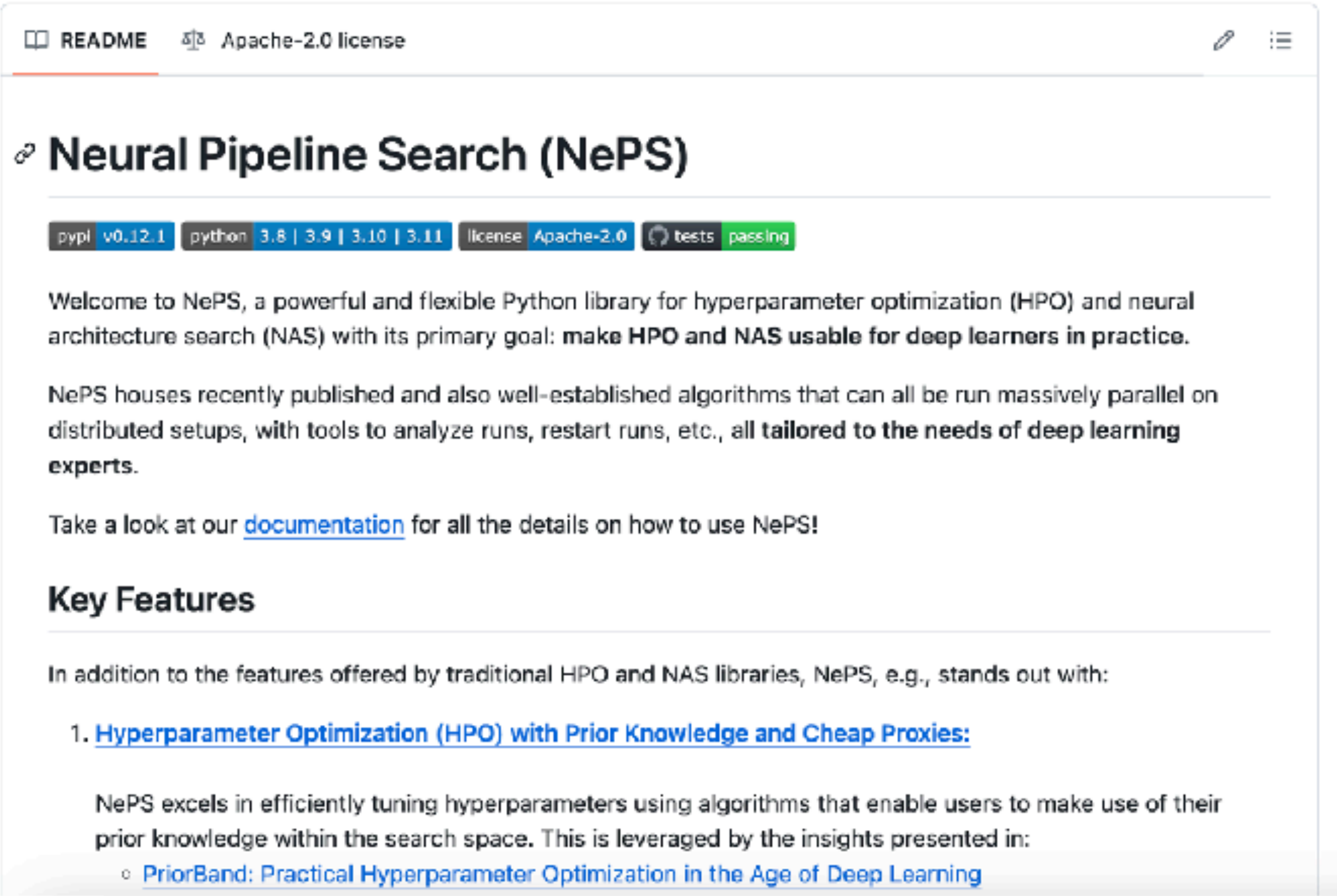
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  - Foundational approach
- Transfer learning can speed HPO significantly!