Auto-Sklearn: Automated Machine Learning in Python

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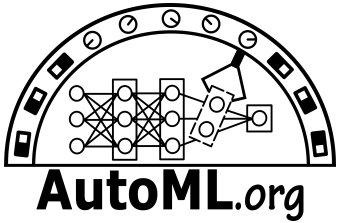


Our Vision

Machine Learning for everyone

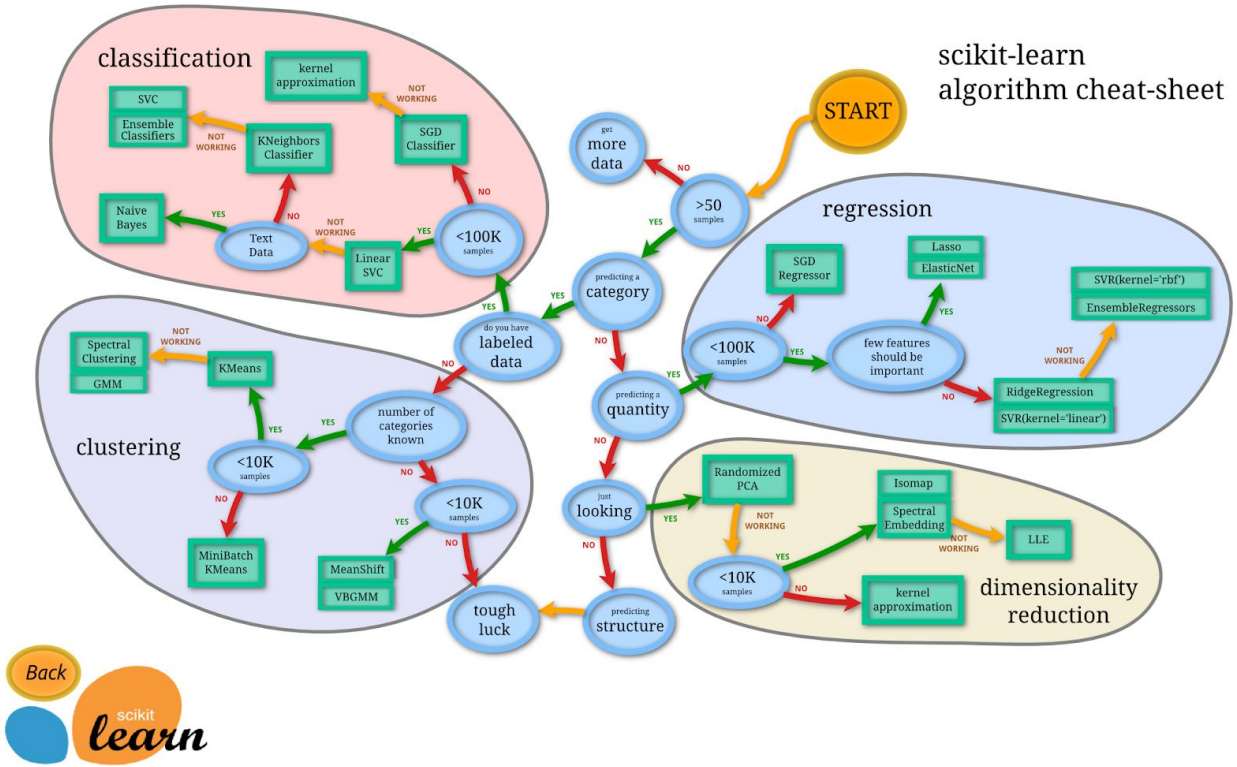
in 4 lines of code

```
import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

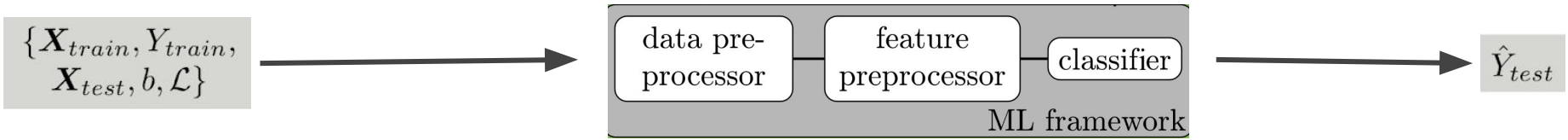
Goals for today

1. Get excited about AutoML
2. Understand how Auto-sklearn works
3. Learn how to apply Auto-sklearn

Why we need AutoML



Design Space: Traditional ML with scikit-learn



Design Space: Traditional ML with scikit-learn

$\{\boldsymbol{X}_{train}, Y_{train}, \boldsymbol{X}_{test}, b, \mathcal{L}\}$

preprocessor	#λ
extreml. rand. trees prepr.	5
fast ICA	4
feature agglomeration	4
kernel PCA	5
rand. kitchen sinks	2
linear SVM prepr.	3
no preprocessing	-
nystroem sampler	5
PCA	2
polynomial	3
random trees embed.	4
select percentile	2
select rates	3
one-hot encoding	2
imputation	1
balancing	1
rescaling	1

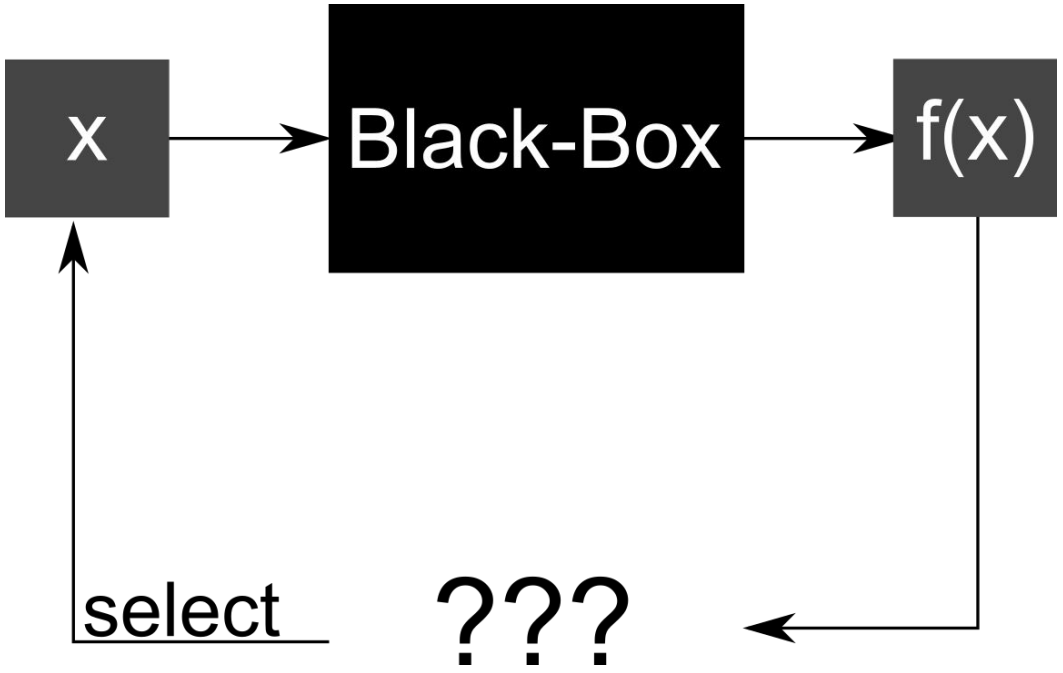
classifier	#λ
AdaBoost (AB)	4
Bernoulli naïve Bayes	2
decision tree (DT)	4
extreml. rand. trees	5
Gaussian naïve Bayes	-
gradient boosting (GB)	6
kNN	3
LDA	4
linear SVM	4
kernel SVM	7
multinomial naïve Bayes	2
passive aggressive	3
QDA	2
random forest (RF)	5
Linear Class. (SGD)	10

$\hat{Y}_{test}$

Black Box Optimization

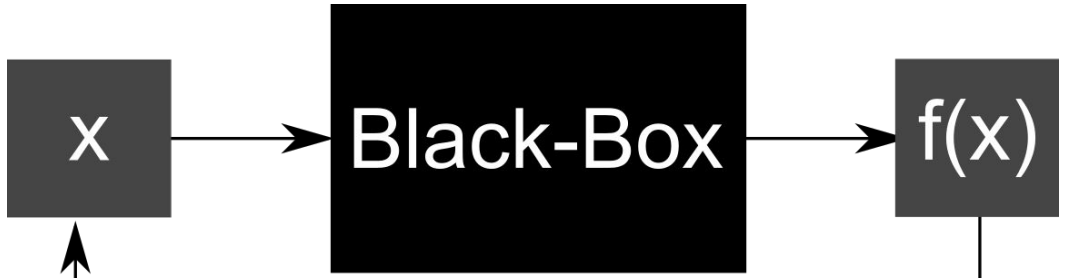
This is your ML pipeline

This is a configuration of a ML pipeline



This measures performance of your pipeline

Black Box Optimization: The Human Optimizer

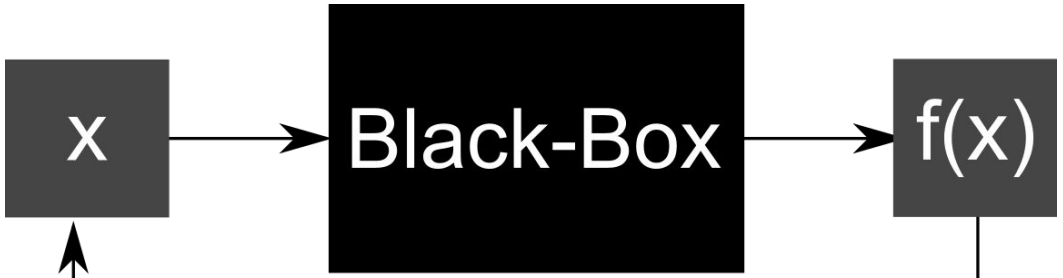


- You'll learn a lot about your system

select

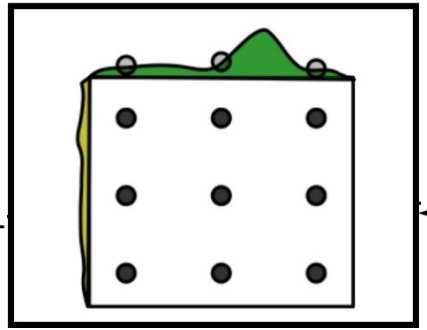
- Not very efficient
- Error-prone
- Requires expert knowledge

Black Box Optimization: Grid Search

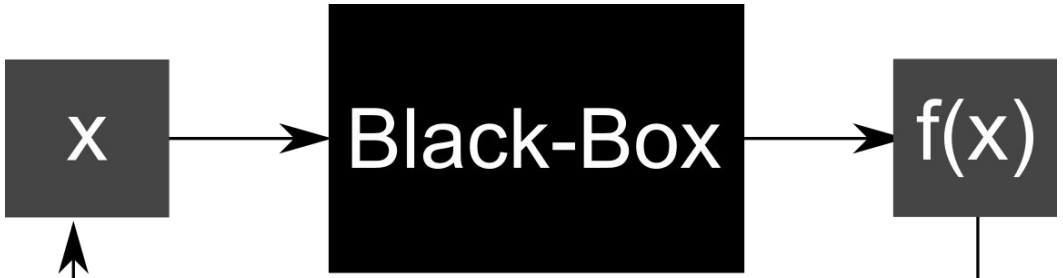


- Very simple approach
- Easily parallelizable
- Can be used to study the problem

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

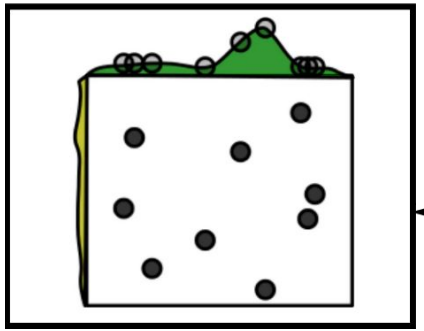


Black Box Optimization: Random Search



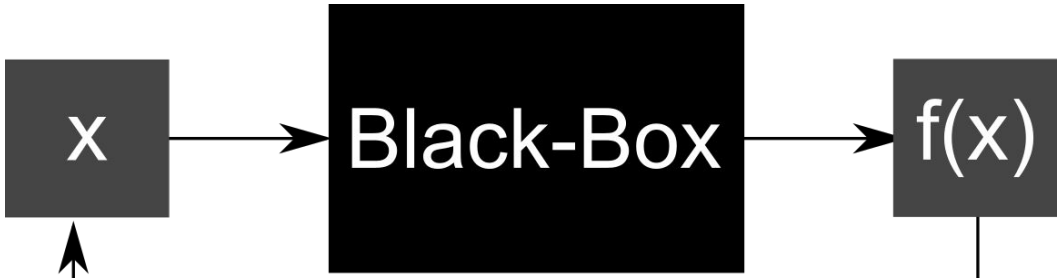
- Even simpler
- Easily parallelizable
- Eventually converges to optimum

select



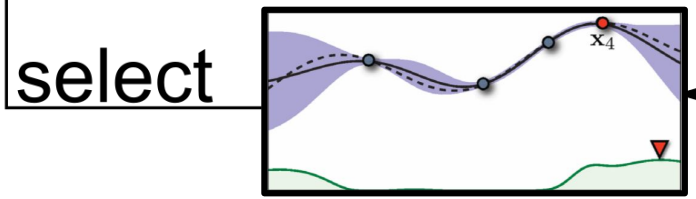
- Not data efficient
- Computationally expensive

Black Box Optimization: Bayesian Optimization

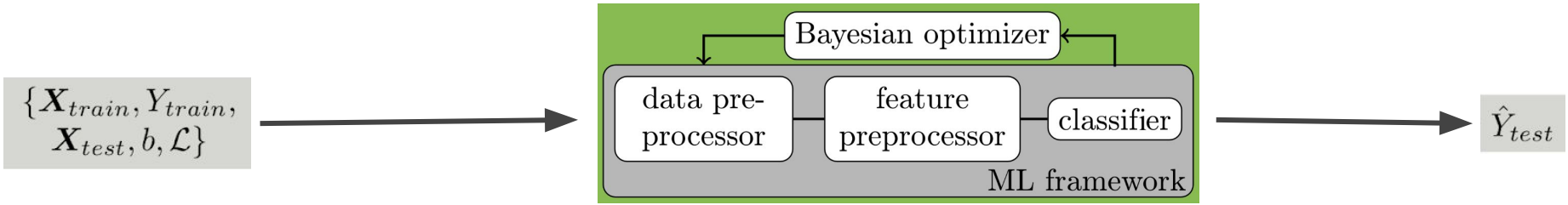


- Trade-off Exploration & Exploitation
- Data efficient
- State-of-the-art

- (Does not scale well with parallel resources)

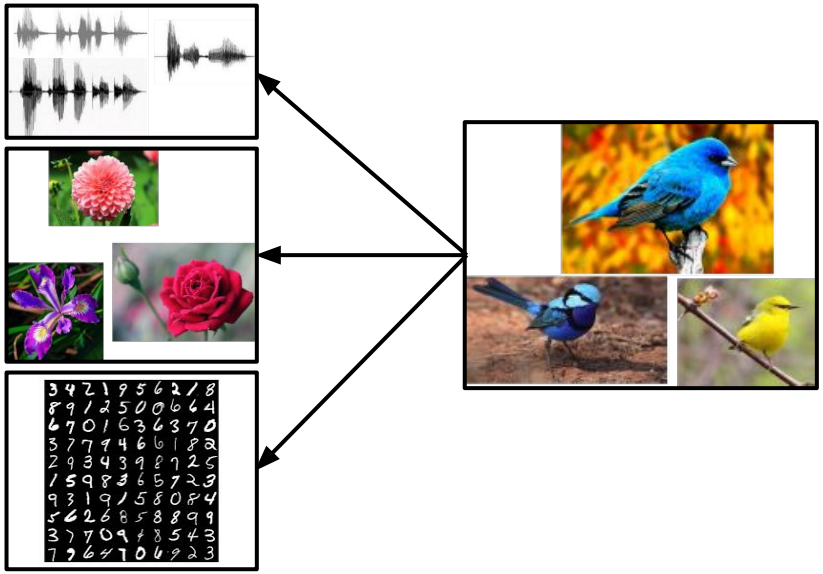


Design Space: Traditional ML with scikit-learn



How to reuse previous experience?

→ Warmstart Bayesian Optimization



Offline / Before:

1) Collect >200 datasets
2) Find the best pipeline on each dataset

Online / For a new dataset:

1) Compute 38 meta-features, select 25 most similar previous datasets
2) Initialize optimization with best pipelines on those datasets

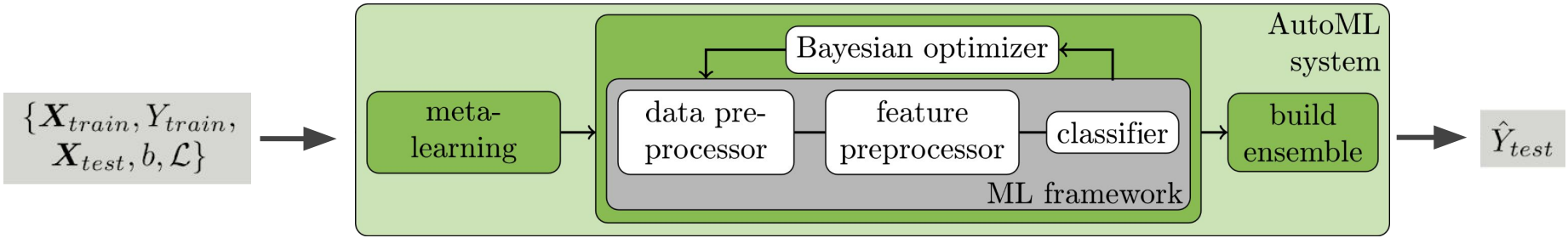
More II: Ensembling

How to get the best out of all evaluated models?

→ **Build an ensemble**

Image credit: Photo by Denisse Leon

Auto-Sklearn 1.0



However, some things to be improved

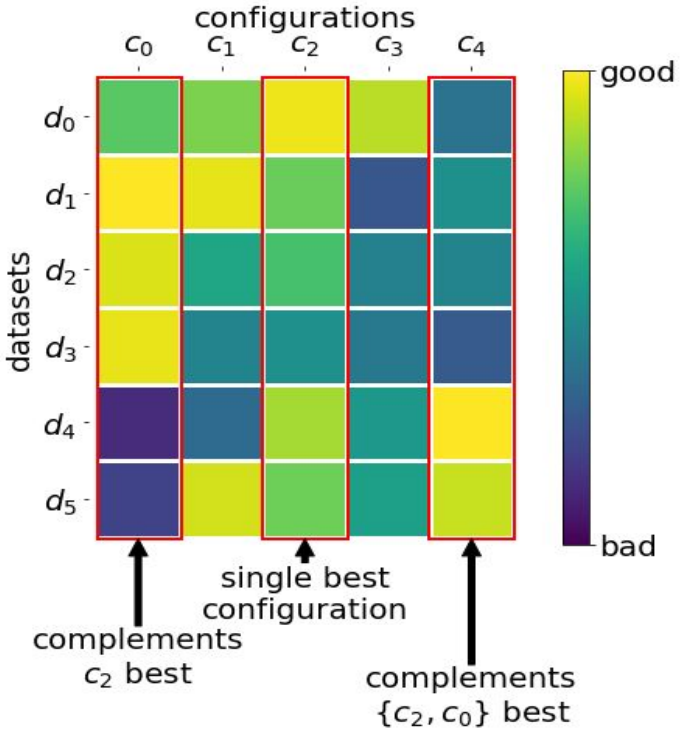
- meta-features can be expensive to compute
- large datasets can be an issue

Feurer et al. (2015): Efficient and Robust Automated Machine Learning (NeurIPS'15)

Even More I: Portfolios

Goal: Meta-Learning without meta-features

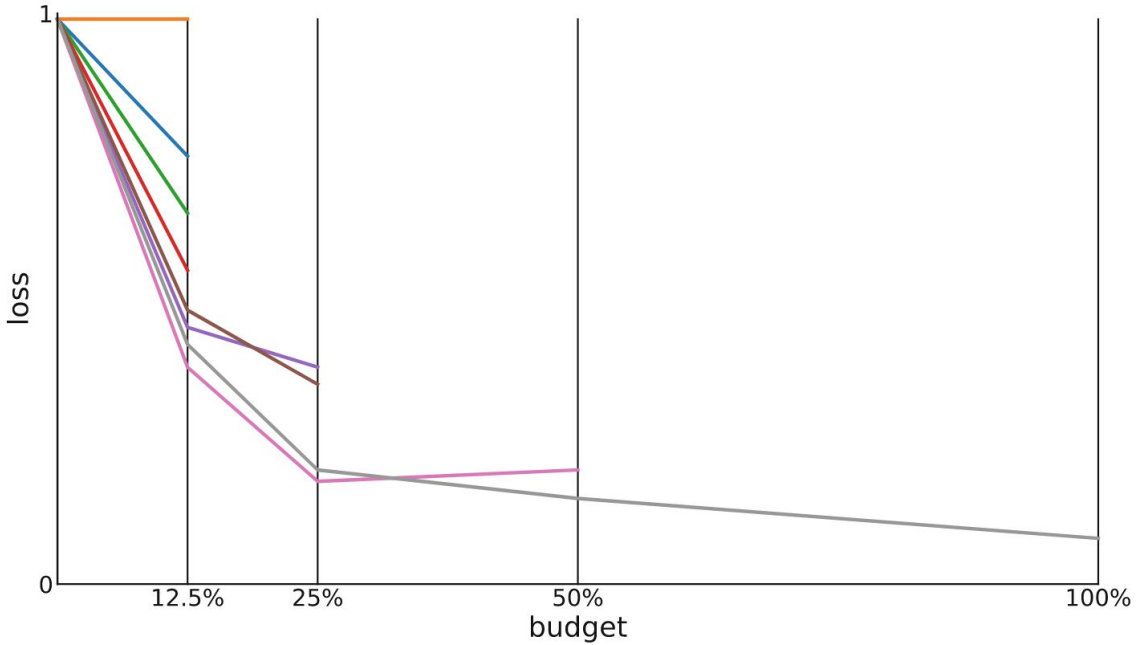
Idea: Construct a Portfolio (a list of diverse pipelines)



Even More II: Successive Halving

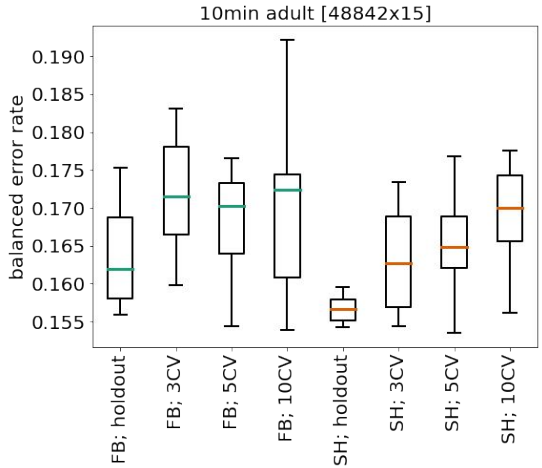
Goal: Scale to large datasets.

Idea: Allocate more resources to promising pipelines



But what about small datasets?

Impact of the Optimization Strategy



But wait … did we make it worse?

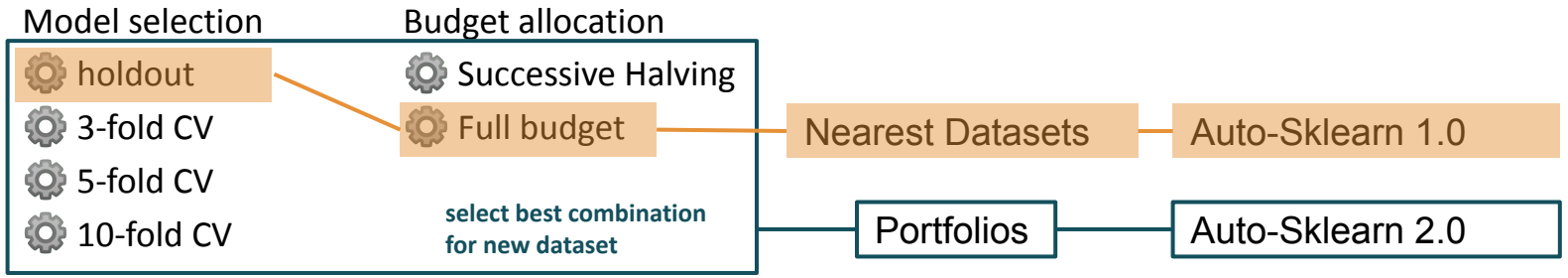
Can we automatically select an optimization policy?

Image Credit - CC BY-NC-ND 2.0; by Beagle Mama

Yes, with a learned selector!

For more details see “Feurer et al. (2021): Auto-Sklearn 2.0: Hands-free AutoML via Meta-Learning“

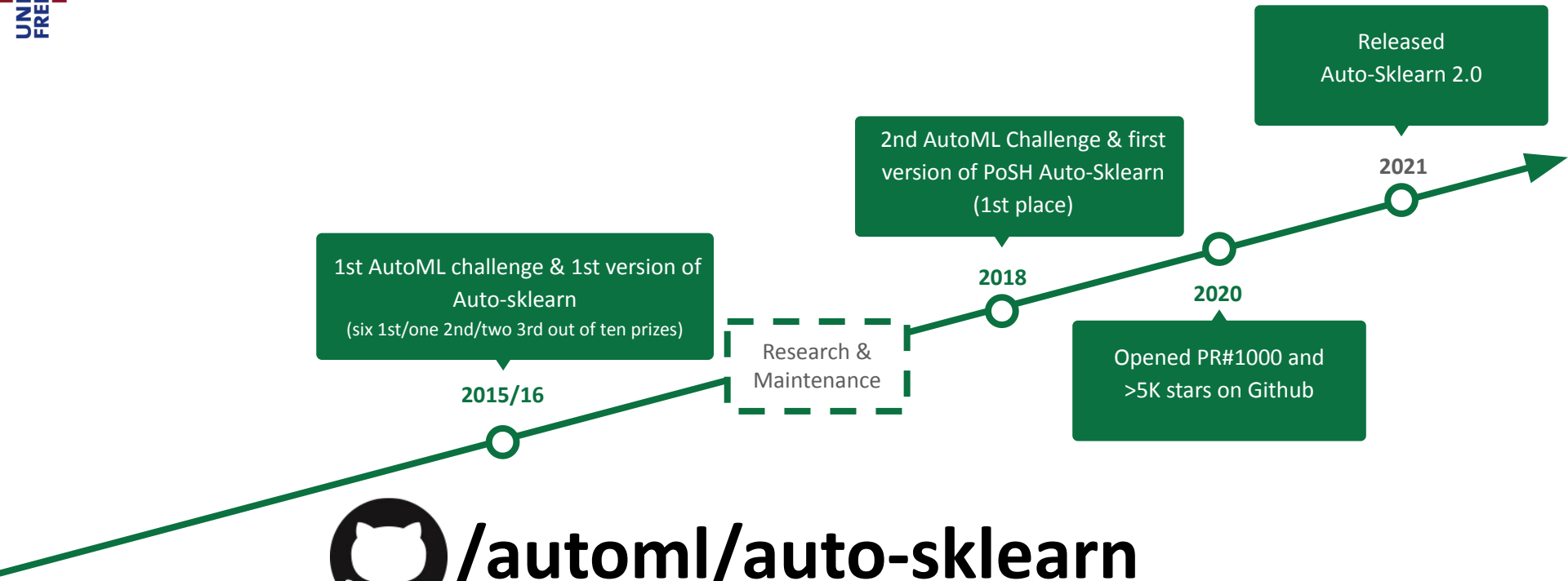
PoSH-Auto-sklearn



	10MIN		60MIN	
	∅	std	∅	std
Auto-sklearn (1.0)	16.21	0.27	7.17	0.30

Feurer et al. (2021): Auto-Sklearn 2.0: Hands-free AutoML via Meta-Learning

Timeline & Success Stories



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Summary

```
import autosklearn.classification
>>> cls = autosklearn.classification.AutoSklearnClassifier()
>>> cls.fit(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

- based on **scikit-learn; simple & familiar API**
- integrates **latest research** (**>1K citations**)
- **>20K** downloads per month

- **BSD-3-Clause** License
- works best under **Linux**
- requires **Python>=3.7**

/automl/auto-sklearn

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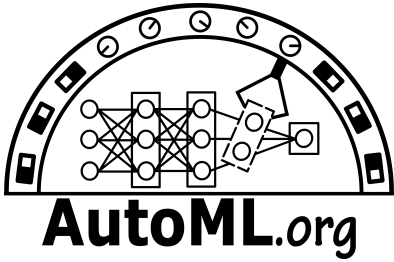
Now: **Demo Session**

/automl/auto-sklearn-talks

Want to learn more?

- automl.org:
  - Book on “AutoML: Methods, Systems, Challenges”
  - Infos on upcoming talks and events

- AutoML Fall School: Nov 8th - 12th 2021
  - hands-on session with open-source packages
  - networking sessions
  - invited talks from leading experts



Thank you!

→ If you like this, leave a star on Github

/automl/auto-sklearn

→ If you're using auto-sklearn, drop us an email

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