Scalable Automatic Machine Learning in H2O

Argentina Data Science Meetup
Oct 3, 2019

H_2O.ai

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@ledell

What is H2O?

H2O.ai, the company

- Founded in 2012
- Advised by Stanford Professors Hastie, Tibshirani & Boyd
- Headquarters: Mountain View, California, USA

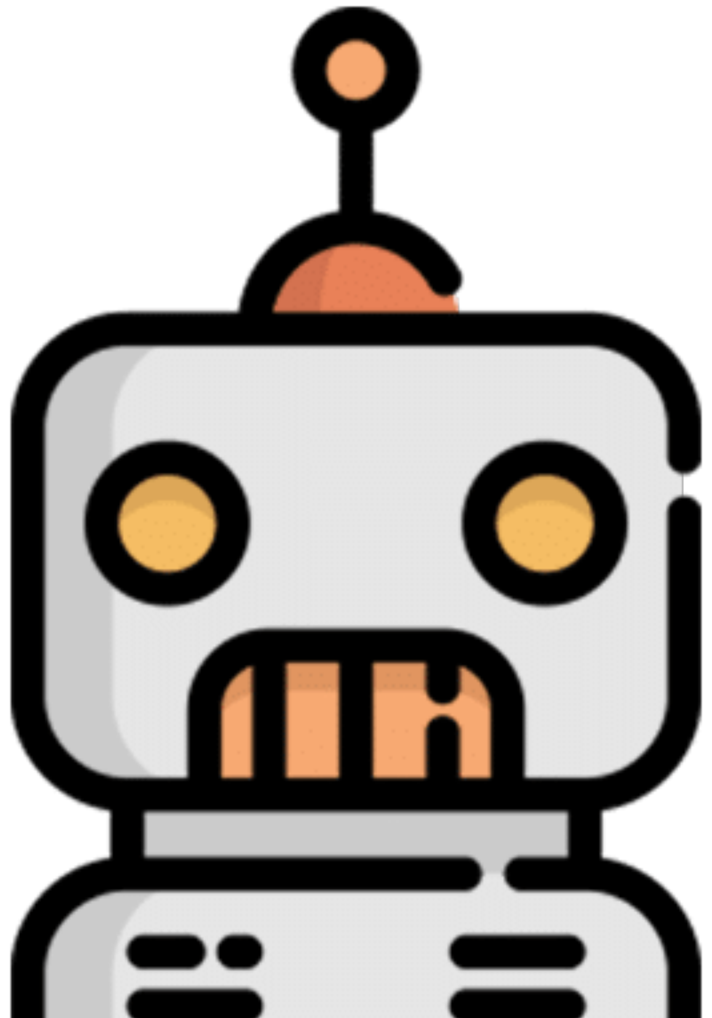
H2O, the platform

- Open Source Software (Apache 2.0 Licensed)
- R, Python, Scala, Java and Web Interfaces
- Distributed Machine Learning Algorithms for Big Data

Agenda

- H2O Platform
- Automatic Machine Learning (AutoML)
- H2O AutoML Overview
- Tutorials

Slides ⬇️ https://tinyurl.com/automl-dsa



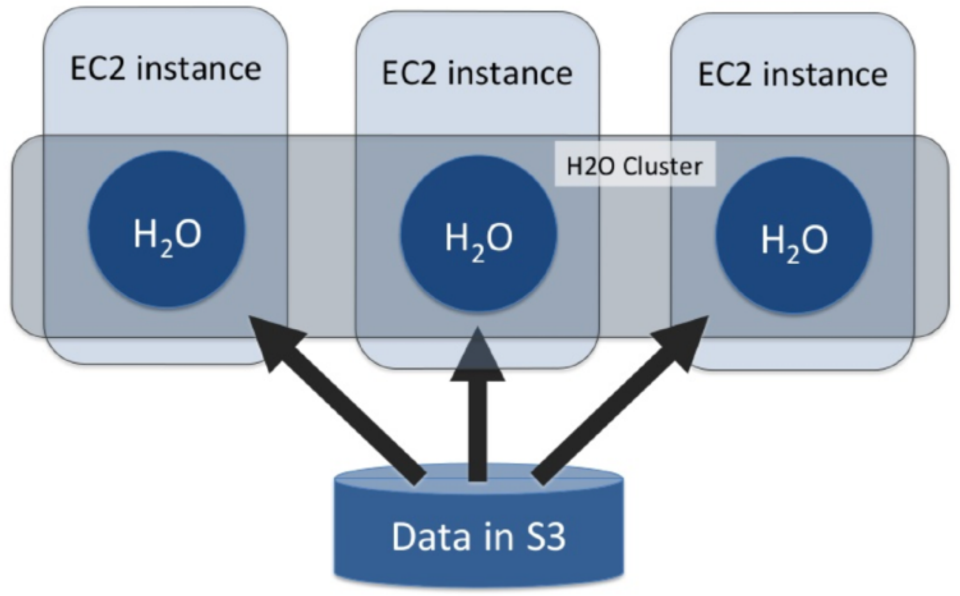
H2O Platform

H2O Machine Learning Platform

- Distributed (multi-core + multi-node) implementations of cutting edge ML algorithms.
- Core algorithms written in high performance Java.
- APIs available in R, Python, Scala; web GUI.
- Easily deploy models to production as pure Java code.
- Works on Hadoop, Spark, EC2, your laptop, etc.

H2O Distributed Computing

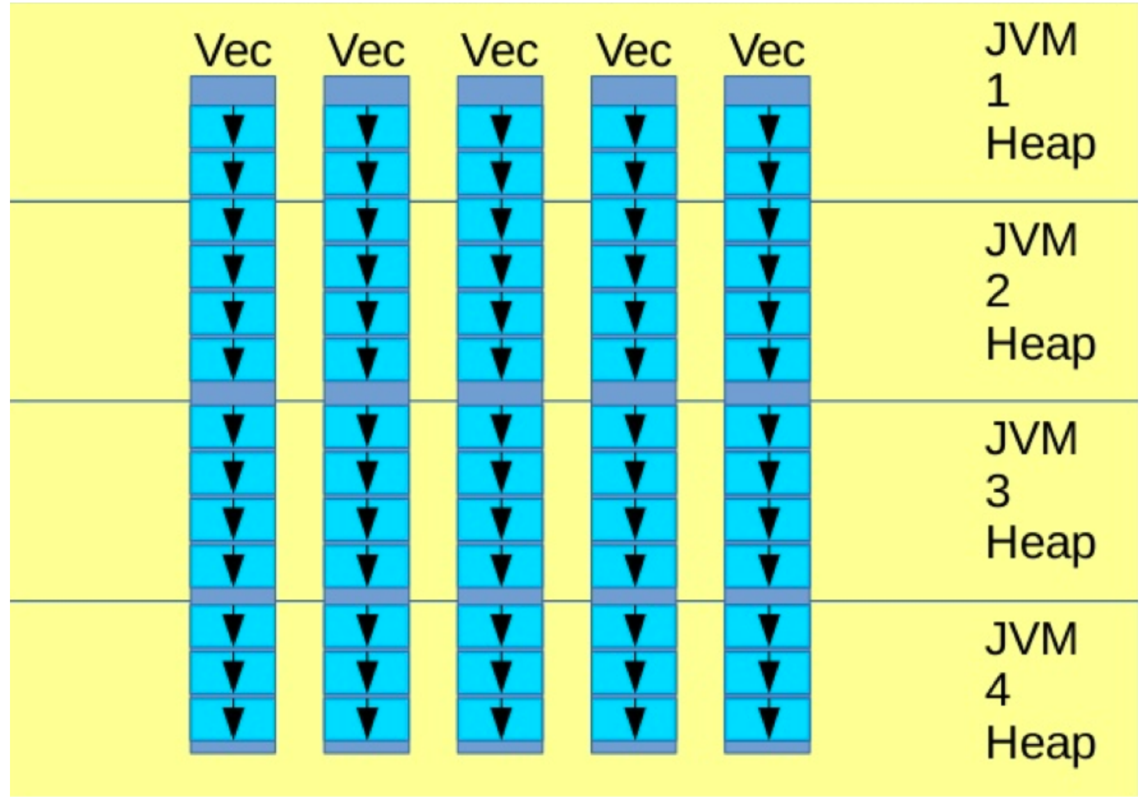
H2O Cluster



- Multi-node cluster with shared memory model.
- All computations in memory.
- Each node sees only some rows of the data.
- No limit on cluster size.

H2O Frame

- Distributed data frames (collection of vectors).
- Columns are distributed (across nodes) arrays.
- Works just like R's data.frame or Python Pandas DataFrame



H2O Machine Learning Features

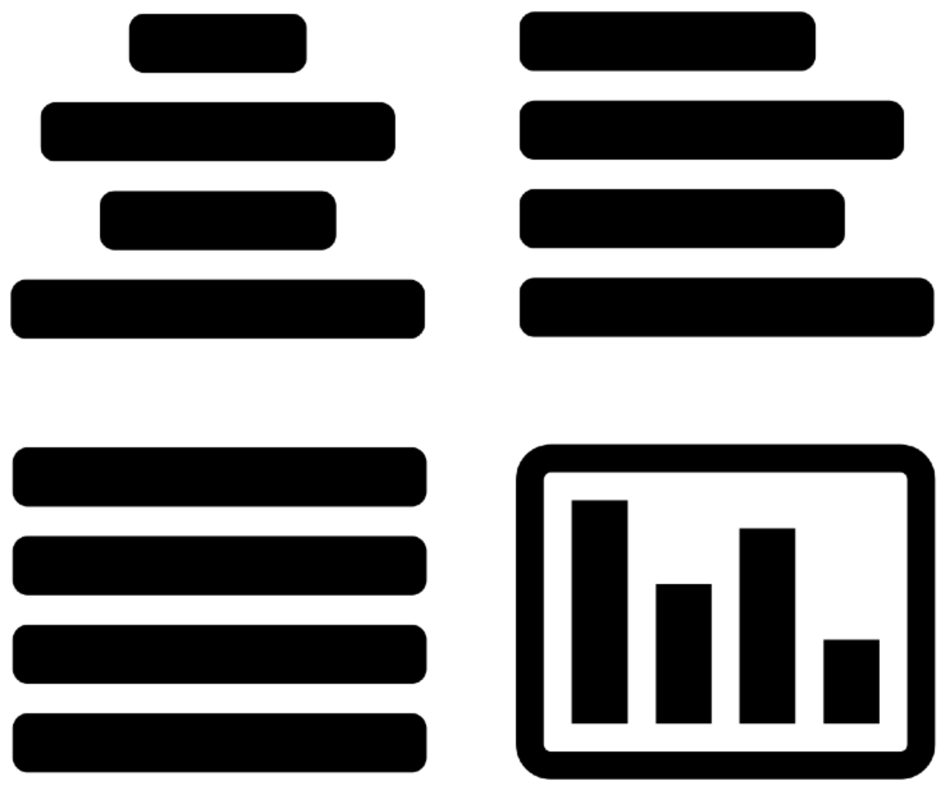
- Supervised & unsupervised machine learning algos (GBM, RF, DNN, GLM, Stacked Ensembles, etc.)
- Imputation, normalization & auto one-hot-encoding
- Automatic early stopping
- Cross-validation, grid search & random search
- Variable importance, model evaluation metrics, plots

Intro to Automatic Machine Learning

Goals & Features of AutoML

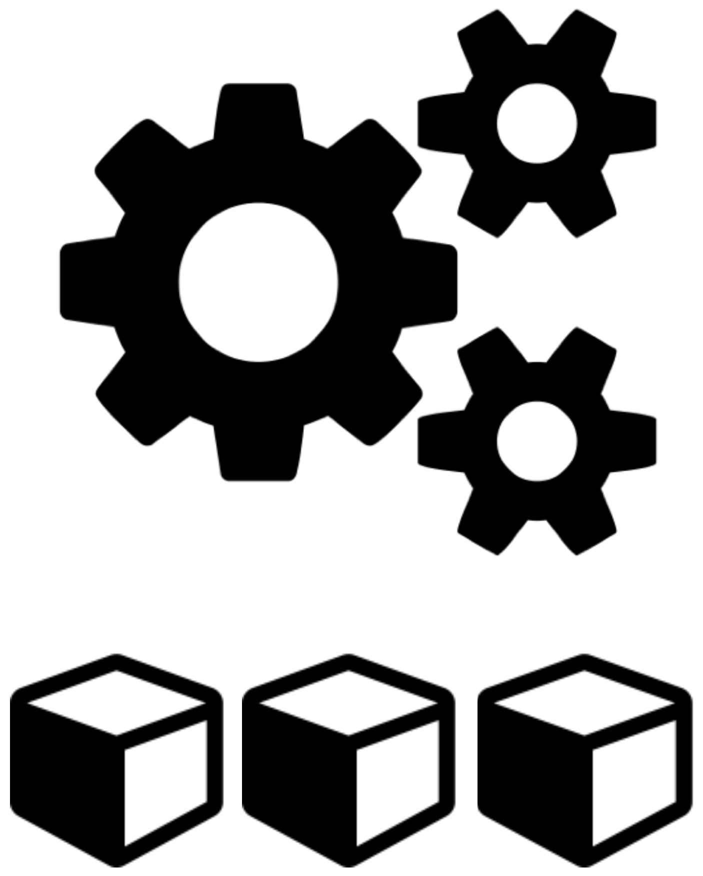
- 🏆 Train the best model in the least amount of time.
- 📉 Reduce the human effort & expertise required in machine learning.
- 📈 Improve the performance of machine learning models.
- 🔄 Increase reproducibility & establish a baseline for scientific research or applications.

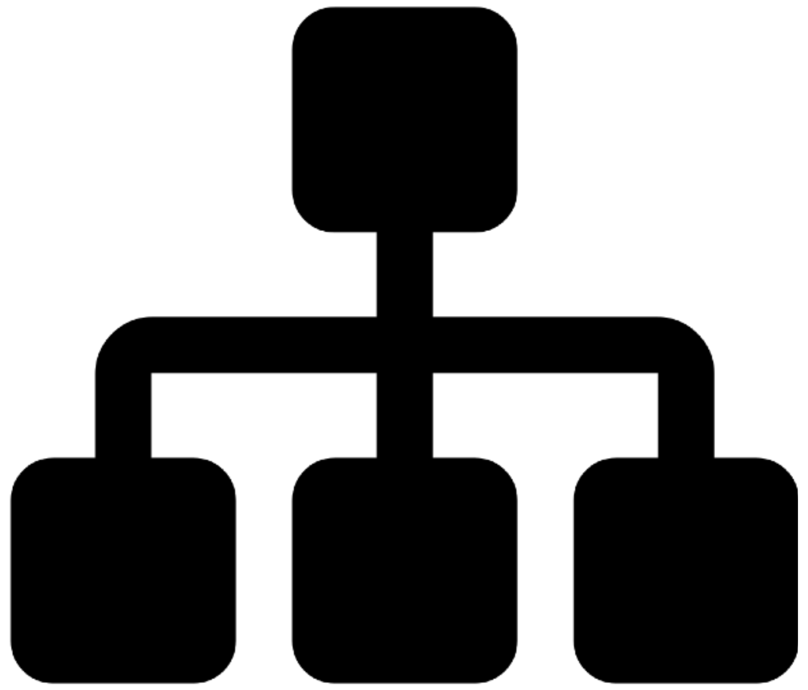
Aspects of Automatic Machine Learning



Data Prep

Model Generation





Ensembles

Aspects of Automatic Machine Learning

Data Preprocessing

- Imputation, one-hot encoding, standardization
- Feature selection and/or feature extraction (e.g. PCA)
- Count/Label/Target encoding of categorical features

Model Generation

- Cartesian grid search or random grid search
- Bayesian Hyperparameter Optimization
- Individual models can be tuned using a validation set

Ensembles

- Ensembles often out-perform individual models
- Stacking / Super Learning (Wolpert, Breiman)
- Ensemble Selection (Caruana)

Different Flavors of AutoML

https://www.h2o.ai/blog/t

67%

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August 15th, 2018

The different flavors of AutoML

Share

Category: AutoML, Data Science, Driverless AI, H2O

By: Erin LeDell

In recent years, the demand for machine learning experts has outpaced the supply, despite the surge of people entering the field. To address this gap, there have been big strides in the development of user-friendly machine learning software (e.g. H2O, scikit-learn, keras). Although these tools have made it easy to train and evaluate machine learning models, there is still a good amount of data science knowledge that's required in order to create the *highest-quality* model, given your dataset. Writing the code to perform a hyperparameter search over many different types of algorithms can also be time consuming and repetitive work.

What is AutoML?

https://tinyurl.com/flavors-of-automl

H2O’s AutoML

H2O AutoML (v3.26)

Data Preprocessing

- Imputation, one-hot encoding, standardization
- Feature selection and/or feature extraction (e.g. PCA)
- Count/Label/Target encoding of categorical features

Model Generation

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Ensembles

- Ensembles often out-perform individual models:
- Stacking / Super Learning (Wolpert, Breiman)
- Ensemble Selection (Caruana)

Random Grid Search & Stacking

- Random Grid Search combined with Stacked Ensembles is a powerful combination.
- Ensembles perform particularly well if the models they are based on (1) are individually strong, and (2) make uncorrelated errors.
- Stacking uses a second-level metalearning algorithm to find the optimal combination of base learners.

H2O AutoML

- Basic data pre-processing (as in all H2O algos).
- Trains a random grid of GBMs, DNNs, GLMs, etc. using a carefully chosen hyper-parameter space.
- Individual models are tuned using cross-validation.
- Two Stacked Ensembles are trained ("All Models" ensemble & a lightweight "Best of Family" ensemble).
- Returns a sorted "Leaderboard" of all models.
- All models can be easily exported to production.

H2O AutoML in Python

Example

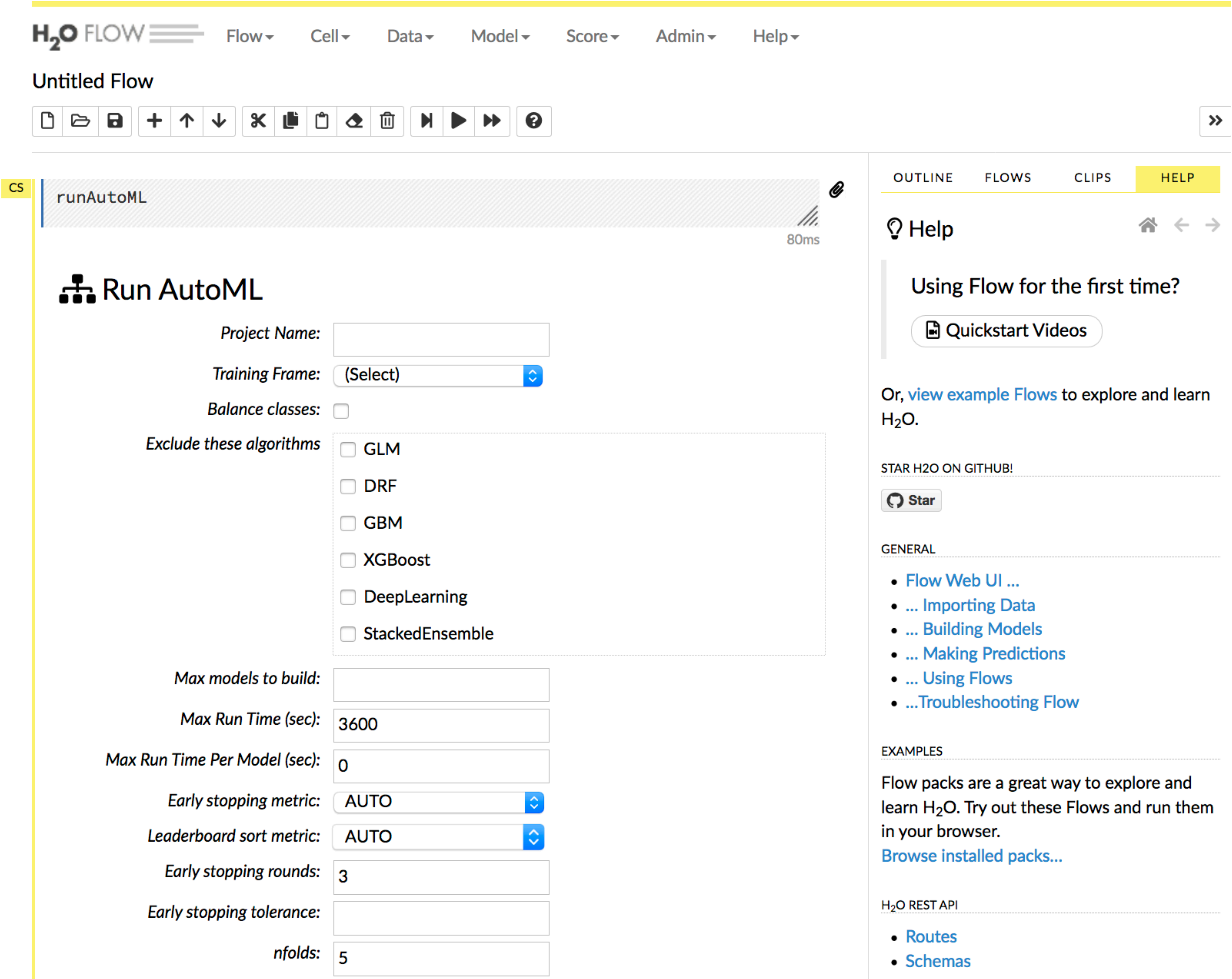
```python
import h2o
from h2o.automl import H2OAutoML
h2o.init()

train = h2o.import_file("train.csv")

aml = H2OAutoML(max_runtime_secs = 600)
aml.train(y = "response_colname",
          training_frame = train)

lb = aml.leaderboard
```

H2O AutoML in R

Example

```r
library(h2o)

h2o.init()

train <- h2o.importFile("train.csv")


aml <- h2o.automl(y = "response_colname",
                  training_frame = train,
                  max_runtime_secs = 600)

lb <- aml@leaderboard
```

H2O AutoML in Flow GUI



H2O AutoML Leaderboard

model_id	auc	logloss	mean_per_class_error	rmse	mse
StackedEnsemble_AllModels_AutoML_20181212_105540	0.7898014	0.5511086	0.3331737	0.4321104	0.1867194
StackedEnsemble_BestOfFamily_AutoML_20181212_105540	0.7884246	0.5521454	0.3231919	0.4326254	0.1871647
XGBoost_1_AutoML_20181212_105540	0.7846510	0.5575305	0.3254707	0.4349489	0.1891806
XGBoost_grid_1_AutoML_20181212_105540_model_4	0.7835232	0.5578542	0.3188188	0.4352486	0.1894413
XGBoost_grid_1_AutoML_20181212_105540_model_3	0.7830043	0.5596125	0.3250808	0.4357077	0.1898412
XGBoost_2_AutoML_20181212_105540	0.7813603	0.5588797	0.3470738	0.4359074	0.1900153
XGBoost_3_AutoML_20181212_105540	0.7808475	0.5595886	0.3307386	0.4361295	0.1902090
GBM_5_AutoML_20181212_105540	0.7808366	0.5599029	0.3408479	0.4361915	0.1902630
GBM_2_AutoML_20181212_105540	0.7800361	0.5598060	0.3399258	0.4364149	0.1904580
GBM_1_AutoML_20181212_105540	0.7798274	0.5608570	0.3350957	0.4366159	0.1906335
GBM_3_AutoML_20181212_105540	0.7786685	0.5617903	0.3255378	0.4371886	0.1911339
XGBoost_grid_1_AutoML_20181212_105540_model_2	0.7744105	0.5750165	0.3228112	0.4427003	0.1959836
GBM_4_AutoML_20181212_105540	0.7714260	0.5697120	0.3374203	0.4410703	0.1945430
GBM_grid_1_AutoML_20181212_105540_model_1	0.7697524	0.5725826	0.3443314	0.4424524	0.1957641
GBM_grid_1_AutoML_20181212_105540_model_2	0.7543664	0.9185673	0.3558550	0.4966377	0.2466490
DRF_1_AutoML_20181212_105540	0.7428924	0.5958832	0.3554027	0.4527742	0.2050045
XRT_1_AutoML_20181212_105540	0.7420910	0.5993457	0.3565826	0.4531168	0.2053148
DeepLearning_grid_1_AutoML_20181212_105540_model_2	0.7417952	0.6014974	0.3682910	0.4549035	0.2069372
XGBoost_grid_1_AutoML_20181212_105540_model_1	0.6935538	0.6207021	0.4058805	0.4657911	0.2169614
DeepLearning_1_AutoML_20181212_105540	0.6913704	0.6379538	0.4093513	0.4717801	0.2225765
DeepLearning_grid_1_AutoML_20181212_105540_model_1	0.6900835	0.6617941	0.4184695	0.4766352	0.2271811
GLM_grid_1_AutoML_20181212_105540_model_1	0.6826481	0.6385205	0.3972341	0.4726827	0.2234290

Example Leaderboard for binary classification

AutoML Benchmarks

Computer Science > Machine Learning

An Open Source AutoML Benchmark

Pieter Gijsbers, Erin LeDell, Janek Thomas, Sébastien Poirier, Bernd Bischl, Joaquin Vanschoren

(Submitted on 1 Jul 2019)

In recent years, an active field of research has developed around automated machine learning (AutoML). Unfortunately, comparing different AutoML systems is hard and often done incorrectly. We introduce an open, ongoing, and extensible benchmark framework which follows best practices and avoids common mistakes. The framework is open-source, uses public datasets and has a website with up-to-date results. We use the framework to conduct a thorough comparison of 4 AutoML systems across 39 datasets and analyze the results.

Comments: Accepted paper at the AutoML Workshop at ICML 2019. Code: this https URL Accompanying website: this https URL

Subjects: **Machine Learning (cs.LG)**; Machine Learning (stat.ML)

Cite as: **arXiv:1907.00909 [cs.LG]**

(or **arXiv:1907.00909v1 [cs.LG]** for this version)

arXiv paper ⬇️

https://tinyurl.com/automlbenchmark

H2O AutoML Tutorials

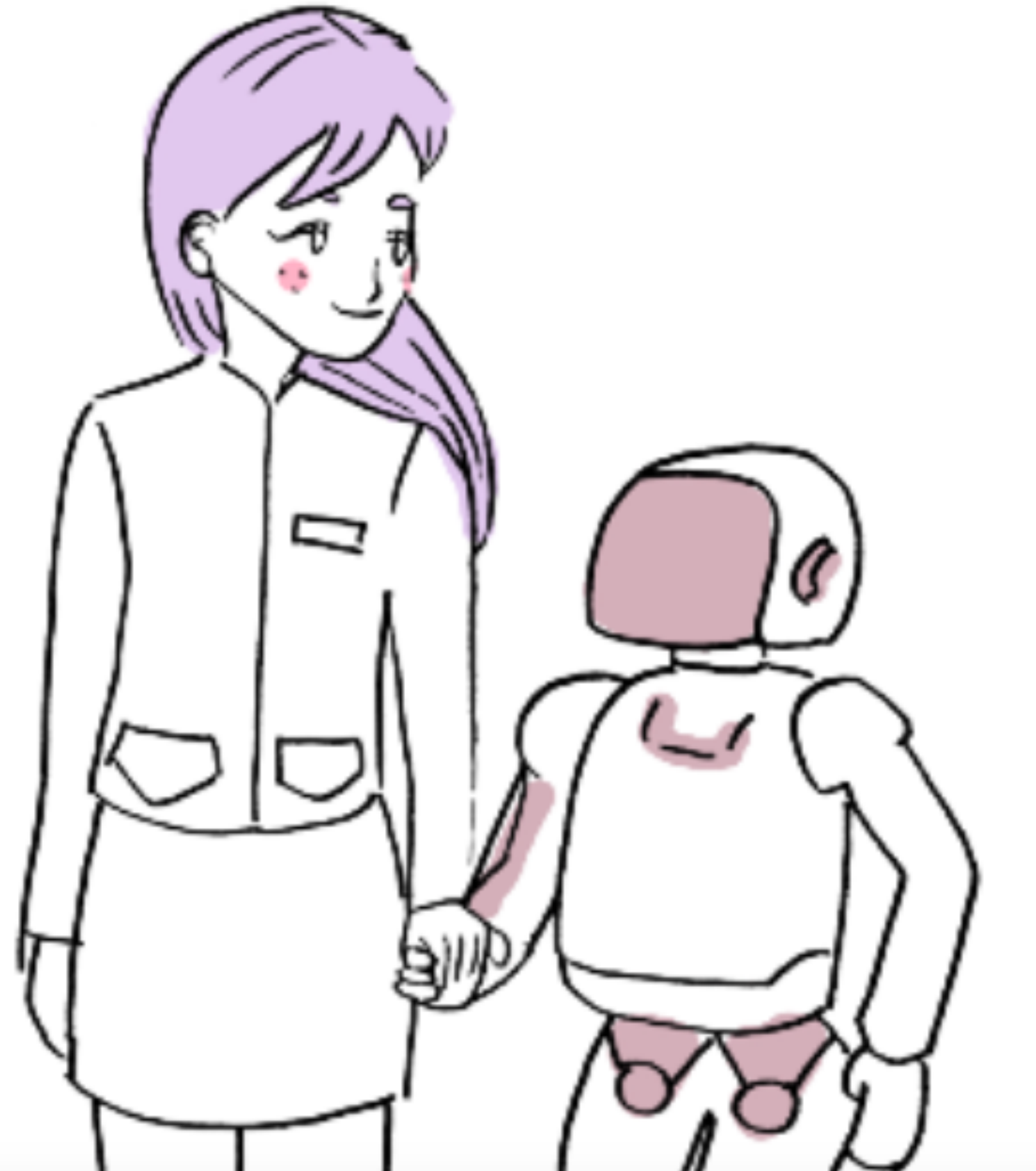
Learn H2O AutoML!

- Docs: https://tinyurl.com/h2o-automl-docs
- R & Py tutorials: https://tinyurl.com/h2o-automl-tutorials
- LatinR H2O tutorial: https://tinyurl.com/latinr-h2o

H2O Resources

- Documentation: http://docs.h2o.ai
- Tutorials: https://github.com/h2oai/h2o-tutorials
- Slidedecks: https://github.com/h2oai/h2o-meetups
- Videos: https://www.youtube.com/user/0xdata
- Stack Overflow: https://stackoverflow.com/tags/h2o
- Google Group: https://tinyurl.com/h2ostream
- Gitter: http://gitter.im/h2oai/h2o-3
- Events & Meetups: http://h2o.ai/events

Thank you!



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