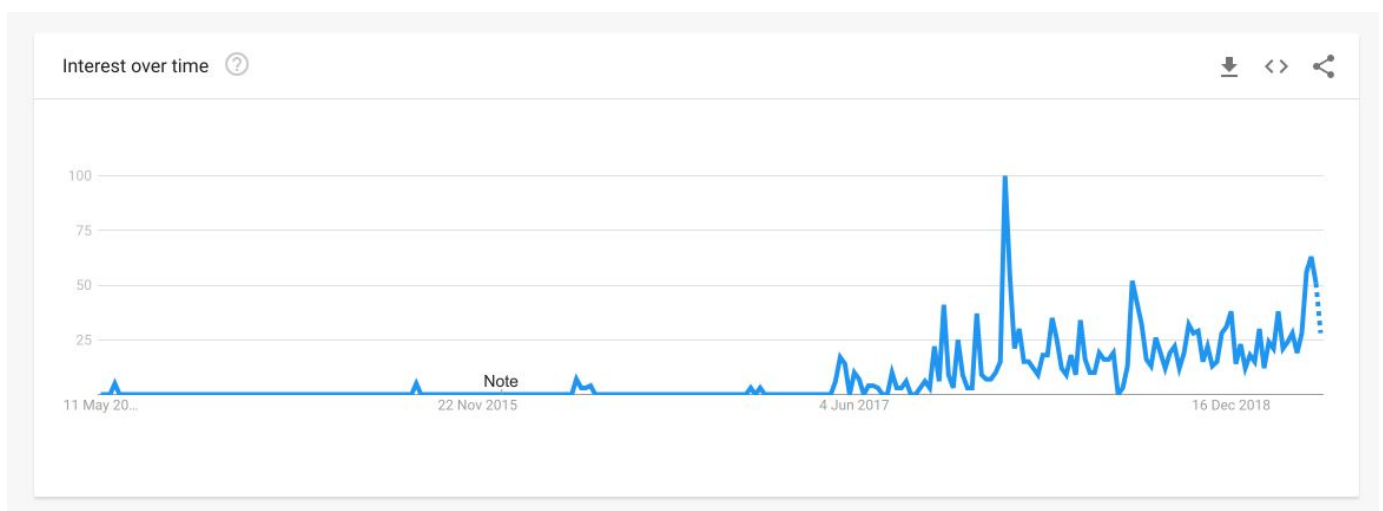


AutoML with h2o

Parameters and Model Optimization

6 minute read

The interest in AutoML is rising over time. This graph shows the trends in Google for the AutoML search term.



AutoML algorithms are reaching really good rankings in data science competitions (see [this article](https://towardsdatascience.com/achieving-a-top-5-position-in-an-ml-competition-with-automl-89a5a6fb8060) (<https://towardsdatascience.com/achieving-a-top-5-position-in-an-ml-competition-with-automl-89a5a6fb8060>))

But *what is* AutoML ? How does it work? And mainly, how can you implement an AutoML in Python?

What is AutoML?

AutoML is a framework whose role is to optimize the machine learning workflow, which includes automatic training and tuning of many models within a user-specified time-limit.

The goal is to fasten the work of the Data Scientist when it comes to model selection and parameter tuning. On the other hand, the user simply inputs the training data, eventually some validation data, and a time limit.



AutoML will automatically try several models, choose the best performing models, tune the parameters of the *leader* models, try to stack them...

AutoML outputs a leaderboard of algorithms, and you can select the best performing algorithm given several criteria that are measured (MSE, RMSE, log loss, Auc...).

Why and when should you use AutoML?

Building models and tuning the hyperparameters is a long process for any data scientist. The search space for the optimal parameters is enormous, and this is only for 1 chosen model.

AutoML can be highly parallelized, so bear in mind that a couple of GPUs will help.

AutoML can be used to :

- Assess the feature importance
- Try a lot of models and parameters as a first guess

Once a model and a set of parameters have been identified, you have 2 options :

- either the model is good enough and satisfies your criteria
- or you can use the selected set of model + parameters as a starting point for a GridSearch or Bayesian HyperOpt

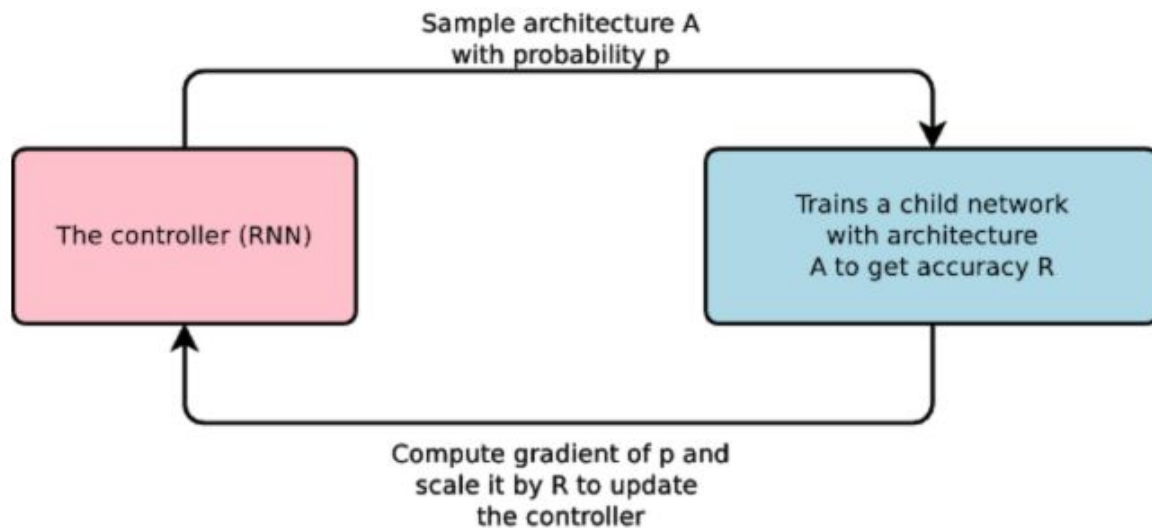
How does AutoML work?

AutoML **does not** use a GIANT double for-loop to test every model and every parameter. It's much smarter than that. It uses Reinforcement Learning.

A controller neural net can propose a "child" model architecture, which can then be trained and evaluated for quality on a particular task. That feedback is then used to inform the controller how to improve its proposals for the next round.

Eventually, the controller learns to assign a high probability to areas of architecture space that achieve better accuracy on a held-out validation dataset, and low probability to areas of architecture space that score poorly.





To make the controller a little more complex, it uses anchor points, and set-selection attention to form skip connections.

At that point, you might think that AutoML frameworks are extremely long to run. In AutoML, each gradient update to the controller parameters θ corresponds to training one child network to convergence.

You're right, training a single child network can take hours. For this reason, according to Google's Blog, AutoML uses distributed training and asynchronous parameter updates to speed up the learning process of the controller. It uses a parameter-server scheme where we have a parameter server of S shards, that store the shared parameters for K controller replicas. Each controller replica samples m different child architectures that are trained in parallel. The controller then collects gradients according to the results of that minibatch of m architectures at convergence and sends them to the parameter server to update the weights across all controller replicas.

Example in Python

Several companies are currently AutoML pipelines. Among them, Google and h2o. In this example, we'll use h2o's solution. I suggest you run this in Google Colab using GPU's, but you can also run it locally.

Start by importing the necessary packages :

```

!pip install requests
!pip install tabulate
!pip install "colorama>=0.3.8"
import h2o
h2o.init(url="http://h2o-release.s3.amazonaws.com/h2o/latest_stable_Py.html")

```



The Data

We'll use the Credit Card Fraud detection, a famous Kaggle dataset that can be found [here](https://www.kaggle.com/mlg-ulb/creditcardfraud) (<https://www.kaggle.com/mlg-ulb/creditcardfraud>).

The dataset contains transactions made by credit cards in September 2013 by European cardholders. This dataset presents transactions that occurred in two days, where we have 492 frauds out of 284,807 transactions. The dataset is highly unbalanced, the positive class (frauds) account for 0.172% of all transactions.

It contains only numerical input variables which are the result of a PCA transformation. Unfortunately, due to confidentiality issues, the original features are not provided. Features V1, V2, ... V28 are the principal components obtained with PCA, the only features which have not been transformed with PCA are 'Time' and 'Amount'. Feature 'Time' contains the seconds elapsed between each transaction and the first transaction in the dataset. The feature 'Amount' is the transaction Amount, this feature can be used for example-dependant cost-sensitive learning. Feature 'Class' is the response variable and it takes value 1 in case of fraud and 0 otherwise.

```
### General
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_csv('creditcard.csv')
df.head()
```

Out[96]:

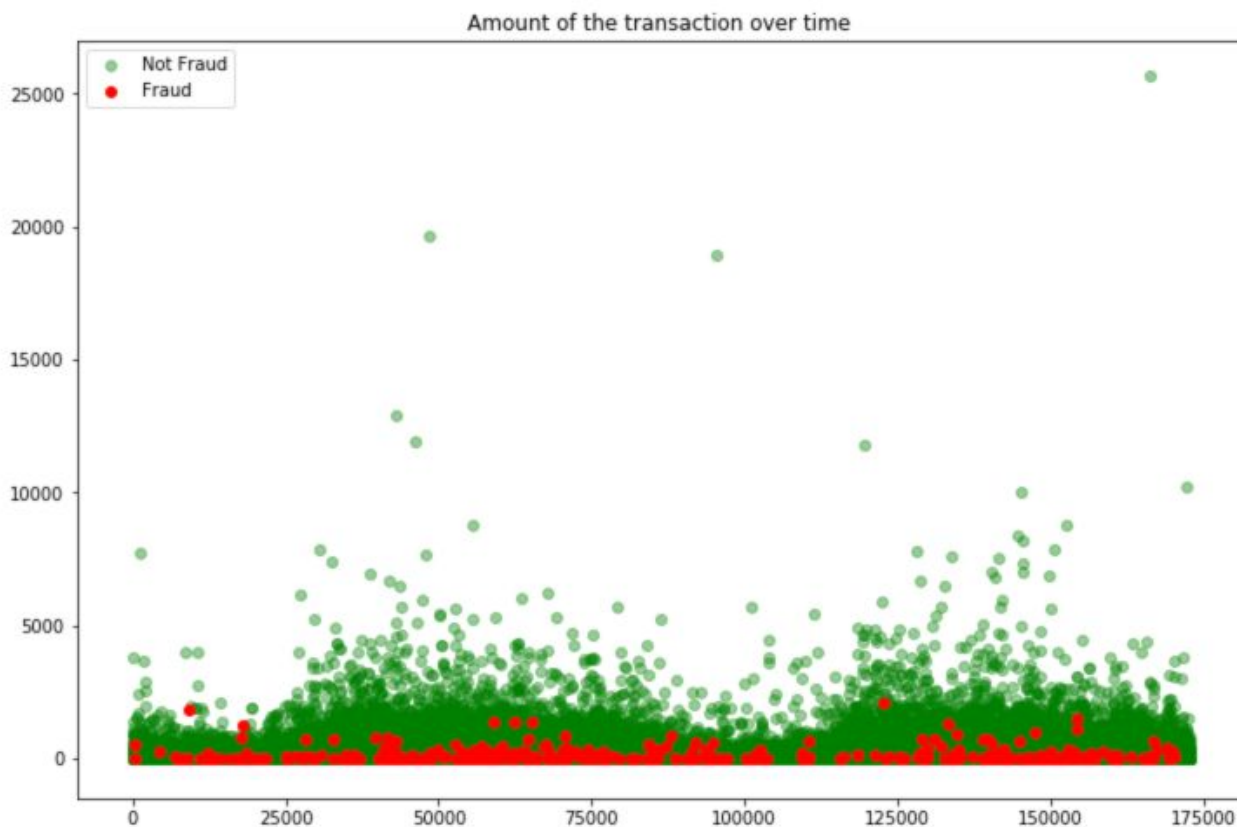
V5	V6	V7	V8	V9	...	V21	V22	V23	V24	V25	V26	V27	V28	Amount	Class
-0.338321	0.462388	0.239599	0.098698	0.363787	...	-0.018307	0.277838	-0.110474	0.066928	0.128539	-0.189115	0.133558	-0.021053	149.62	0
0.060018	-0.082361	-0.078803	0.085102	-0.255425	...	-0.225775	-0.638672	0.101288	-0.339846	0.167170	0.125895	-0.008983	0.014724	2.69	0
-0.503198	1.800499	0.791461	0.247676	-1.514654	...	0.247998	0.771679	0.909412	-0.689281	-0.327642	-0.139097	-0.055353	-0.059752	378.66	0
-0.010309	1.247203	0.237609	0.377436	-1.387024	...	-0.108300	0.005274	-0.190321	-1.175575	0.647376	-0.221929	0.062723	0.061458	123.50	0
-0.407193	0.095921	0.592941	-0.270533	0.817739	...	-0.009431	0.798278	-0.137458	0.141267	-0.206010	0.502292	0.219422	0.215153	69.99	0

If you explore the data, you'll notice that only 0.17% of the transactions are fraudulent. We'll use the F1-Score metric, a harmonic mean between the precision and the recall.

To understand the nature of the fraudulent transactions, simply plot the following graph :



```
plt.figure(figsize=(12,8))
plt.scatter(df[df.Class == 0].Time, df[df.Class == 0].Amount, c='green', alpha=0.4, label="Not
Fraud")
plt.scatter(df[df.Class == 1].Time, df[df.Class == 1].Amount, c='red', label="Fraud")
plt.title("Amount of the transaction over time")
plt.legend()
plt.show()
```



Fraudulent transactions have a limited amount. We can guess that these transactions must remain "unseen" and not attracting too much attention.

h2o AutoML

Now, let's import h2o AutoML :

```
### h2o AutoML
import h2o
from h2o.estimators.gbm import H2OGradientBoostingEstimator
from h2o.automl import H2OAutoML
```



h2o session :

If you're running this locally, you should see something like this :

Checking whether there is an H2O instance running at <http://localhost:54321> . connected.

H2O cluster uptime:	05 secs
H2O cluster timezone:	Europe/Paris
H2O data parsing timezone:	UTC
H2O cluster version:	3.24.0.2
H2O cluster version age:	18 days
H2O cluster name:	H2O_from_python_maelfabien_z2x0sv
H2O cluster total nodes:	1
H2O cluster free memory:	3.546 Gb
H2O cluster total cores:	4
H2O cluster allowed cores:	4
H2O cluster status:	locked, healthy
H2O connection url:	http://localhost:54321
H2O connection proxy:	None
H2O internal security:	False
H2O API Extensions:	Amazon S3, XGBoost, Algos, AutoML, Core V3, Core V4
Python version:	3.6.5 final

If you follow the local link to the instance, you can access the h2o Flow :

The screenshot displays the H2O Flow web interface. The top navigation bar includes 'H2O FLOW' and menu items like 'Flow', 'Cell', 'Data', 'Model', 'Score', 'Admin', and 'Help'. Below the navigation bar is a toolbar with icons for file operations and execution. The main area is titled 'Untitled Flow' and shows an 'assist' sidebar on the left with a list of routines and their descriptions. On the right, there's a 'HELP' sidebar with sections for 'Using Flow for the first time?', 'STAR H2O ON GITHUB!', 'GENERAL' (with links to various topics), and 'EXAMPLES'.

I'll write the Flow in another article, but Flow aims to do the same thing with a visual interface. You need to import the dataset as an h2o object, and use built-in functions to process it.

```
# Load the data
df = h2o.import_file("/Users/maelfabien/Desktop/LocalDB/CreditCard/creditcard.csv")

d = df.split_frame(ratios = [0.8], seed = 1234)
df_train = d[0] # using 80% for training
df_test = d[1] #rest 20% for testing
```

We then define a list of the columns we'll use as predictors :

```
# Predictor columns
predictors = list(df.columns)
predictors.remove('Time')
predictors.remove('Class')
```

As you might have guessed, we're facing a binary classification problem here. The default case is regression in AutoML. To "cast" a column type to integer, use this :

```
# Cast binary
df_train['Class'] = df_train['Class'].asfactor()
```

We are now ready to define the model and train it. We specify the maximal number of models to test, and the overall maximal runtime in seconds.

```
aml = H2OAutoML(max_models = 50, seed = 1, max_runtime_secs=21000)
aml.train(x = predictors, y = 'Class', training_frame = df_train, validation_frame = df_test)
```

By default, the maximal runtime is 1 hour. Your model will be training for 21'000 seconds now (I left it to train overnight). Now, let's display all the models that have been tested and their performance :

```
print(aml.leaderboard)
```

	model_id	auc	logloss	mean_per_class_error	rmse	mse
	GBM_grid_1_AutoML_20190506_000950_model_8	0.981646	0.00279929	0.105491	0.0217763	0.000474206
	GBM_grid_1_AutoML_20190506_000950_model_13	0.97855	0.00278203	0.106747	0.0212029	0.000449564
	GLM_grid_1_AutoML_20190506_000950_model_1	0.977505	0.00403073	0.111985	0.0260326	0.000677699
	GBM_grid_1_AutoML_20190506_000950_model_10	0.97727	0.0027134	0.0977369	0.0202304	0.000409271
	GBM_grid_1_AutoML_20190506_000950_model_16	0.976829	0.00273863	0.0977566	0.0208157	0.000433294
	GBM_grid_1_AutoML_20190506_000950_model_5	0.969094	0.00313117	0.100327	0.0217719	0.000474017
	GBM_grid_1_AutoML_20190506_000950_model_17	0.963728	0.00304207	0.101602	0.0220067	0.000484294
	GBM_grid_1_AutoML_20190506_000950_model_6	0.95929	0.00727195	0.105513	0.0240526	0.000578527
	GBM_grid_1_AutoML_20190506_000950_model_4	0.954595	0.00835674	0.114497	0.0240522	0.00057851
	GBM_grid_1_AutoML_20190506_000950_model_3	0.952148	0.0103404	0.106811	0.0246377	0.000607014

The leaderboard is established using Cross Validation, which more or less guarantees that the top performing models are indeed consistently performing well.

To display only the best model, use `print(aml.leader)`.

We can now make a prediction using the leader model, simply using:

```
aml.leader.predict(new_data)
```

We can then save the best model :

```
h2o.save_model(aml.leader, path = "./model_credit_card")
```

Once your work is over, shut down the session :

```
h2o.shutdown()
```

In this simple example, h2o outperformed the tuning I manually did.

Conclusion : *I hope this article on AutoML was interesting. It's a really hot topic, and I do expect large improvements to be made over the next years in this field.*

Sources :

- [How AutoML works](https://medium.com/@gangele397/how-does-automl-works-b0f9e45fbb24) (<https://medium.com/@gangele397/how-does-automl-works-b0f9e45fbb24>).
- [Google AI Blog](https://ai.googleblog.com/2017/05/using-machine-learning-to-explore.html?m=1) (<https://ai.googleblog.com/2017/05/using-machine-learning-to-explore.html?m=1>).
- [H2o package exercises](http://eric.univ-lyon2.fr/~ricco/tanagra/fichiers/fr_Tanagra_Package_H2O_Python.pdf) (http://eric.univ-lyon2.fr/~ricco/tanagra/fichiers/fr_Tanagra_Package_H2O_Python.pdf).

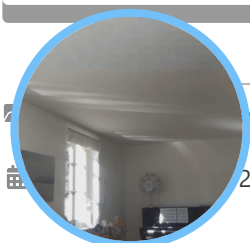


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Best,
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Maël Fabien Mod ➔ Márcio Basgalupp • 2 years ago

Hi Márcio,

You are right ! I'll update the article accordingly, I never noticed this mistake. Thanks :)

Maël

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