Better than Deep Learning: Gradient Boosting Machines (GBM)

Szilard Pafka, PhD
Chief Scientist, Epoch (USA)

DSPT Day Conference, Porto, Portugal
Oct 2019

Szilard [Deeper than Deep Learning]

@DataScienceLA

physics PhD, chief (data) scientist, meetup organizer, datascience.la, (visiting) professor, machine learning benchmarks 🇺🇸🇭🇺🇪🇺

Santa Monica, California linkedin.com/in/szilard

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Disclaimer:

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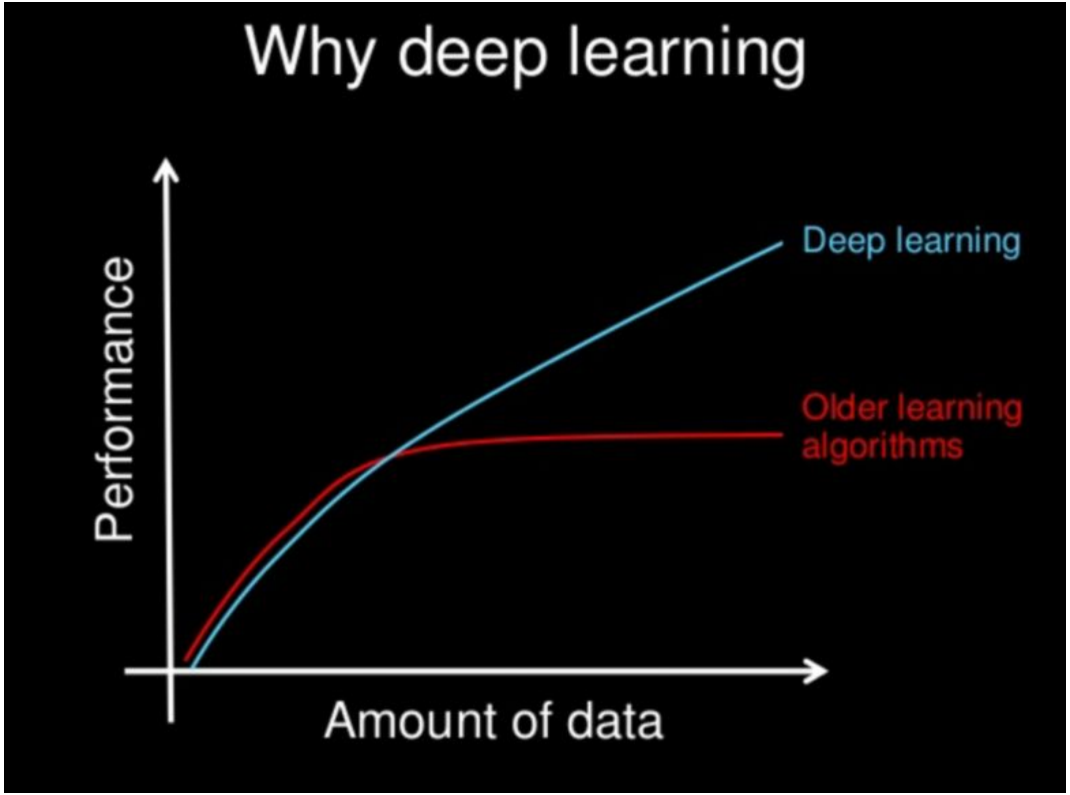
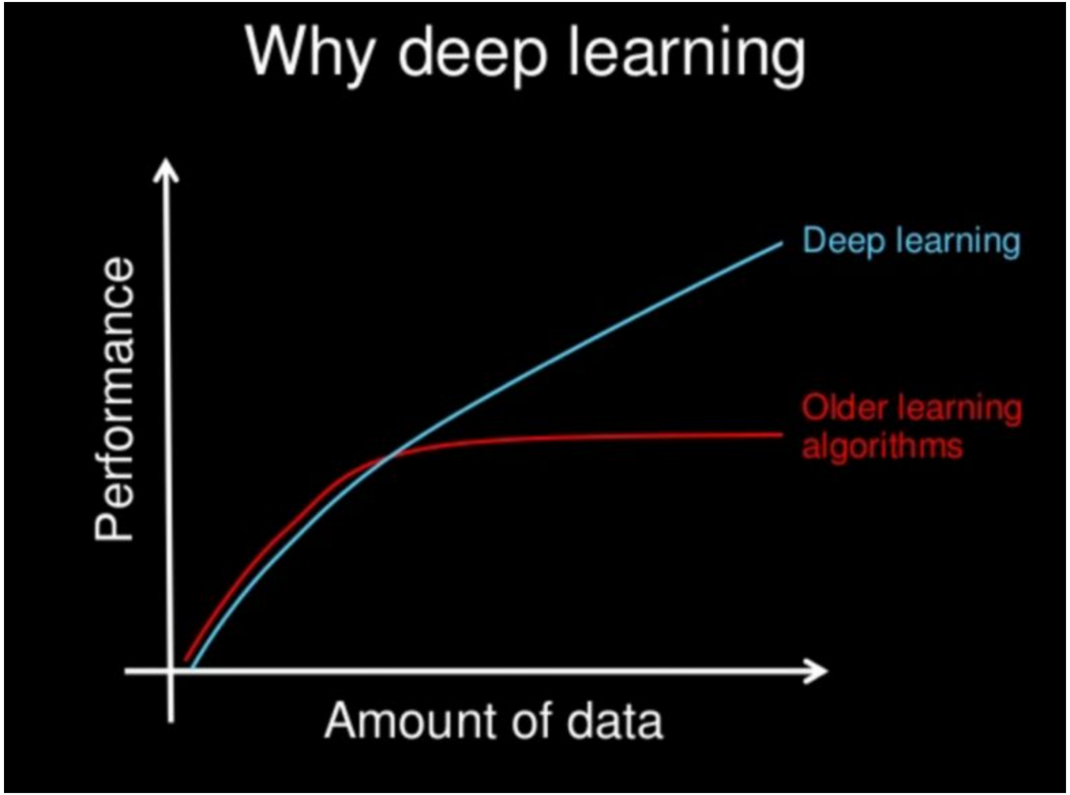
I cannot confirm nor deny if Epoch is using any of the methods, tools, results etc. mentioned in this talk



Source: Andrew Ng



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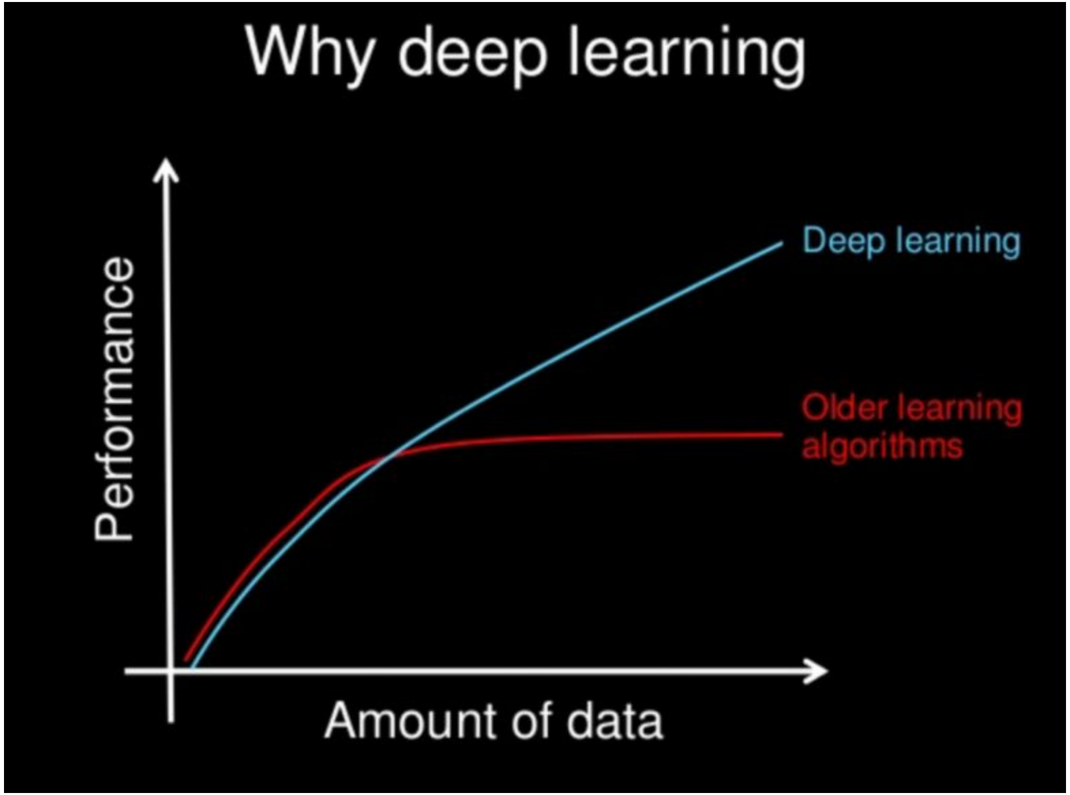

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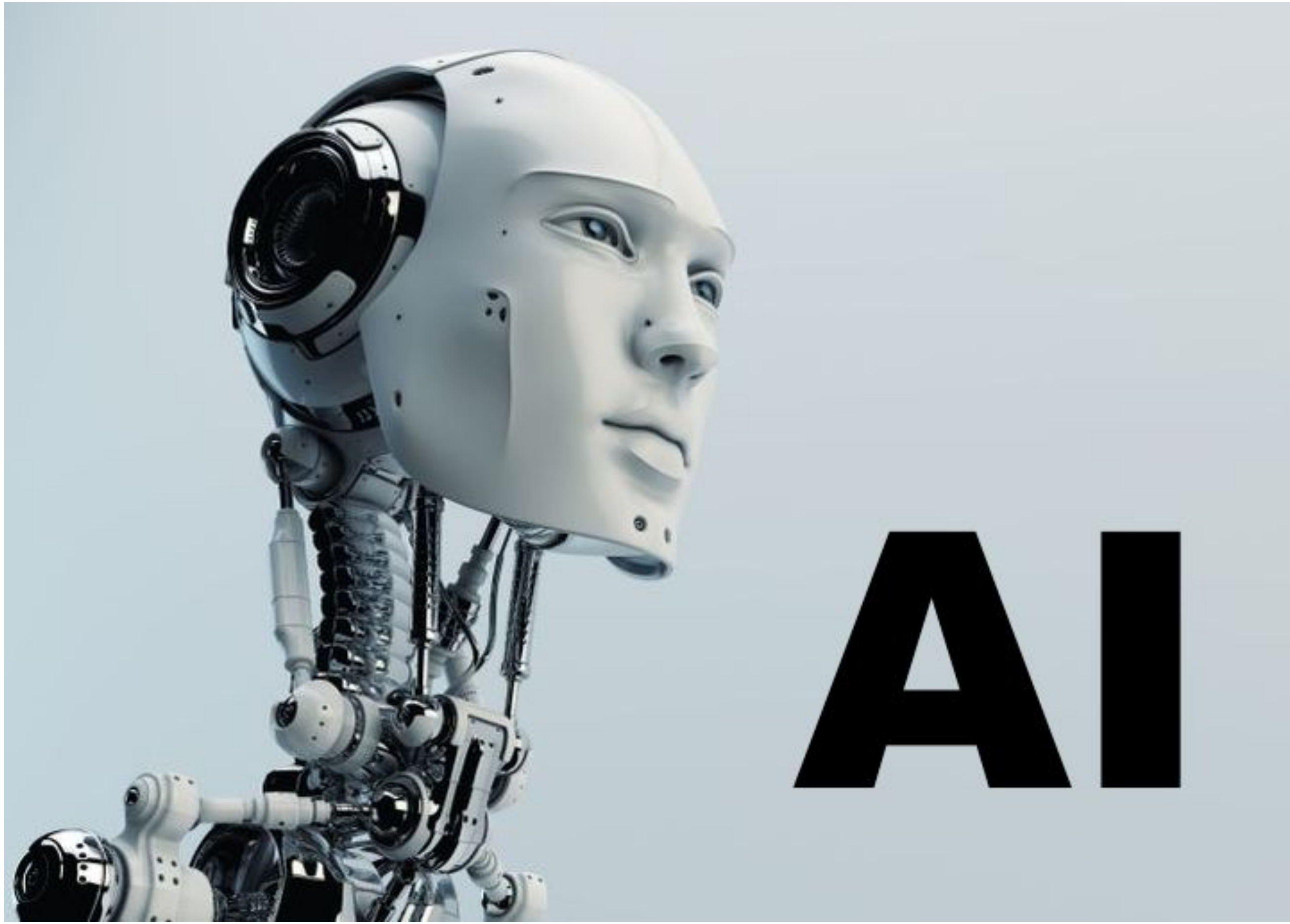
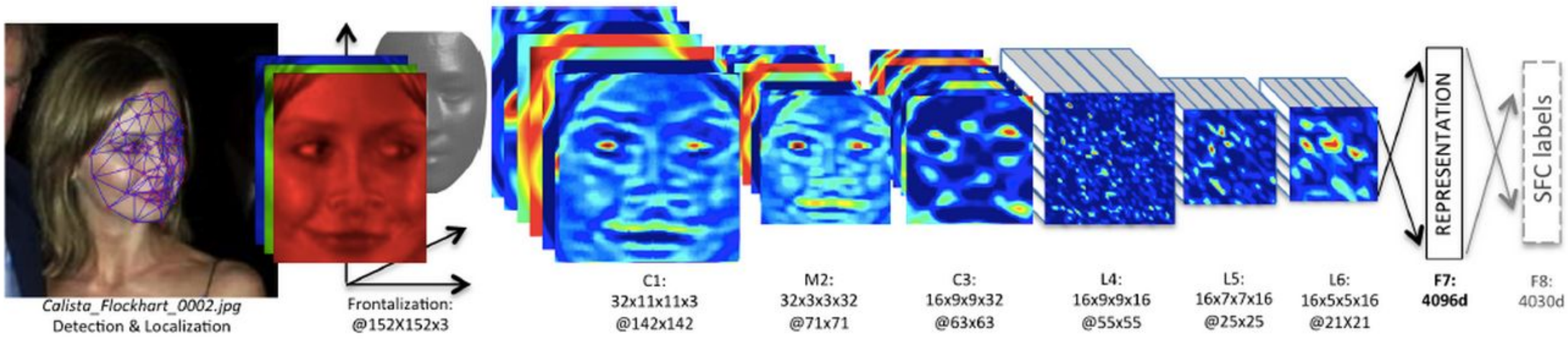
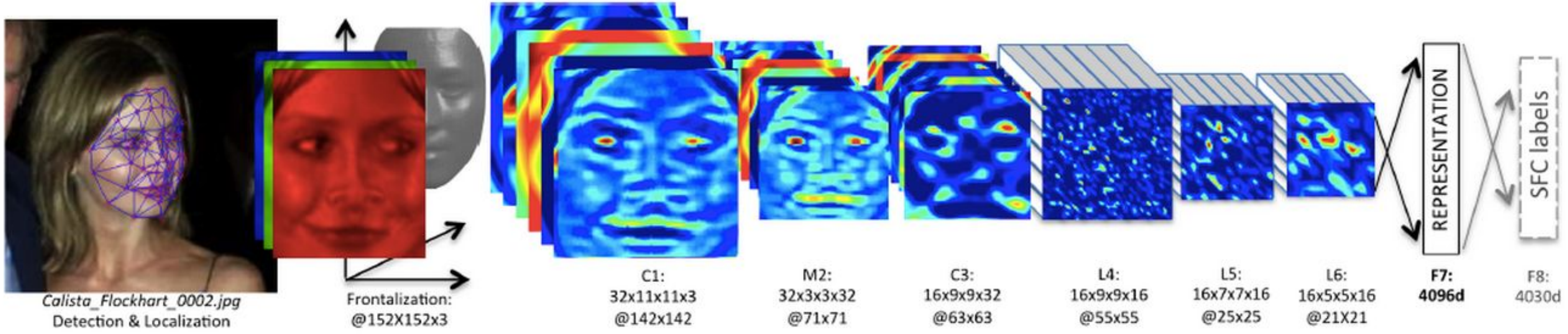

AI



Calista_Flockhart_0002.jpg
Detection & Localization
Frontalization:
@152X152x3
C1:
32x11x11x3
@142x142
M2:
32x3x3x32
@71x71
C3:
16x9x9x32
@63x63
L4:
16x9x9x16
@55x55
L5:
16x7x7x16
@25x25
L6:
16x5x5x16
@21X21
REPRESENTATION
F7:
4096d
SFC labels
F8:
4030d



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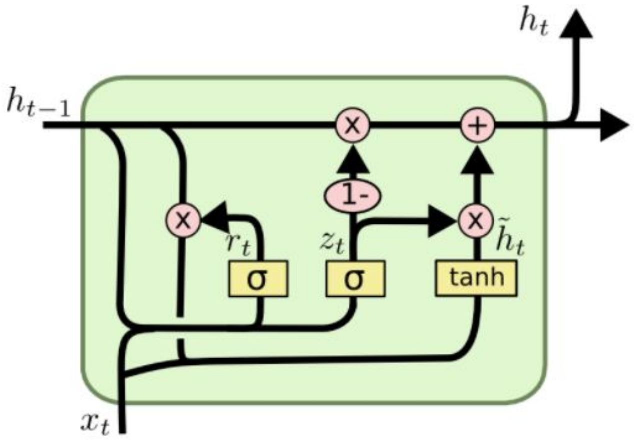

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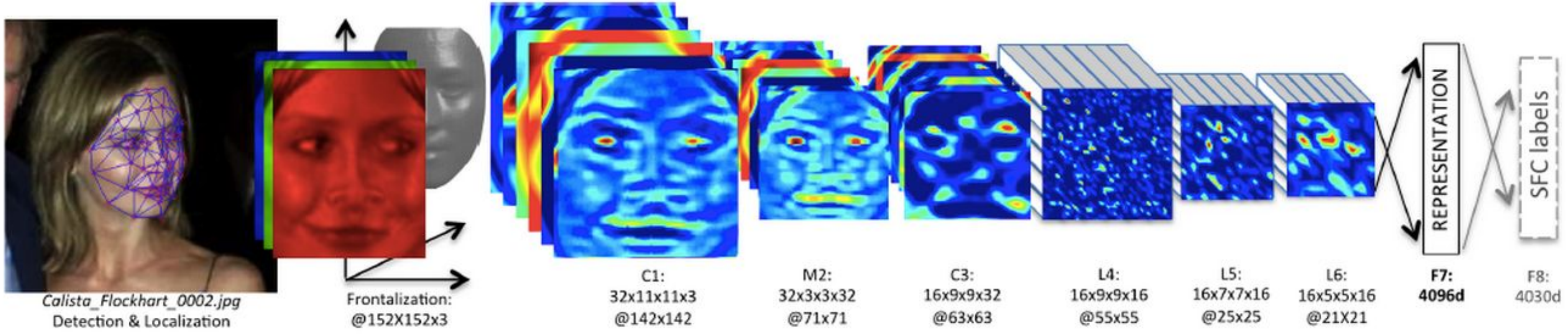
h_{t-1}
1-
r_t
z_t
$\tilde{h}_t$
σ
σ
tanh
x_t



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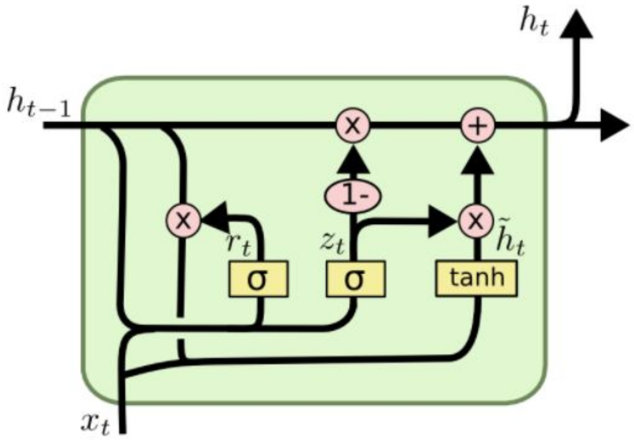

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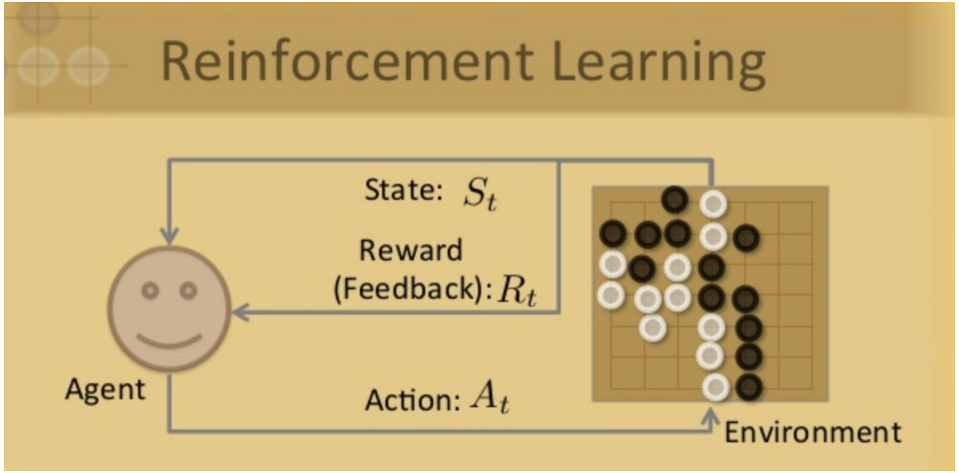


Reinforcement Learning
State: S_t
Reward
(Feedback): R_t
Agent
Action: A_t
Environment

Source: https://twitter.com/iamdevloper/


FRAUD
FRAUD


710
POOR
GOOD


marketing
client
delivering
customers
profit
solution
concept
creating
relationships
techniques
activities
strategy
brand
value
offer
business
management
development
organization
communicating
satisfaction
build
activity
strong
long term
focus
society
competitor
production
identify


FRAUD
FRAUD


710
POOR
GOOD


marketing
client
delivering
customers
profit
solution
concept
creating
techniques
society
activities
strategy
business
management
development
offer
value
brand
build
activity
strong
communicating
satisfaction

Params	AUC	Time (s)	Epochs
default: `activation = "Rectifier", hidden = c(200,200)`	73.1	270	1.8
`hidden = c(50,50,50,50), input_dropout_ratio = 0.2`	73.2	140	2.7
`hidden = c(50,50,50,50)`	73.2	110	1.9
`hidden = c(20,20)`			
`hidden = c(20)`			

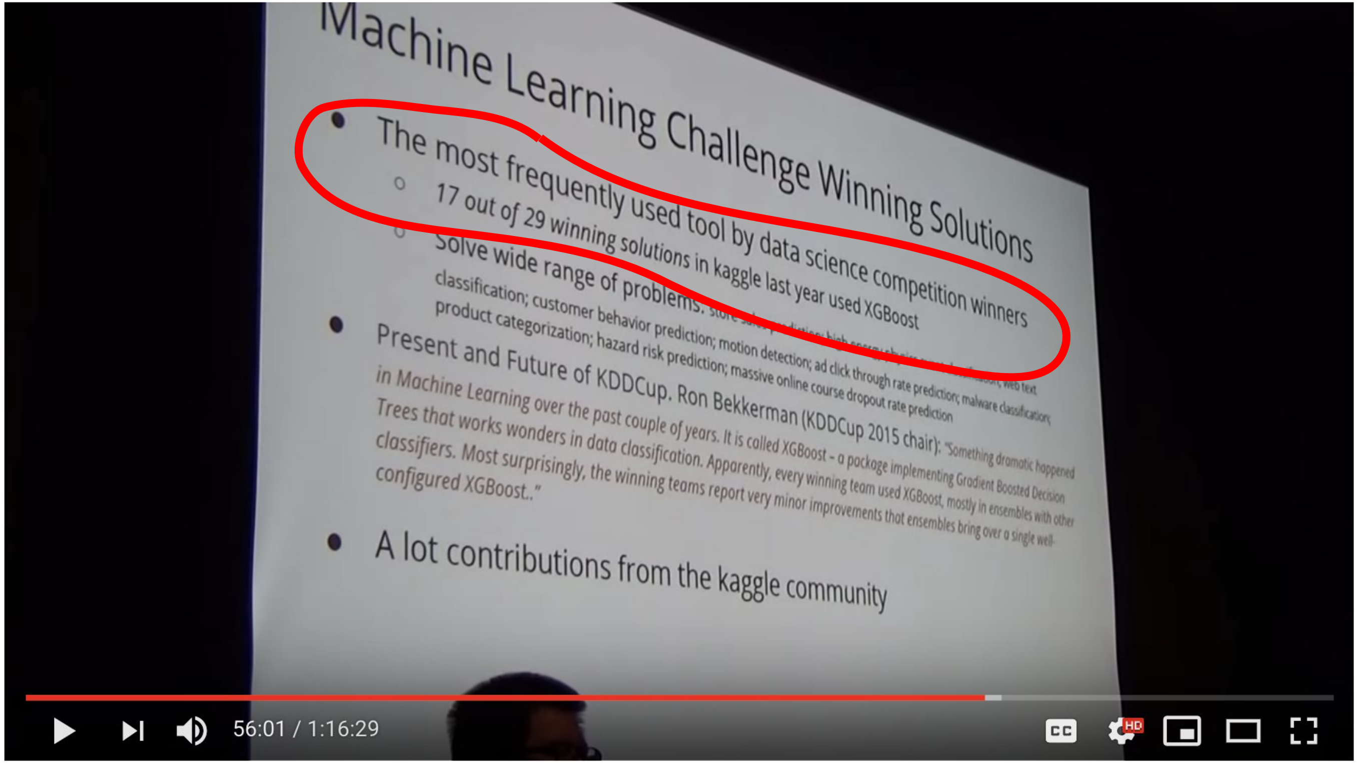
szilard commented Nov 27, 2015

Trying to see if DL can match RF/GBM in accuracy on the airline dataset (wh
years 2005-2006, while validation and test sets sampled disjunctly from 20
kept categorical artificially and are intentionally not encoded as ordinal varia
structure of business datasets).

`RectifierWithDropout, c(200,200,20`			
`ADADELTA rho = 0.95, epsilon = 1e-`			
`rho = 0.999, epsilon = 1e-08`	73.3	270	1.9
`adaptive = FALSE` default: `rate = 0.005, decay = 1, momentum = 0`	73.0	340	1.1
`rate = 0.001, momentum = 0.5 / 1e5 / 0.99`	73.2	410	0.7
`rate = 0.01, momentum = 0.5 / 1e5 / 0.99`	73.3	280	0.9
`rate = 0.01, rate_annealing = 1e-05, momentum = 0.5 / 1e5 / 0.99`	73.5	360	1
`rate = 0.01, rate_annealing = 1e-04, momentum = 0.5 / 1e5 / 0.99`	72.7	3700	8.7
`rate = 0.01, rate_annealing = 1e-05, momentum = 0.5 / 1e5 / 0.9`	73.4	350	0.9

szilard / **benchm-ml**

kaggle



XGBoost A Scalable Tree Boosting System June 02, 2016

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DataScience.LA
Published on Jun 3, 2016

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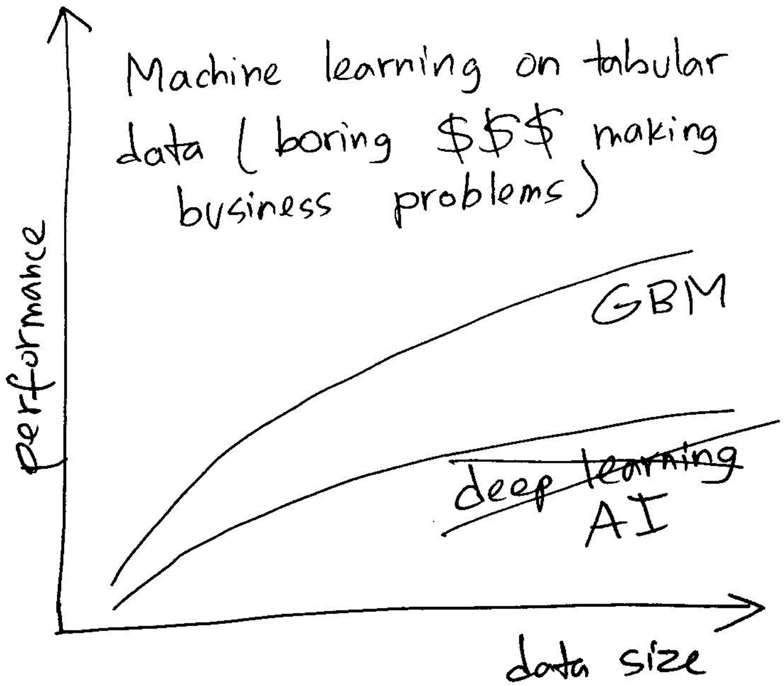
Can anyone **beat** GBMs with deep learning (ahem, AI) on the airline dataset (or generally tabular/business data)? github.com/szilard/benchm…



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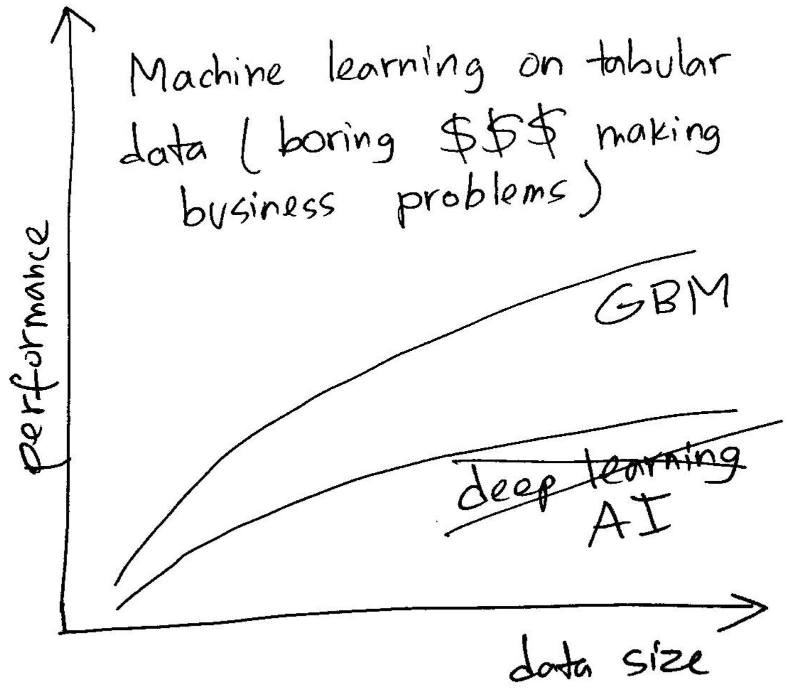

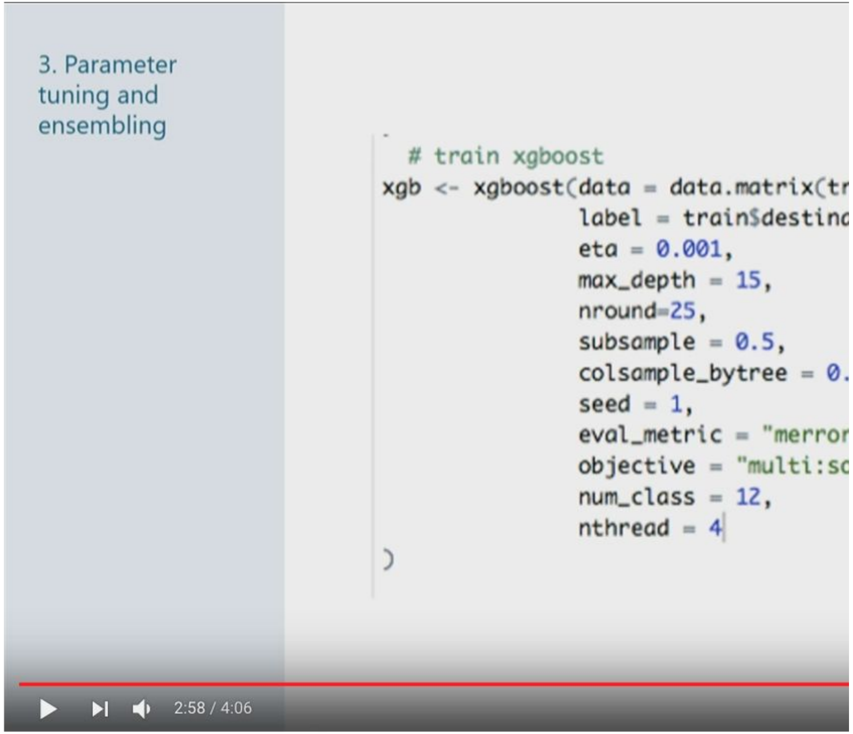

What Kaggle has learned from almost a million data scientists - Anthony Goldbloom

18,153 views

O'Reilly

Published on May 25, 2017

MODEL	1ST	2ND
BST-DT	0.580	0.228
RF	0.390	0.525
BAG-DT	0.030	0.232
SVM	0.000	0.008
ANN	0.000	0.007
KNN	0.000	0.000
BST-STMP	0.000	0.000
DT	0.000	0.000
LOGREG	0.000	0.000
NB	0.000	0.000

AVG	1ST	2ND
RF	0.727	0.207
ANN	0.053	0.172
BSTDT	0.059	0.228
SVM	0.043	0.195
LR	0.089	0.132
BAGDT	0.002	0.012
KNN	0.023	0.045
BSTST	0.004	0.009
PRC	0	0
NB	0	0

An Empirical Comparison of Supervised Learning Algorithms

http://www.cs.cornell.edu/~alexn/papers/empirical.icml06.pdf

An Empirical Evaluation of Supervised Learning in High Dimensions

http://lowrank.net/nikos/pubs/empirical.pdf

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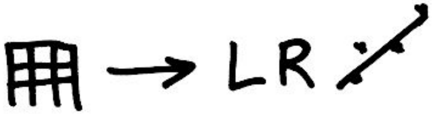
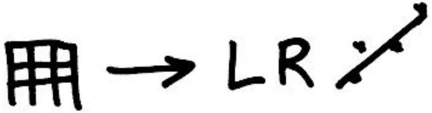
GBM
RF


GBM
RF


LR


GBM
RF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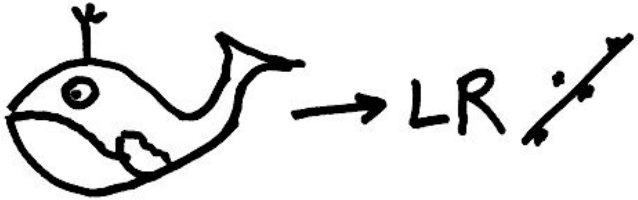
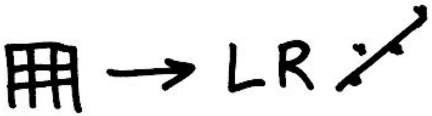

LR


GBM
RF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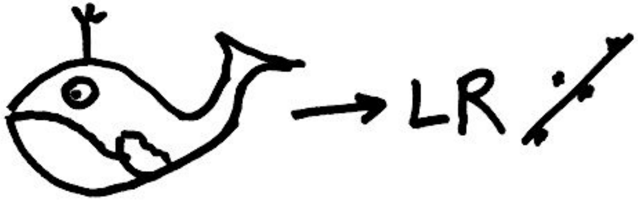
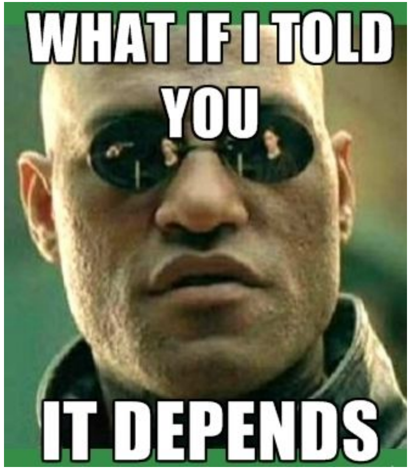

LR


DL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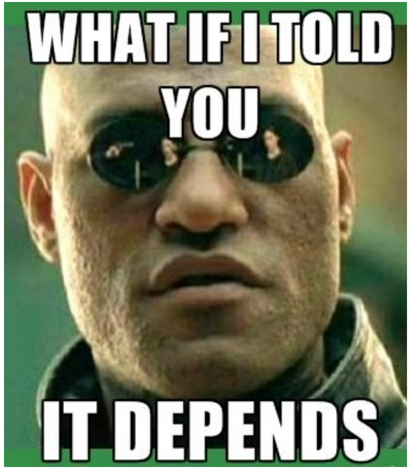
IT DEPENDS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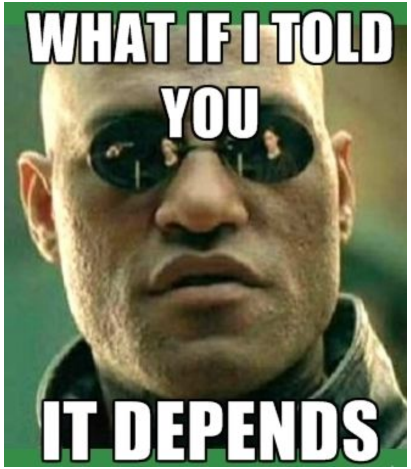
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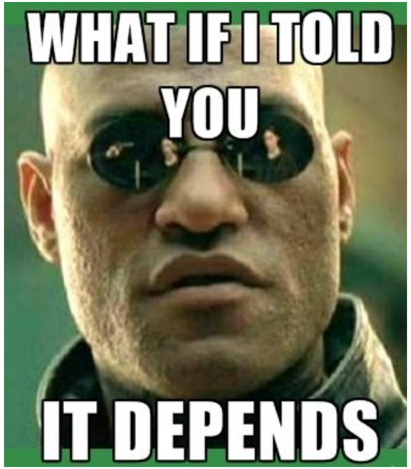
Hyperparameter
tuning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Hyperparameter
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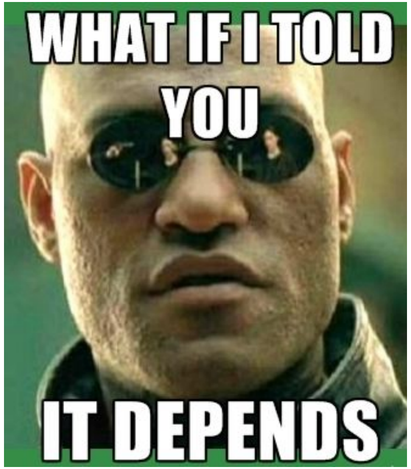
WHAT IF I TOLD YOU
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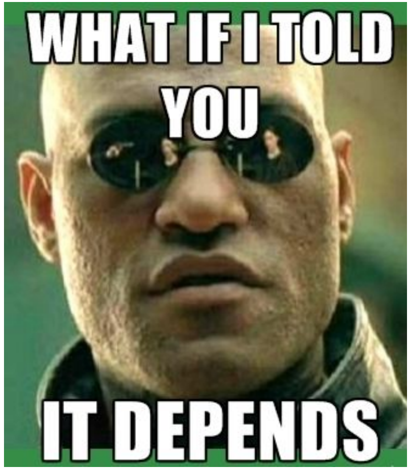
Hyperparameter tuning


Features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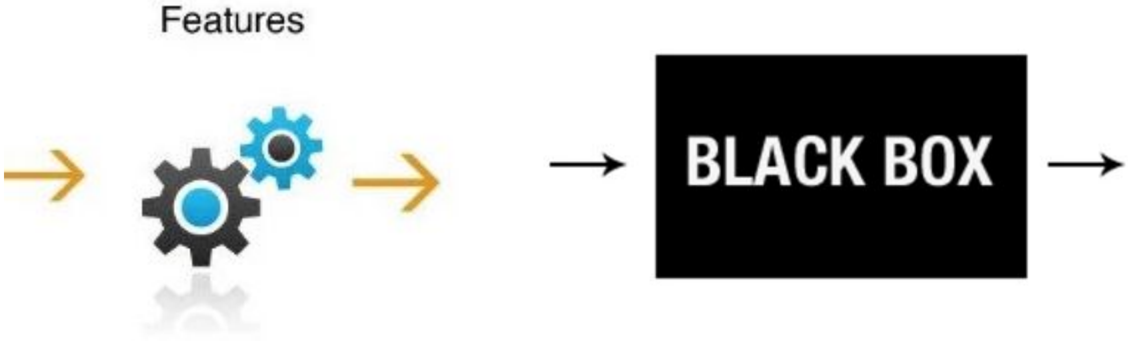
Hyperparameter tuning


Features
BLACK BOX


GBM?
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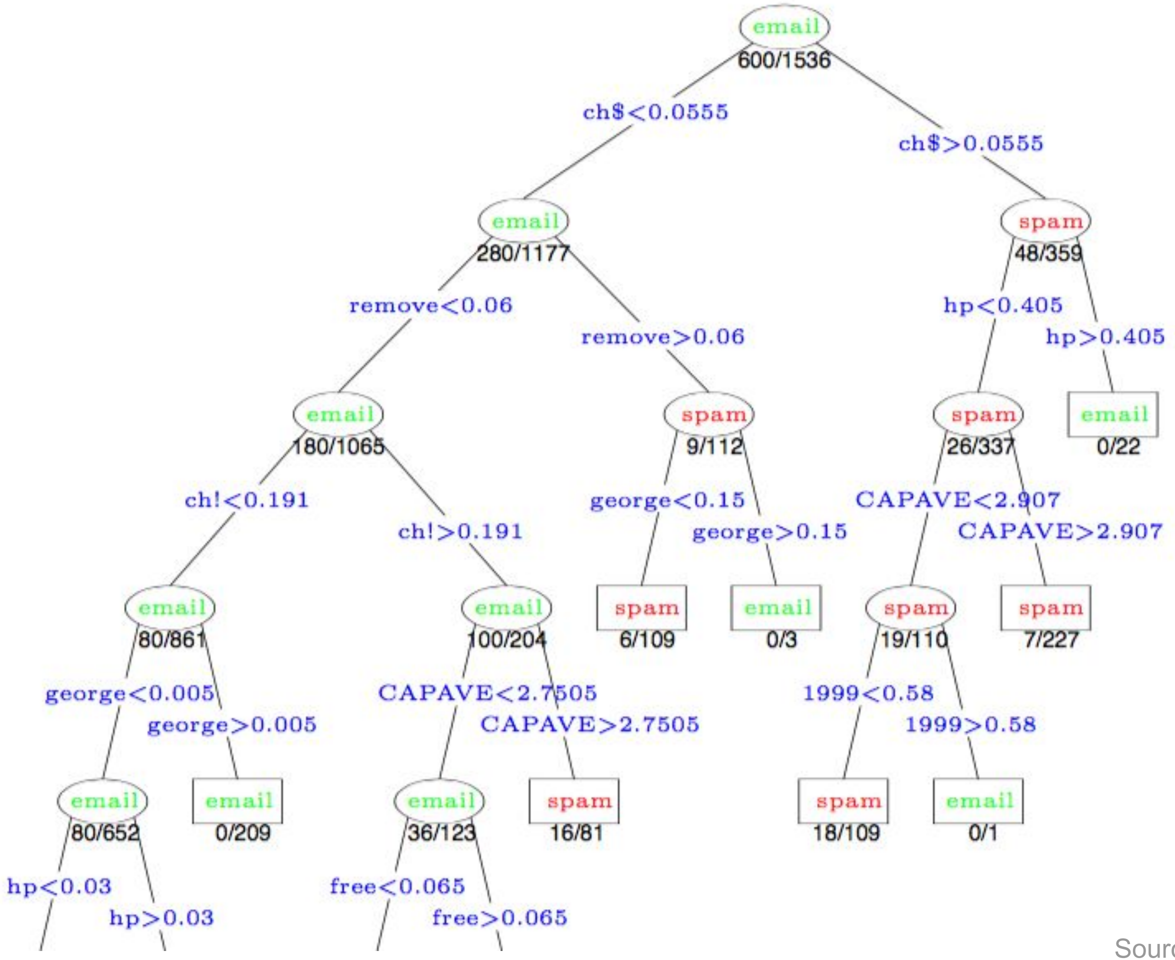

Source: Hastie etal, ESL 2ed

Algorithm 10.1 *AdaBoost.M1.*

1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))],\ i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

Source: Hastie etal, ESL 2ed

- R packages
- Python scikit-learn
- Vowpal Wabbit
- H2O
- xgboost
- Spark MLlib
- a few others

open source

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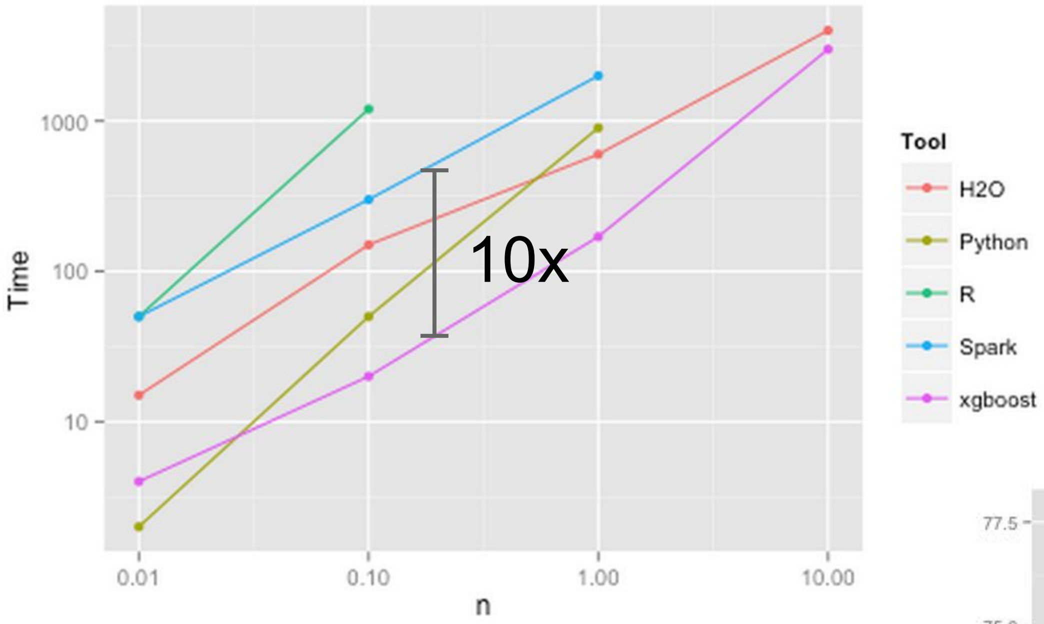
Simple/limited/incomplete benchmark



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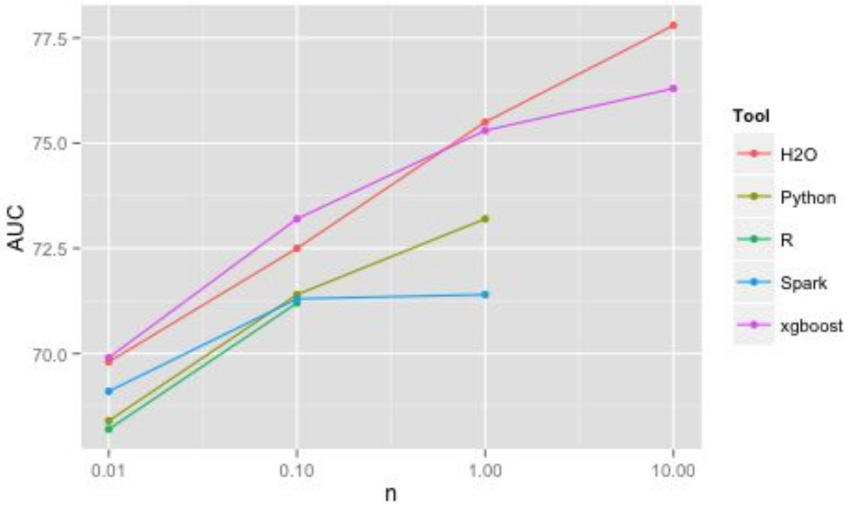
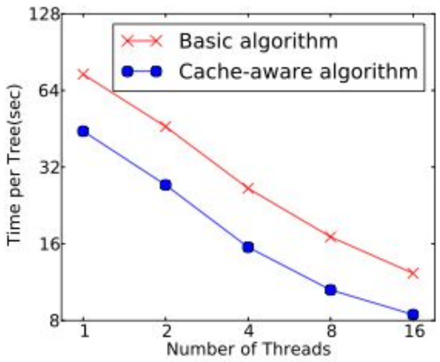


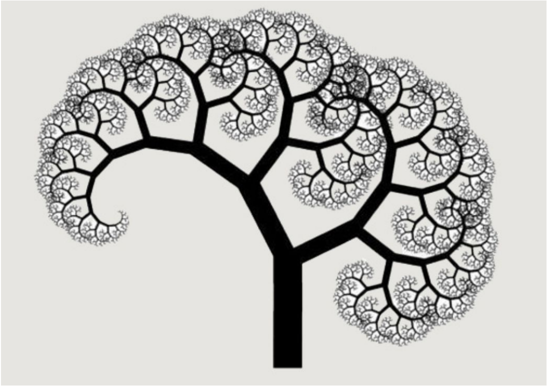
arXiv.org > cs > arXiv:1603.02754

Computer Science > Learning

XGBoost: A Scalable Tree Boosting System



H_2O.ai



Microsoft / LightGBM

arXiv.org > cs > arXiv:1603.02754

Computer Science > Learning

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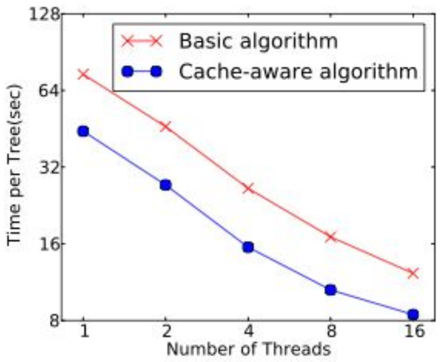

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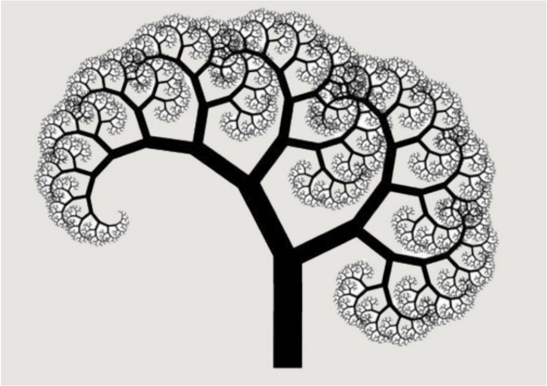


Microsoft / **LightGBM**

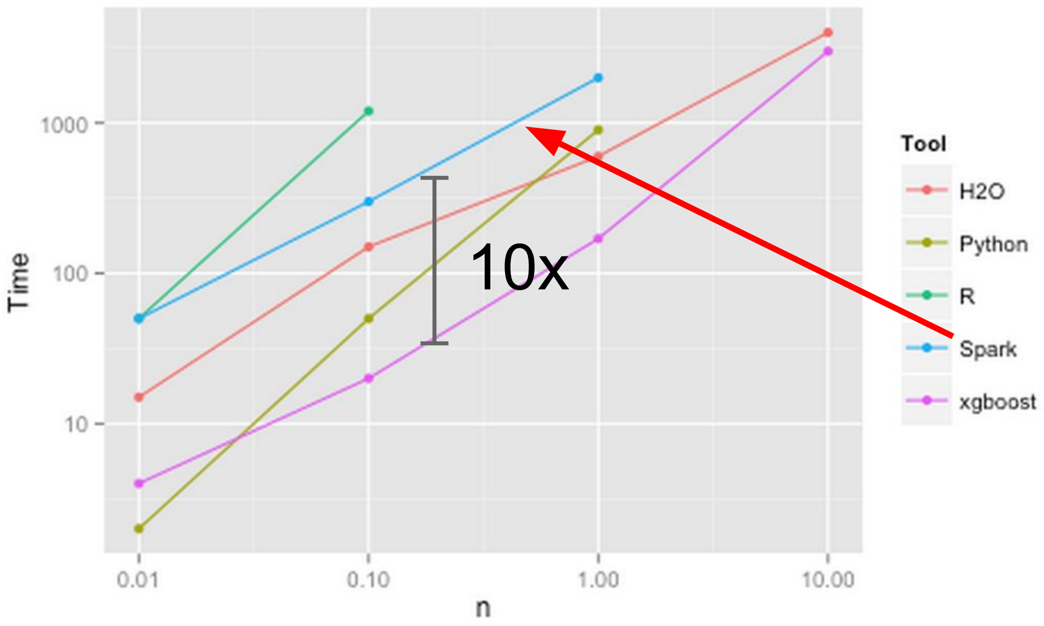
https://cran.r-project.org/web/pa

xgboost: Extreme Gradient Boosting

https://cran.r-project.org/

h2o: R Interface for H2O

PyData



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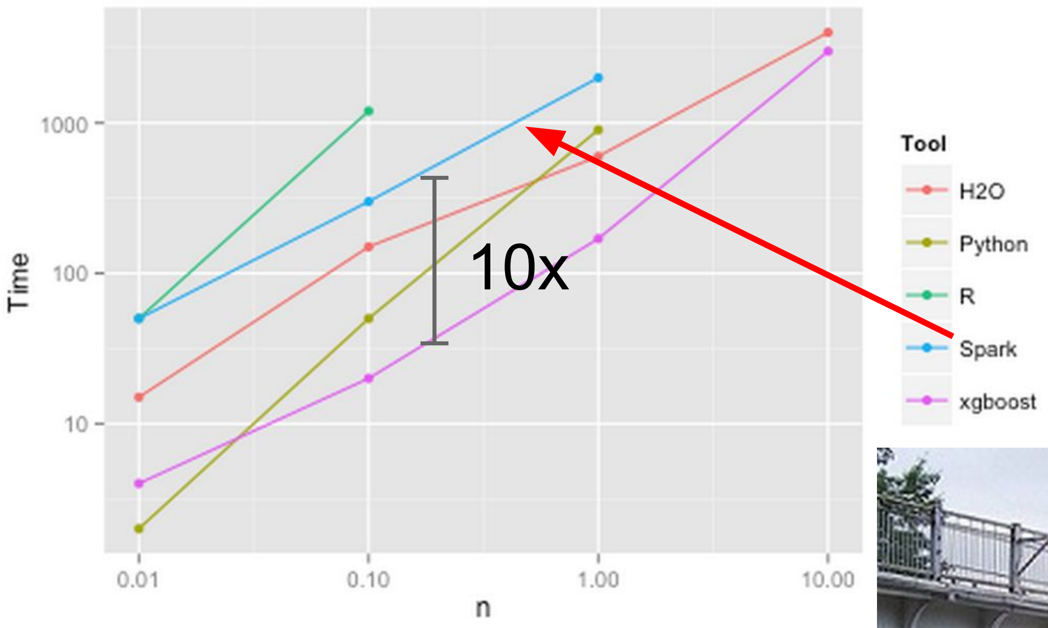

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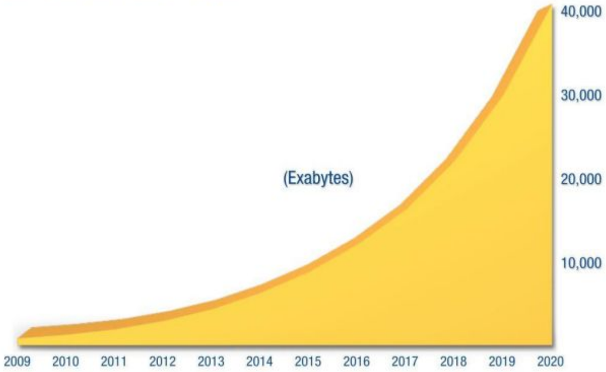
Figure 1

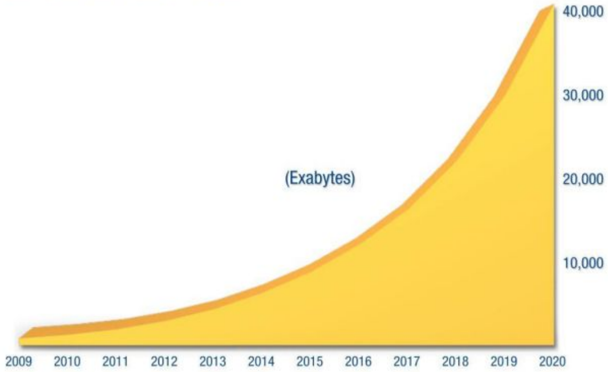
The Digital Universe: 50-fold Growth from the Beginning of 2010 to the End of 2020



Source: IDC's Digital Universe Study, sponsored by EMC, December 2012

Figure 1

The Digital Universe: 50-fold Growth from the Beginning of 2010 to the End of 2020



Source: IDC's Digital Universe Study, sponsored by EMC, December 2012

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@hadleywickham

Following

"It takes a big man to admit his data is small" — @jcheng

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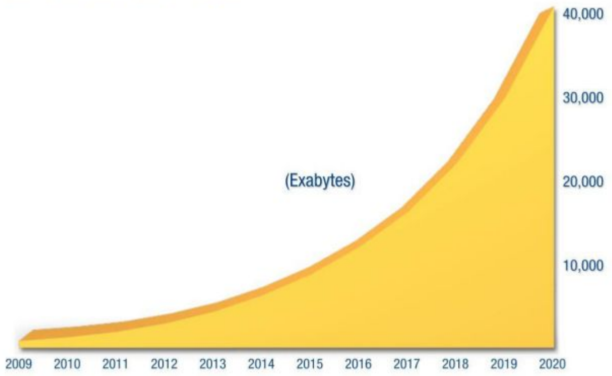
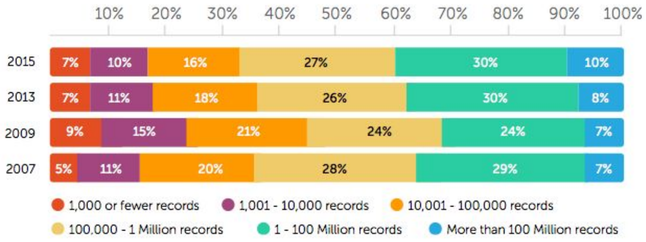


Source: IDC's Digital Universe Study, sponsored by EMC, December 2012

TYPICAL SIZE OF DATASETS



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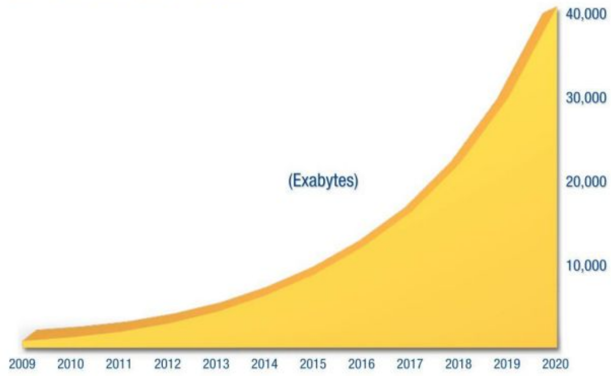

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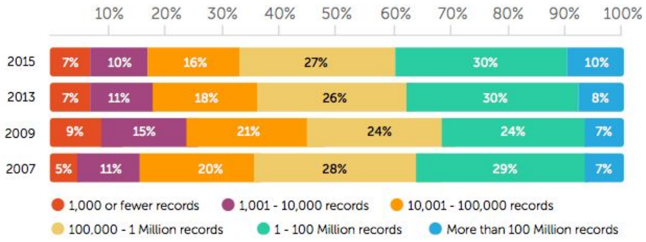

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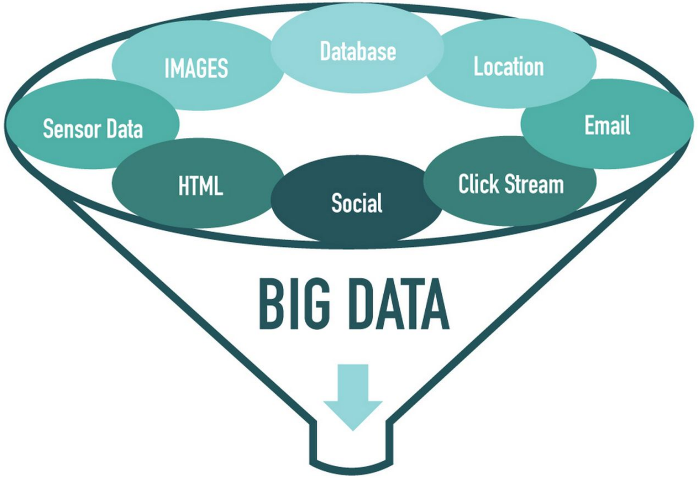
Following

"It takes a big man to admit his data is small" — @jcheng



Kingston Technology Value RAM 128GB Kit (4x32GB) 2133MHz DDR4 ECC Reg CL15 (KVR21R15D4K4/128)

by Kingston Technology

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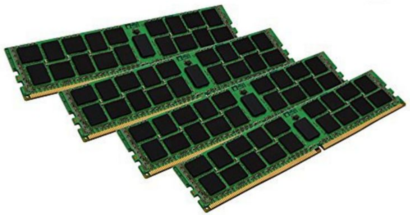
Was: ~~$743.99~~

Price: $743.96 & **FREE Shipping**. Details



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amazon web services

Model	vCPU	Mem (GiB)
r3.8xlarge	32	244
x1e.32xlarge	128	3,904
u-12tb1.metal	448	12 **(TiB)**

Szilard @DataScienceLA · Aug 3

I wish my #machinelearning worked... ("both" is not a choice 😃) #bigdata #datascience #rstats #pydata cc @h2o @databricks @cloudera @kaggle

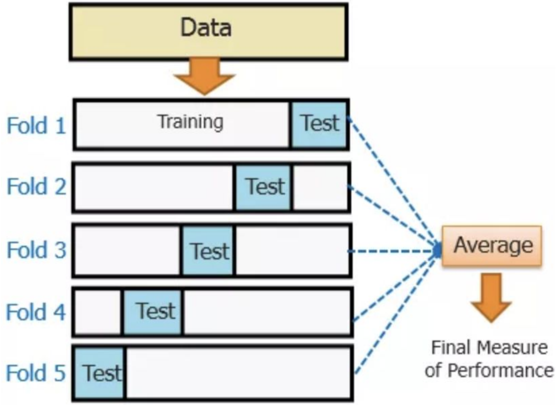
10% on 10x bigger data

70% 10x faster

20% I don't care about either

104 votes • Final results


16
MISSION
WINNOW
MAHLE


Data
Fold 1
Training
Test
Fold 2
Test
Fold 3
Test
Fold 4
Test
Fold 5
Test
Average
Final Measure
of Performance


Hyperparameter
tuning

szilard / GBM-perf

```
git clone https://github.com/szi
cd GBM-perf/cpu
sudo docker build -t gbmperf_cpu
sudo docker run --rm gbmperf_cpu
```

r4.8xlarge (32 cores, but run on physical cores only/no hyperthreading) with software as of

Tool	Time[s] 100K	Time[s] 1M	Time[s] 10M	AUC 1M	AUC 10M
h2o	16	20	100	0.762	0.776
xgboost	3.8	12	78	0.749	0.755
lightgbm	**2.4**	**5.2**	42	0.764	0.774
catboost	5.4	50	490	0.740	0.744

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catboost	5.4	50	490	0.740	0.744

p3.2xlarge (1 GPU, Tesla V100) with software as of 2019-04-29:

Tool	Time[s] 100K	Time[s] 1M	Time[s] 10M	AUC 1M	AUC 10M
h2o xgboost	9	14	60	0.749	0.756
xgboost	**2.4**	**4.8**	**13**	0.750	0.756
lightgbm	10	16	67	0.766	0.774
catboost	3.9	10	135	0.742	0.750

100M records and RAM usage

CPU (m5.12xlarge):

Tool	time [s]	AUC	RAM train [GB]
h2o	520	0.775	8
xgboost	510	0.751	15
lightgbm	**310**	0.774	**5**
catboost	3360	0.723 ?!	140

100M records and RAM usage

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xgboost	510	0.751	15
lightgbm	**310**	**0.774**	**5**
catboost	3360	0.723 ?!	140

GPU (Tesla V100):

Tool	time [s]	AUC	GPU mem [GB]	extra RAM [GB]
h2o xgboost	270	0.755	4	30
xgboost	**80**	0.756	6	**0**
lightgbm	400	0.774	3	6
catboost	crash (OOM)		>16	14

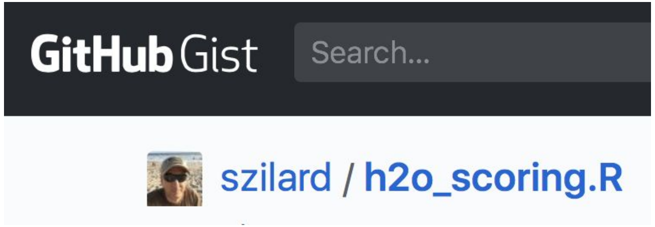
```
## exporting model for scoring

h2o.download_mojo(md_rf, path = "./h2o")
```

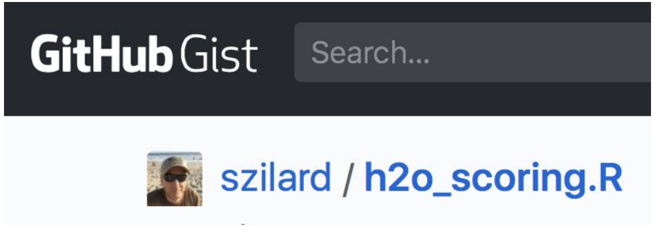
```
## building prediction service

# (need jetty-runner.jar ROOT.war from Steam)
java -jar jetty-runner.jar ROOT.war

curl -X POST --form mojo=@h2o_RF.zip --form jar=@h2o-genmodel.jar \
             localhost:8080/makewar > h2o_RF_MOJO.war
```



H2O.ai

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```

```bash
## run prediction service

java -jar jetty-runner.jar --port 20000 h2o_RF_MOJO.war
```

```bash
## score via REST API

time curl "http://localhost:20000/predict?Month=c-8&DayofMonth=c-21&Da
# (fast scoring needs JVM to warm up with a few requests)
```

```r
## read CSV (e.g. data.table::fread) or get data from database (SQL connector)
## do one-hot-encoding of categorical variables (e.g. Matrix::sparse.model.matrix)

## special optimized data structure
dxgb_train <- xgb.DMatrix(data = X_train, label = y_train)

## TRAIN
md <- xgb.train(data = dxgb_train,
                objective = "binary:logistic",
                nround = 100, max_depth = 10, eta = 0.1,
                tree_method = "hist")

## SCORE
yhat <- predict(md, newdata = X_test)

## evaluation (score distribution, ROC curve, AUC etc.)
```

```r
h2o.gbm(x, y, training_frame, model_id, checkpoint, ignore_const_cols = TRUE,
  distribution = c("AUTO", "gaussian", "bernoulli", "multinomial", "poisson",
  "gamma", "tweedie", "laplace", "quantile", "huber"), quantile_alpha = 0.5,
  tweedie_power = 1.5, huber_alpha = 0.9, ntrees = 50, max_depth = 5,
  min_rows = 10, learn_rate = 0.1, learn_rate_annealing = 1,
  sample_rate = 1, sample_rate_per_class, col_sample_rate = 1,
  col_sample_rate_change_per_level = 1, col_sample_rate_per_tree = 1,
  nbins = 20, nbins_top_level = 1024, nbins_cats = 1024,
  validation_frame = NULL, balance_classes = FALSE, class_sampling_factors,
  max_after_balance_size = 5, seed, build_tree_one_node = FALSE,
  nfolds = 0, fold_column = NULL, fold_assignment = c("AUTO", "Random",
  "Modulo", "Stratified"), keep_cross_validation_predictions = FALSE,
  keep_cross_validation_fold_assignment = FALSE,
  score_each_iteration = FALSE, score_tree_interval = 0,
  stopping_rounds = 0, stopping_metric = c("AUTO", "deviance", "logloss",
  "MSE", "AUC", "misclassification", "mean_per_class_error"),
  stopping_tolerance = 0.001, max_runtime_secs = 0, offset_column = NULL,
  weights_column = NULL, min_split_improvement = 1e-05,
  histogram_type = c("AUTO", "UniformAdaptive", "Random", "QuantilesGlobal",
  "RoundRobin"), max_abs_leafnode_pred, pred_noise_bandwidth = 0,
  categorical_encoding = c("AUTO", "Enum", "OneHotInternal", "OneHotExplicit",
  "Binary", "Eigen"))
```

blog.h2o.ai/2016/06/h2o-gbm-tuning-tutorial-for-r/

Arno Candel in GBM, R, Technical, Tutorials | June 16, 2016

H2O GBM Tuning Tutorial for R

In this tutorial, we show how to build a well-tuned H2O GBM model for a supervised classification task. and use a small dataset to allow you to reproduce these results in a few minutes on a laptop. This script ca dreds of GBs large and H2O clusters with dozens of compute nodes.

---

machinelearningmastery.com/configure-gradient-boosting-algorithm/

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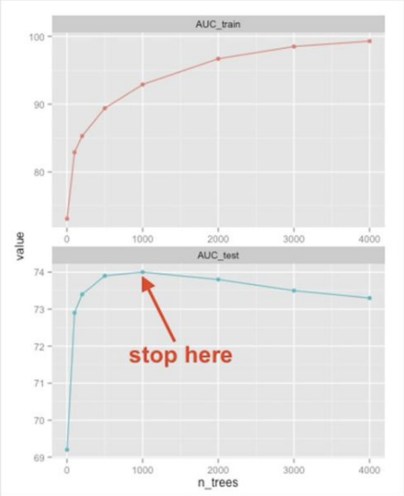
How to Configure the Gradient Boosting Algorithm

by **Jason Brownlee** on September 12, 2016 in **XGBoost**

Szilard [Deeper than Deep Learning]
@DataScienceLA

GBM/GBDT tip of the day: If it's not using early stopping, it's crap. 😬😬😬 (early stopping: checking accuracy metric on a validation set and stopping when it starts deteriorating by X) If not, you are either overfitting or wasting CPU/training time (or both). Don't do either!



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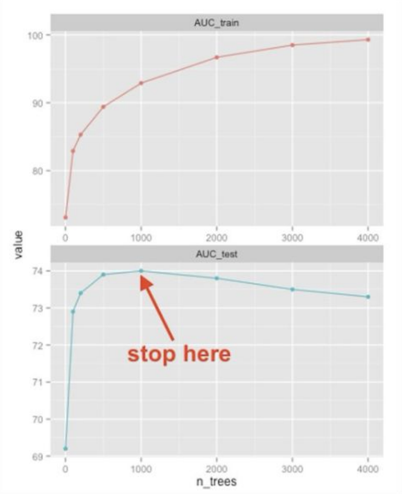


Szilard [Deeper than Deep Learning]
@DataScienceLA

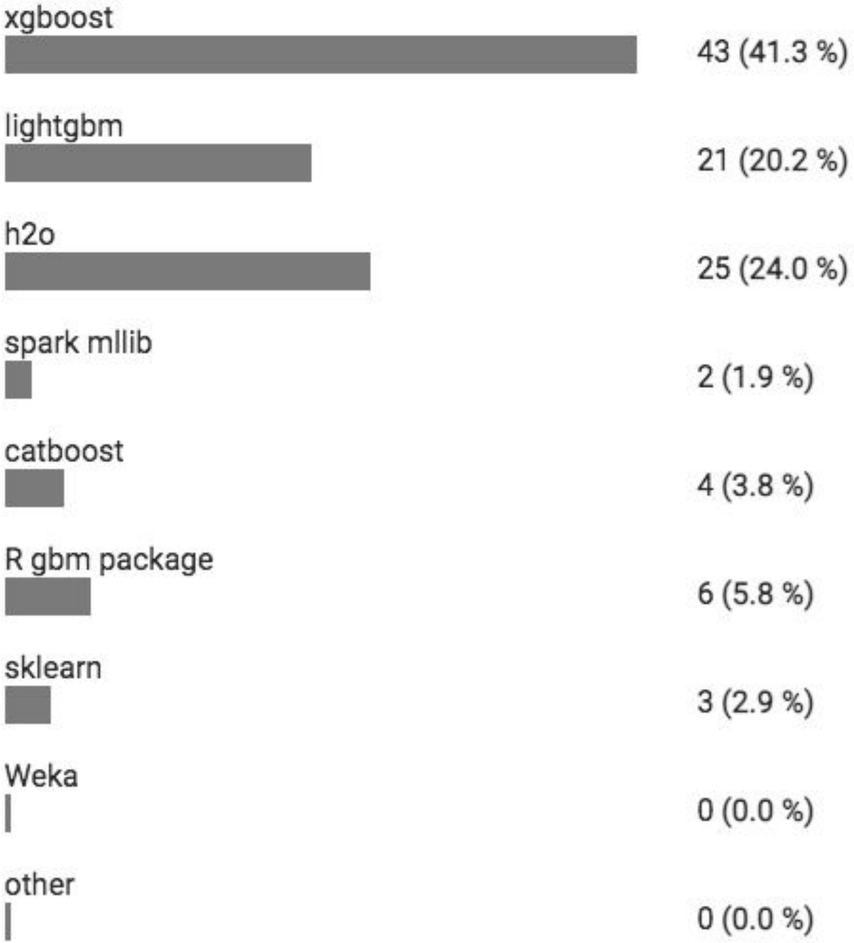
in all 3 top GBM implementations (#xgboost, #lightgbm, #h2oai) all you have to do (for early stopping) is to set a few params in the training function

```
md <- xgb.train(data = dxgb_train,
+               objective = "binary:logistic",
+               max_depth = 10, eta = 0.1,
+               nround = 10000, early_stopping_rounds = 10, watchlist = list(valid=dxgb_valid),
+               tree_method = "hist")

[1]     valid-error:0.207010
Will train until valid_error hasn't improved in 10 rounds.

[2]     valid-error:0.203230
[3]     valid-error:0.202950
[4]     valid-error:0.202810
[5]     valid-error:0.202550
[6]     valid-error:0.202380
[7]     valid-error:0.202410
[8]     valid-error:0.202380
....
[113]   valid-error:0.197940
[114]   valid-error:0.197960
[115]   valid-error:0.197940
[116]   valid-error:0.197950
[117]   valid-error:0.197820
Stopping. Best iteration:
[107]   valid-error:0.197750
```

	gbm (R pkg)	xgboost	lightgbm	h2o
easy R install	cran	cran	linux OK	java+cran
maintained	retired	yes	yes	yes
preprocessing	not needed	1-hot	1-hot/categ int	not needed
new cats scoring	yes	no	no	yes
early stopping	no	yes	yes	yes
speed (CPU)	1 core	ok	fastest	slow (small data)
GPU supported	no	yes	yes	via xgboost
speed GPU	NA	fastest	ok/slow	indirectly/slower
REST scoring	no	no	no	yes
other algos	no	RF	RF	RF/GLM/NN
best for	teaching/historic	Kaggle	Kaggle	prod/real-time



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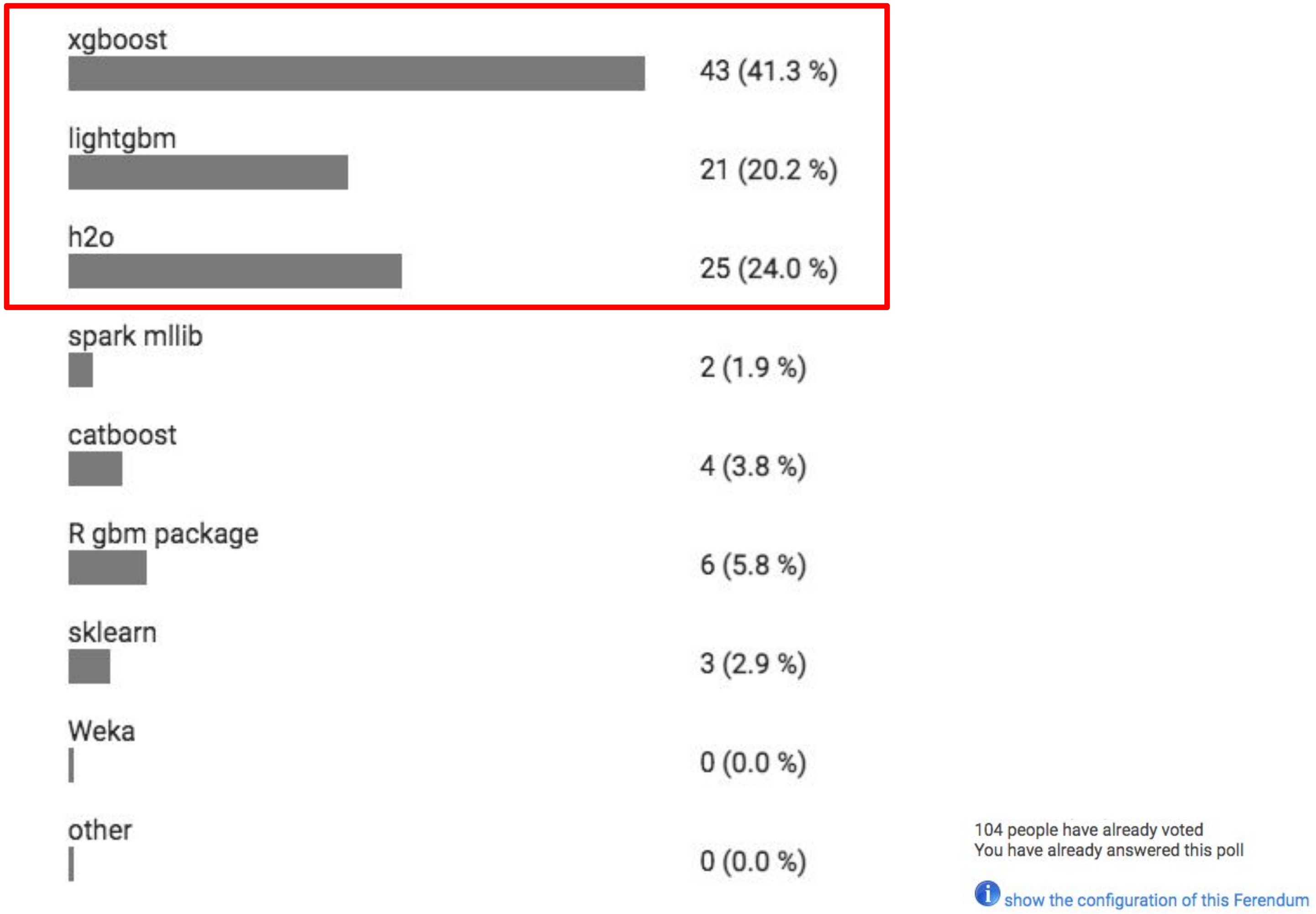
xgboost
43 (41.3 %)
lightgbm
21 (20.2 %)
h2o
25 (24.0 %)
spark mllib
2 (1.9 %)
catboost
4 (3.8 %)
R gbm package
6 (5.8 %)
sklearn
3 (2.9 %)
Weka
0 (0.0 %)
other
0 (0.0 %)
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Winning Solution of KaggleDays 2019 Competition in San Francisco

Source: https://www.linkedin.com/pulse/winning-solution-kaggledays-2019-competition-san-francisco-mark-peng/

Winning Solution of KaggleDays 2019 Competition in San Francisco

During the first two to three hours of the competition, we focused on exploratory data analysis (EDA). We first analyzed the distributions of raw features between train and test

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For model training, LightGBM is chosen as the baseline model for doing quick experiments on raw and engineered features. It turned out that our engineered features improved AUC in

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Based on the LightGBM baseline notebook, I created other notebooks for Xgboost, Logistic Regression, Random Forests and Extra Trees models. To save some time, I ran Random

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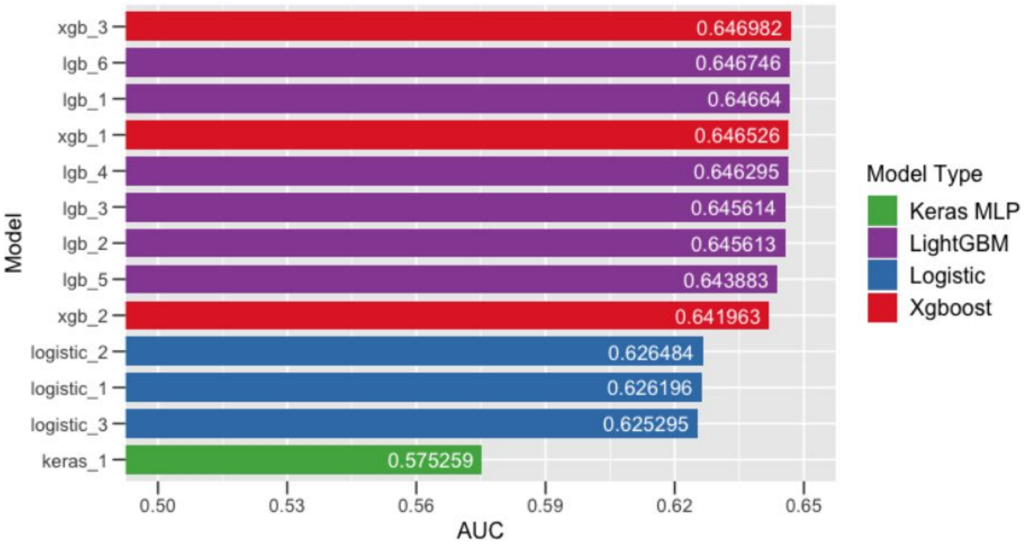

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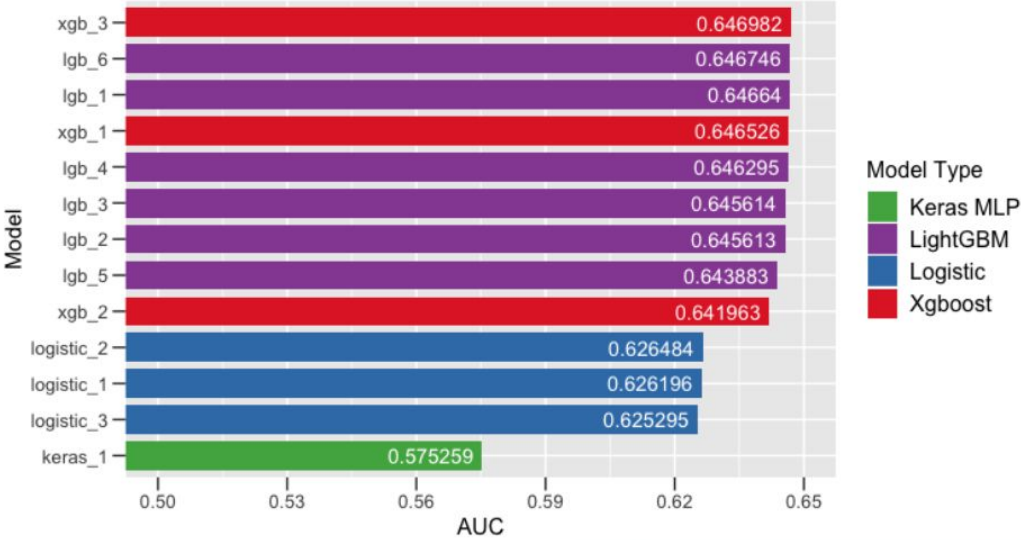

For blending and stacking, we looked for diverse models that perform relatively well, but are not highly correlated with each other. Xgboost and LightGBM had very similar

Source: https://www.linkedin.com/pulse/winning-solution-kaggledays-2019-competition-san-francisco-mark-peng/


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In the last 5 years I gave about 50 talks at various data science and machine learning conferences and meetups.

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