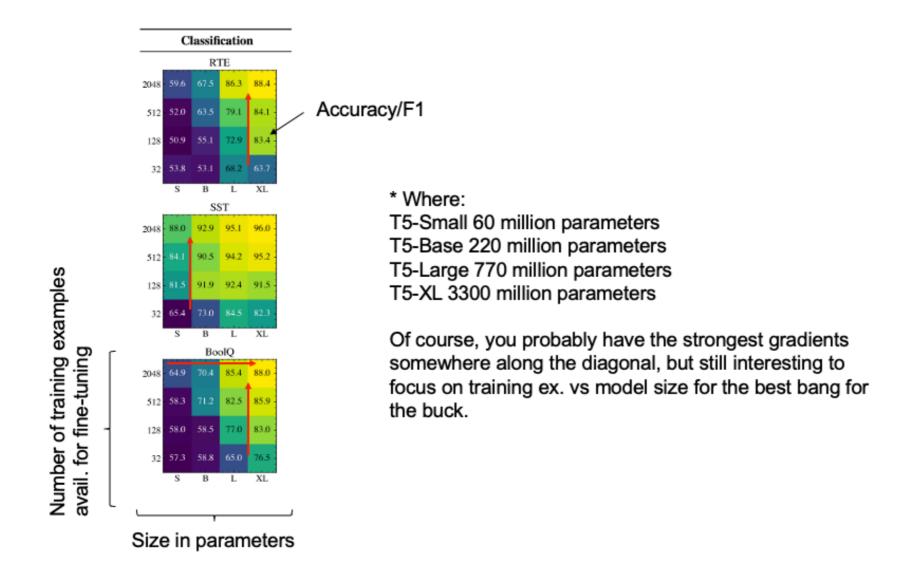
#### Computer Science > Computation and Language

[Submitted on 8 Oct 2021]

#### A Few More Examples May Be Worth Billions of Parameters

Yuval Kirstain, Patrick Lewis, Sebastian Riedel, Omer Levy

https://arxiv.org/abs/2110.04374



#### Lecture 07

### **Ensemble Methods Part 2/3**

STAT 451: Machine Learning, Fall 2021

Sebastian Raschka

### Overview

Majority Voting

Bagging

Boosting

Random Forests

Stacking

**Ensemble Methods** 

- 7.1 Ensemble Methods -- Intro and Overview
- 7.2 Majority Voting
- 7.3 Bagging
- 7.4 Boosting

### 7.5 Gradient Boosting

- 7.6 Random Forests
- 7.7 Stacking

## Gradient Boosting

# Gradient Boosting

Gradient boosting is somewhat similar to AdaBoost:

- trees are fit sequentially to improve error of previous trees
- boost weak learners to a strong learner

The way how the trees are fit sequentially differs in AdaBoost and Gradient Boosting, though ...

Friedman, J. H. (1999). "Greedy Function Approximation: A Gradient Boosting Machine".

### **Gradient Boosting -- Conceptual Overview**

- Step 1: Construct a base tree (just the root node).
- Step 2: Build next tree based on errors of the previous tree.
- Step 3: Combine tree from step 1 with trees from step 2. Go back to step 2.

				ars
x1# Rooms	x2=City	x3=Age	y=Price	
5	Boston	30	1.5	
10	Madison	20	0.5	
6	Lansing	20	0.25	
5	Waunakee	10	0.1	

Step 1: Construct a base tree (just the root node)

$$\hat{y}_1 = \frac{1}{n} \sum_{i=1}^n y^{(i)} = 0.5875$$

In million LIC Dollars

 Step 2: Build next tree based on errors of the previous tree

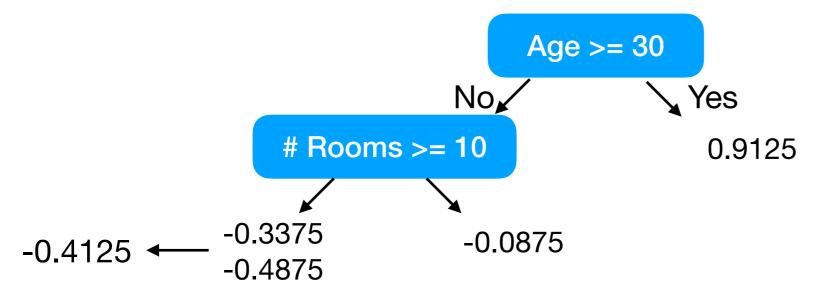
First, compute (pseudo) residuals:  $r_1 = y_1 - \hat{y}_1$ 

x1#	x2=City	x3=Age	y=Price	r1=Res	
5	Boston	30	1.5	1.5 - 0.5875 = 0.9125	
10	Madison	20	0.5	0.5 - 0.5875 = -0.0875	
6	Lansing	20	0.25	0.25 - 0.5875 = -0.3375	
5	Waunake	10	0.1	0.1 - 0.5875 = -0.4875	

Step 2: Build next tree based on errors of the previous tree

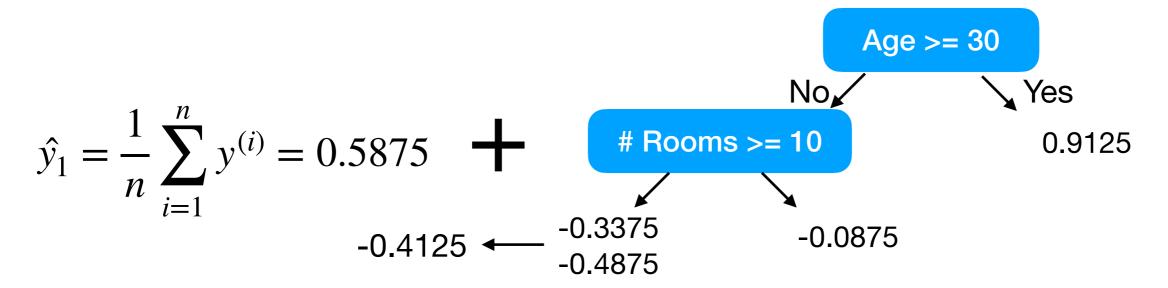
That is, create a tree based on  $x_1, \ldots, x_m$  to fit the residuals

x1#	x2=City	x3=Age	y=Price	r1=Residual
5	Boston	30	1.5	1.5 - 0.5875 = 0.9125
10	Madison	20	0.5	0.5 - 0.5875 = -0.0875
6	Lansing	20	0.25	0.25 - 0.5875 = -0.3375
5	Waunake	10	0.1	0.1 - 0.5875 = -0.4875



**Step 3:** Combine tree from step 1 with trees from step 2

x1#	x2=City	x3=Age	y=Price	r1=Res
5	Boston	30	1.5	1.5 - 0.5875 = 0.9125
10	Madison	20	0.5	0.5 - 0.5875 = -0.0875
6	Lansing	20	0.25	0.25 - 0.5875 = -0.3375
5	Waunake	10	0.1	0.1 - 0.5875 = -0.4875



• Step 3: Combine tree from step 1 with trees from step 2

	x1#	x2=City	x3=Age	y=Price	r1=Res
	5	Boston	30	1.5	1.5 - 0.5875 = 0.9125
E.g.,	10	Madison	20	0.5	0.5 - 0.5875 = -0.0875
predict -	6	Lansing	20	0.25	0.25 - 0.5875 = -0.3375
Lansing	5	Waunakee	10	0.1	0.1 - 0.5875 = -0.4875

$$\hat{y_1} = \frac{1}{n} \sum_{i=1}^{n} y^{(i)} = 0.5875 + \text{\#Rooms} >= 10$$
 0.9125 
$$-0.4125 \leftarrow -0.3375 -0.0875$$

E.g., predict Lansing

predict  $0.5875 + \alpha \times (-0.4125)$ 

where  $\alpha$  learning rate between 0 and 1 (if  $\alpha = 1$ , low bias but high variance)

### **Gradient Boosting -- Algorithm Overview**

**Step 0:** Input data  $\{\langle \mathbf{x}^{(i)}, y^{(i)} \rangle\}_{i=1}^n$ 

Differentiable Loss function  $L(y^{(i)}, h(\mathbf{x}^{(i)}))$ 

**Step 1:** Initialize model  $h_0(\mathbf{x}) = \underset{\hat{y}}{\operatorname{argmin}} \sum_{i=1}^{n} L(y^{(i)}, \hat{y})$ 

Step 2:

### **Gradient Boosting -- Algorithm Overview**

Step 2: for 
$$t = 1$$
 to  $T$ 

**A.** Compute pseudo residual 
$$r_{i,t} = -\left[\frac{\partial L(\mathbf{y}^{(i)}, h(\mathbf{x}^{(i)}))}{\partial h(\mathbf{x}^{(i)})}\right]_{h(\mathbf{x}) = h_{t-1}(\mathbf{x})}$$

for i = 1 to n

- **B.** Fit tree to  $r_{i,t}$  values, and create terminal nodes  $R_{j,t}$  for  $j=1,...,J_t$
- C. for  $j = 1,...,J_t$ , compute

$$\hat{y}_{j,t} = \underset{\hat{y}}{\operatorname{argmin}} \sum_{\mathbf{x}^{(i)} \in R_{i,j}} L(y^{(i)}, h_{t-1}(\mathbf{x}^{(i)}) + \hat{y})$$

**D.** Update 
$$h_t(\mathbf{x}) = h_{t-1}(\mathbf{x}) + \alpha \sum_{j=1}^{J_t} \hat{y}_{j,t} \, \mathbb{I} \left( \mathbf{x} \in R_{j,t} \right)$$

### **Step 3:** Return $h_t(\mathbf{x})$

### **Step 0:** Input data $\{\langle \mathbf{x}^{(i)}, y^{(i)} \rangle\}_{i=1}^n$

Differentiable Loss function  $L(y^{(i)}, h(\mathbf{x}^{(i)}))$ 

E.g., Sum-squared error in regression

$$SSE' = \frac{1}{2} \left( y^{(i)} - h(\mathbf{x}^{(i)}) \right)^2$$

$$\frac{\partial}{\partial h(\mathbf{x}^{(i)})} \frac{1}{2} \left( y^{(i)} - h(\mathbf{x}^{(i)}) \right)^2 \quad \text{[chain rule]}$$

$$= 2 \times \frac{1}{2} (y^{(i)} - h(\mathbf{x}^{(i)})) \times (0 - 1) = - (y^{(i)} - h(\mathbf{x}^{(i)}))$$

[neg. residual]

**Step 1:** Initialize model 
$$h_0(\mathbf{x}) = \underset{\hat{y}}{\operatorname{argmin}} \sum_{i=1}^n L(y^{(i)}, \hat{y})$$
 pred. target

turns out to be the average (in regression)

$$\frac{1}{n} \sum_{i=1}^{n} y^{(i)}$$

Loop to make T trees (e.g., T=100)

**Step 2:** for 
$$t = 1$$
 to  $T$ 

**A.** Compute pseudo residual 
$$r_{i,t} = -$$

pseudo residual of the *t*-th tree and *i*-th example

$$-\left[\frac{\partial L(\mathbf{y}^{(t)}, h(\mathbf{x}^{(t)}))}{\partial h(\mathbf{x}^{(i)})}\right]_{h(\mathbf{x}) = h_{t-1}(\mathbf{x})}$$
for  $i = 1$  to  $n$ 

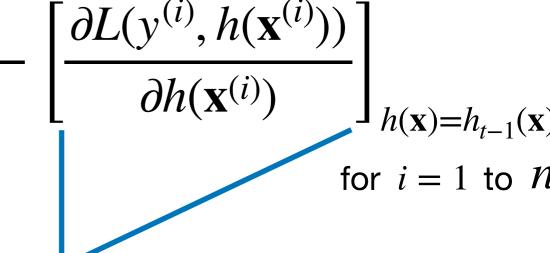
Derivative of the loss function

Loop to make T trees (e.g., T=100)

**Step 2:** for 
$$t = 1$$
 to  $T$ 

**A.** Compute pseudo residual  $r_{i,t} = -$ 

pseudo residual of the *t*-th tree and *i*-th example



Derivative of the loss function

**B.** Fit tree to  $r_{i,t}$  values, and create terminal nodes  $R_{j,t}$  for  $j=1,...,J_t$ Use features in dataset to fit tree  $R_{1,t} = \frac{R_{1,t}}{-0.4125} -\frac{0.0875}{R_{2,t}}$ 0.9125  $R_{3,t} = \frac{R_{1,t}}{-0.4875} -\frac{0.0875}{R_{2,t}}$ 

Sebastian Raschka

STAT 451: Intro to ML

Lecture 7: Ensemble Methods

for t=1 to TStep 2:

**A.** Compute pseudo residual  $r_{i,t} = -\left[\frac{\partial L(y^{(i)}, h(\mathbf{x}^{(i)}))}{\partial h(\mathbf{x}^{(i)})}\right]_{h(\mathbf{x}) = h_{t-1}(\mathbf{x})}$ 

for 
$$i = 1$$
 to  $n$ 

- **B.** Fit tree to  $r_{i,t}$  values, and create terminal nodes  $R_{i,t}$  for  $j = 1,...,J_t$
- C. for  $j = 1,...,J_t$ , compute



Compute the prediction for each leaf node

$$\hat{y}_{j,t} = \underset{\hat{y}}{\operatorname{argmin}} \sum_{\mathbf{x}^{(i)} \in R_{i,j}} L(y^{(i)}, h_{t-1}(\mathbf{x}^{(i)}) + \hat{y})$$
Only consider

Only consider examples at that leaf node

Like step 1 but add previous prediction

Lecture 7: Ensemble Methods STAT 451: Intro to ML Sebastian Raschka

Step 2: for 
$$t = 1$$
 to  $T$ 

**A.** Compute pseudo residual 
$$r_{i,t} = -\left[\frac{\partial L(y^{(i)}, h(\mathbf{x}^{(i)}))}{\partial h(\mathbf{x}^{(i)})}\right]_{h(\mathbf{x}) = h_{t-1}(\mathbf{x})}$$

for 
$$i = 1$$
 to  $n$ 

- **B.** Fit tree to  $r_{i,t}$  values, and create terminal nodes  $R_{i,t}$  for  $j = 1,...,J_t$
- C. for  $j = 1,...,J_t$ , compute

$$\hat{y}_{j,t} = \underset{\hat{y}}{\operatorname{argmin}} \sum_{\mathbf{x}^{(i)} \in R_{i,j}} L(y^{(i)}, h_{t-1}(\mathbf{x}^{(i)}) + \hat{y})$$

D. Update 
$$h_t(\mathbf{x}) = h_{t-1}(\mathbf{x}) + \alpha \sum_{j=1}^{\infty} \hat{y}_{j,t} \, \mathbb{I} \left( \mathbf{x} \in R_{j,t} \right)$$
learning rate between 0 and 1 (usually 0.1)

Summation just in case examples end up in multiple nodes

For prediction, combine all T trees, e.g.,

$$h_0(\mathbf{x}) = \underset{\hat{y}}{\operatorname{argmin}} \sum_{i=1}^n L(y^{(i)}, \hat{y})$$

$$+\alpha \hat{y}_{j,t=1} = \underset{\hat{y}}{\operatorname{argmin}} \sum_{\mathbf{x}^{(i)} \in R_{i,j}} L(y^{(i)}, h_{(t=1)-1}(\mathbf{x}^{(i)}) + \hat{y})$$

• • •

$$+\alpha \hat{y}_{j,T} = \underset{\hat{y}}{\operatorname{argmin}} \sum_{\mathbf{x}^{(i)} \in R_{i,j}} L(\mathbf{y}^{(i)}, h_{T-1}(\mathbf{x}^{(i)}) + \hat{y})$$

For prediction, combine all T trees, e.g.,

$$h_0(\mathbf{x}) = \underset{\hat{y}}{\operatorname{argmin}} \sum_{i=1}^n L(y^{(i)}, \hat{y})$$

$$+\alpha \hat{y}_{j,t=1}$$

The idea is that we decrease the pseudo residuals by a small amount at each step

. . .

$$+\alpha \hat{y}_{j,T}$$

### **XGBoost**

rearring system for tree boosting. The system is available as an open source package<sup>2</sup>. The impact of the system has been widely recognized in a number of machine learning and data mining challenges. Take the challenges hosted by the machine learning competition site Kaggle for example. Among the 29 challenge winning solutions <sup>3</sup> published at Kaggle's blog during 2015, 17 solutions used XGBoost. Among these solutions, eight solely used XGBoost to train the model, while most others combined XGBoost with neural nets in ensembles. For comparison, the second most popular method, deep neural nets, was used in 11 solutions. The success of the system was also witnessed in KDDCup 2015, where XGBoost was used by every winning team in the top-10. Moreover, the winning teams reported that ensemble

Chen, T., & Guestrin, C. (2016, August). Xgboost: A scalable tree boosting system. In *Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining* (pp. 785-794). ACM.

### **XGBoost**

Table 1: Comparison of major tree boosting systems.

System	exact greedy	approximate global	approximate local	out-of-core	sparsity aware	parallel
XGBoost	yes	yes	yes	yes	yes	yes
pGBRT	no	no	yes	no	no	yes
Spark MLLib	no	yes	no	no	partially	yes
H2O	no	yes	no	no	partially	yes
scikit-learn	yes	no	no	no	no	no
R GBM	yes	no	no	no	partially	no

Table 3: Comparison of Exact Greedy Methods with 500 trees on Higgs-1M data.

Method	Time per Tree (sec)	Test AUC
XGBoost	0.6841	0.8304
XGBoost (colsample=0.5)	0.6401	0.8245
scikit-learn	28.51	0.8302
R.gbm	1.032	0.6224

Chen, T., & Guestrin, C. (2016, August). XGBoost: A scalable tree boosting system. In *Proceedings of the 22nd International Conference on Knowledge Discovery and Data Mining* (pp. 785-794). ACM.

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### **XGBoost**

#### Summary and Main Points:

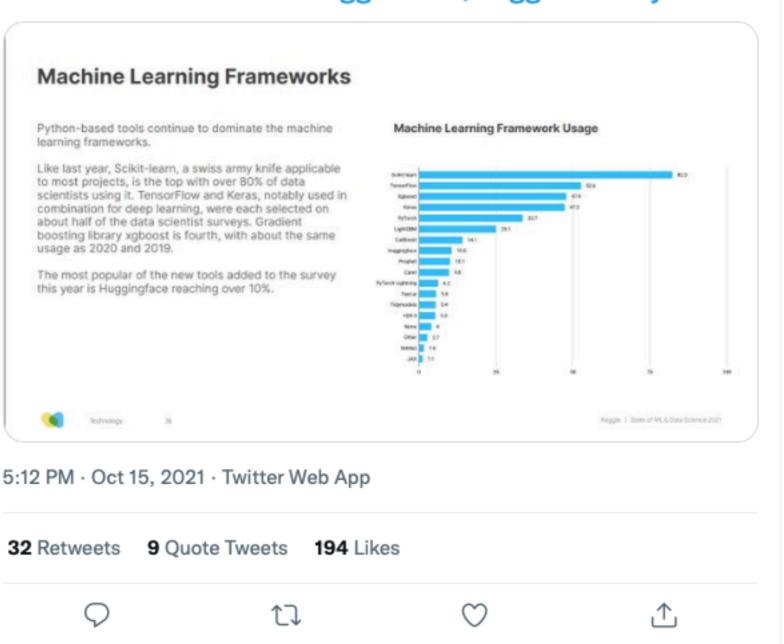
- scalable implementation of gradient boosting
- Improvements include: regularized loss, sparsity-aware algorithm, weighted quantile sketch for approximate tree learning, caching of access patterns, data compression, sharding
- Decision trees based on CART
- Regularization term for penalizing model (tree) complexity
- Uses second order approximation for optimizing the objective
- Options for column-based and row-based subsampling
- Single-machine version of XGBoost supports the exact greedy algorithm

Chen, T., & Guestrin, C. (2016, August). XGBoost: A scalable tree boosting system. In *Proceedings of the 22nd International Conference on Knowledge Discovery and Data Mining* (pp. 785-794). ACM.

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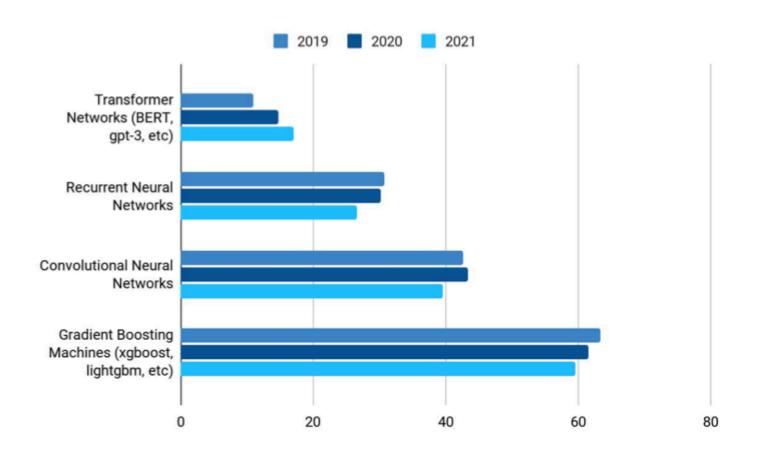
@kaggle State of machine learning annual survey. XGboost, as usual, is among the top framework choices. Glad that we can help to make ml and data science better together with collection of other awesome frameworks kaggle.com/kaggle-survey-...



#### Methods & Algorithms (cont.)

We also saw strong year-over-year growth in the use of large language models such as transformer networks (BERT, GPT-3, etc).

#### **Popular ML Algorithms**



Technology

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https://www.kaggle.com/kaggle-survey-2021

Sebastian Raschka STAT 451: Intro to ML Lecture 7: Ensemble Methods

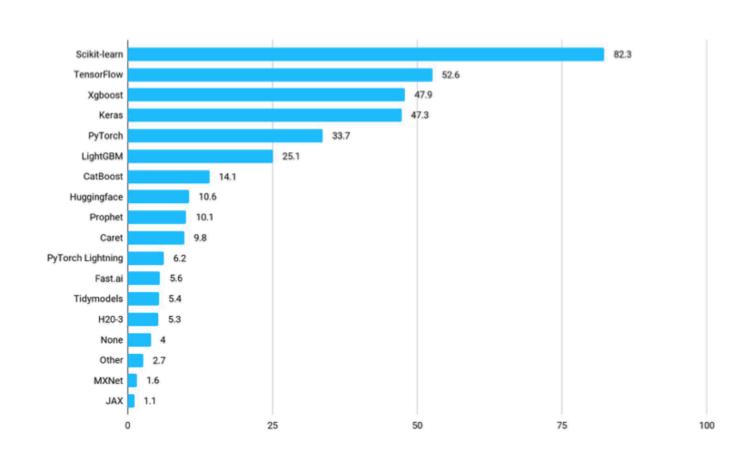
#### **Machine Learning Frameworks**

Python-based tools continue to dominate the machine learning frameworks.

Like last year, Scikit-learn, a swiss army knife applicable to most projects, is the top with over 80% of data scientists using it. TensorFlow and Keras, notably used in combination for deep learning, were each selected on about half of the data scientist surveys. Gradient boosting library xgboost is fourth, with about the same usage as 2020 and 2019.

The most popular of the new tools added to the survey this year is Huggingface reaching over 10%.

#### **Machine Learning Framework Usage**





Technology

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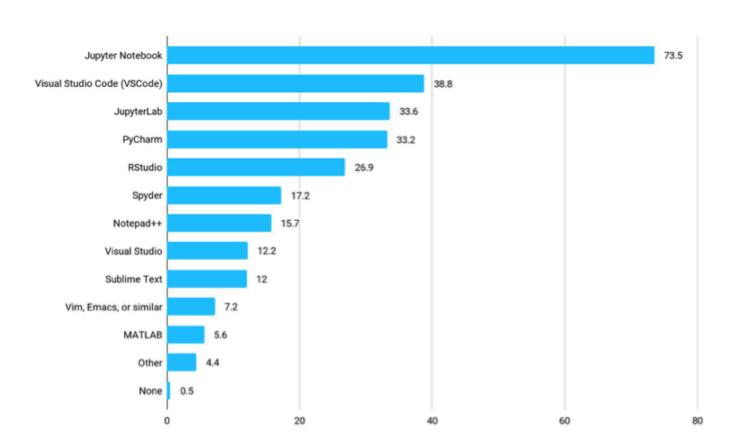
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#### **Interactive Development Environments**

Jupyter-based IDEs continue to be the go-to tool for data scientists, with around three-quarters of Kaggle data scientists using it. However, Visual Studio Code is in the second spot with 38%.

#### **IDE Popularity**



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#### Speed

We compared speed using only the training task without any test or metric output. We didn't count the time for IO. For the ranking tasks, since XGBoost and LightGBM implement different ranking objective functions, we used <a href="regression">regression</a> objective for speed benchmark, for the fair comparison.

The following table is the comparison of time cost:

Data	xgboost	xgboost_hist	LightGBM
Higgs	3794.34 s	165.575 s	130.094 s
Yahoo LTR	674.322 s	131.462 s	76.229 s
MS LTR	1251.27 s	98.386 s	70.417 s
Expo	1607.35 s	137.65 s	62.607 s
Allstate	2867.22 s	315.256 s	148.231 s

LightGBM ran faster than xgboost on all experiment data sets.

#### **Accuracy**

We computed all accuracy metrics only on the test data set.

Data	Metric	xgboost	xgboost_hist	LightGBM
Higgs	AUC	0.839593	0.845314	0.845724
	NDCG <sub>1</sub>	0.719748	0.720049	0.732981
Yahoo LTR	NDCG <sub>3</sub>	0.717813	0.722573	0.735689
Talloo LTK	NDCG <sub>5</sub>	0.737849	0.740899	0.75352
	NDCG <sub>10</sub>	0.78089	0.782957	0.793498
	NDCG <sub>1</sub>	0.483956	0.485115	0.517767
MS LTR	NDCG <sub>3</sub>	0.467951	0.47313	0.501063
IVIS LIK	NDCG <sub>5</sub>	0.472476	0.476375	0.504648
	NDCG <sub>10</sub>	0.492429	0.496553	0.524252
Expo	AUC	0.756713	0.776224	0.776935
Allstate	AUC	0.607201	0.609465	0.609072

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https://lightgbm.readthedocs.io/en/latest/Experiments.html

#### 2.2 Histogram-based Split Finding

Both XGBoost and LightGBM support **histogram-based** algorithm for split finding. As mentioned in XGBoost paper, the exact-greedy (brute-force) split find algorithm is time consuming: for current feature to search, need to sort feature values and iterate through. For faster training, histogram-based algorithm is used, which bucket continuous feature into discrete bins. This speeds up training and reduces memory usage.

LightGBM is using histogram-based algorithm. Related parameters are:

- max\_bin : max number of bins that feature values will be bucketed in.
- min\_data\_in\_bin : minimal number of data inside one bin.
- bin\_construct\_sample\_cnt : number of data that sampled to construct histogram bins.

XGBoost has options to choose histogram-based algorithm, it is specified by tree\_method with options:

- auto: (default) use heuristic to choose the fastest method.
- exact: exact greedy algorithm.
- approx: approximate greedy algorithm using quantile sketch and gradient histogram.
- hist: fast histogram optimized approximate greedy algorithm, with this option enabled, max bin (default 256) could be tuned

#### https://bangdasun.github.io/2019/03/21/38-practical-comparison-xgboost-lightgbm/

### More GBM Implementations

#### **LightGBM, Light Gradient Boosting Machine**

#### From <a href="https://github.com/Microsoft/LightGBM">https://github.com/Microsoft/LightGBM</a>:

- Faster training speed and higher efficiency
- Lower memory usage
- Better accuracy
- Support of parallel and GPU learning
- Capable of handling large-scale data

Ke, G., Meng, Q., Finley, T., Wang, T., Chen, W., Ma, W., ... & Liu, T. Y. (2017). Lightgbm: A highly efficient gradient boosting decision tree. In *Advances in Neural Information Processing Systems* (pp. 3146-3154).

#### https://scikit-learn.org/stable/whats\_new.html#version-0-21-0

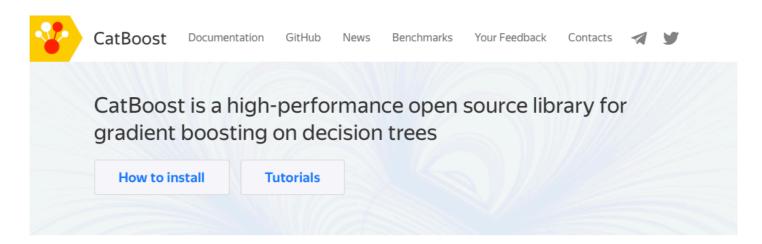
sklearn.ensemble ¶

Major Feature Add two new implementations of gradient boosting trees:
 ensemble.HistGradientBoostingClassifier and ensemble.HistGradientBoostingRegressor. The implementation of these estimators is inspired by LightGBM and can be orders of magnitude faster than ensemble.GradientBoostingRegressor and ensemble.GradientBoostingClassifier when the number of samples is larger than tens of thousands of samples. The API of these new estimators is slightly different, and some of the features from ensemble.GradientBoostingClassifier and ensemble.GradientBoostingRegressor are not yet supported.

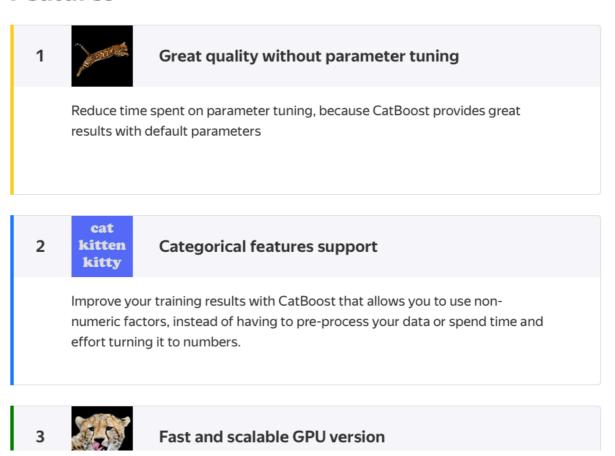
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#### **CatBoost**

#### https://catboost.ai



#### **Features**



```
from sklearn import model_selection
from sklearn.model_selection import train_test_split
from sklearn import datasets

data = datasets.load_breast_cancer()
X, y = data.data, data.target

X_temp, X_test, y_temp, y_test = \
    train_test_split(X, y, test_size=0.3, random_state=123, stratify=y)

X_train, X_valid, y_train, y_valid = \
    train_test_split(X_temp, y_temp, test_size=0.2, random_state=123, stratify=y_temp)

print('Train/Valid/Test sizes:', y_train.shape[0], y_valid.shape[0], y_test.shape[0])
```

Train/Valid/Test sizes: 318 80 171

#### Original gradient boosting

```
from sklearn.ensemble import GradientBoostingClassifier

boost = GradientBoostingClassifier(
    learning_rate=0.1,
    n_estimators=100,
    max_depth=8,
    random_state=1)

boost.fit(X_train, y_train)

print("Training Accuracy: %0.2f" % boost.score(X_train, y_train))
print("Validation Accuracy: %0.2f" % boost.score(X_valid, y_valid))
print("Test Accuracy: %0.2f" % boost.score(X_test, y_test))
```

Training Accuracy: 1.00 Validation Accuracy: 0.90 Test Accuracy: 0.92

#### HistGradientBoostingClassifier (inspired by LightGBM)

```
#from sklearn.experimental import enable_hist_gradient_boosting
from sklearn.ensemble import HistGradientBoostingClassifier

boost = HistGradientBoostingClassifier(
    learning_rate=0.1,
    #n_estimators=100,
    #max_depth=8,
    random_state=1)

boost.fit(X_train, y_train)

print("Training Accuracy: %0.2f" % boost.score(X_train, y_train))
print("Validation Accuracy: %0.2f" % boost.score(X_valid, y_valid))
print("Test Accuracy: %0.2f" % boost.score(X_test, y_test))
```

Training Accuracy: 1.00 Validation Accuracy: 0.96

Test Accuracy: 0.97

#### **XGBoost**

```
# https://xgboost.readthedocs.io/en/latest/build.html

#!pip install xgboost

import numpy as np
import xgboost as xgb

boost = xgb.XGBClassifier()

boost.fit(X_train, y_train)

print("Training Accuracy: %0.2f" % boost.score(X_train, y_train))
print("Validation Accuracy: %0.2f" % boost.score(X_valid, y_valid))
print("Test Accuracy: %0.2f" % boost.score(X_test, y_test))

[07:41:34] WARNING: ../src/learner.cc:1061: Starting in XGBoost 1.3.0, the default eval om 'error' to 'logloss'. Explicitly set eval_metric if you'd like to restore the old be Training Accuracy: 1.00
Validation Accuracy: 0.98
```

#### LightGBM

```
# https://lightgbm.readthedocs.io/en/latest/Installation-Guide.html
# conda install -c conda-forge lightgbm
```

```
import lightgbm as lgb

boost = lgb.LGBMClassifier()

boost.fit(X_train, y_train)

print("Training Accuracy: %0.2f" % boost.score(X_train, y_train))
print("Validation Accuracy: %0.2f" % boost.score(X_valid, y_valid))
print("Test Accuracy: %0.2f" % boost.score(X_test, y_test))
```

Training Accuracy: 1.00 Validation Accuracy: 0.96

Test Accuracy: 0.98

#### CatBoost

```
# https://catboost.ai
# conda install -c conda-forge catboost

from catboost import CatBoostClassifier

boost = CatBoostClassifier(verbose=0)

boost.fit(X_train, y_train)

print("Training Accuracy: %0.2f" % boost.score(X_train, y_train))
print("Validation Accuracy: %0.2f" % boost.score(X_valid, y_valid))
print("Test Accuracy: %0.2f" % boost.score(X_test, y_test))

Training Accuracy: 1.00
```

Validation Accuracy: 0.97

# Show Jupyter Notebook with Categorical Examples

- 7.1 Ensemble Methods -- Intro and Overview
- 7.2 Majority Voting
- 7.3 Bagging
- 7.4 Boosting
- 7.5 Gradient Boosting
- 7.6 Random Forests
- 7.7 Stacking

### Overview

Majority Voting

Bagging

Boosting

Random Forests

Stacking

**Ensemble Methods**