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A Gentle Introduction to XGBoost for Applied Machine Learning

by Jason Brownlee on August 17, 2016 in [XGBoost](#)

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Last Updated on August 21, 2019

XGBoost is an algorithm that has recently been dominating applied machine learning and Kaggle competitions for structured or tabular data.

XGBoost is an implementation of gradient boosted decision trees designed for speed and performance.

In this post you will discover XGBoost and get a gentle introduction to what is, where it came from and how you can learn more.

After reading this post you will know:

- What XGBoost is and the goals of the project.
- Why XGBoost must be apart of your machine learning toolkit.
- Where you can learn more to start using XGBoost on your next machine learning project.

Discover how to configure, fit, tune and evaluation gradient boosting models with XGBoost [in my new book](#), with 15 step-by-step tutorial lessons, and full python code.

Let's get started.

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A Gentle Introduction to XGBoost
Photo by [Sigfrid Lundström](#)

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What is XGBoost?

XGBoost stands for eXtreme Gradient Boosting.



The name `xgboost`, though, actually refers to the engineering goal to push the limit of computations resources for boosted tree algorithms. Which is the reason why many people use `xgboost`.

— Tianqi Chen, in answer to the question “What is the difference between the R `gbm` (gradient boosting machine) and `xgboost` (extreme gradient boosting)?” on Quora

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It is an implementation of gradient boosting machines created by [Tianqi Chen](#), now with contributions from many developers. It belongs to a broader collection of tools under the umbrella of the Distributed Machine Learning Community or [DMLC](#) who are also the creators of the popular [mxnet deep learning library](#).

Tianqi Chen provides a brief and interesting back story on the creation of XGBoost in the post [Story and Lessons Behind the Evolution of XGBoost](#).

XGBoost is a software library that you can download and install on your machine, then access from a variety of interfaces. Specifically, XGBoost supports the following main interfaces:

- Command Line Interface (CLI).
- C++ (the language in which the library is written)
- Python interface as well as a model in scikit-learn
- R interface as well as a model in the caret package
- Julia.
- Java and JVM languages like Scala and platforms

XGBoost Features

The library is laser focused on computational speed and frills. Nevertheless, it does offer a number of advanced features.

Model Features

The implementation of the model supports the features of the scikit-learn and R implementations, with new additions like regularization. Three main forms of gradient boosting are supported:

- **Gradient Boosting** algorithm also called gradient boosting machine including the learning rate.
- **Stochastic Gradient Boosting** with sub-sampling at the row, column and column per split levels.
- **Regularized Gradient Boosting** with both L1 and L2 regularization.

System Features

The library provides a system for use in a range of computing environments, not least:

- **Parallelization** of tree construction using all of your CPU cores during training.
- **Distributed Computing** for training very large models using a cluster of machines.
- **Out-of-Core Computing** for very large datasets that don't fit into memory.
- **Cache Optimization** of data structures and algorithm to make best use of hardware.

Algorithm Features

The implementation of the algorithm was engineered for efficiency of compute time and memory resources. A design goal was to make the best use of available resources to train the model. Some key algorithm implementation features include:

- **Sparse Aware** implementation with automatic handling of missing data values.
- **Block Structure** to support the parallelization
- **Continued Training** so that you can further build on a trained model.

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XGBoost is free open source software available for use under the permissive Apache-2 license.

Why Use XGBoost?

The two reasons to use XGBoost are also the two goals of the project:

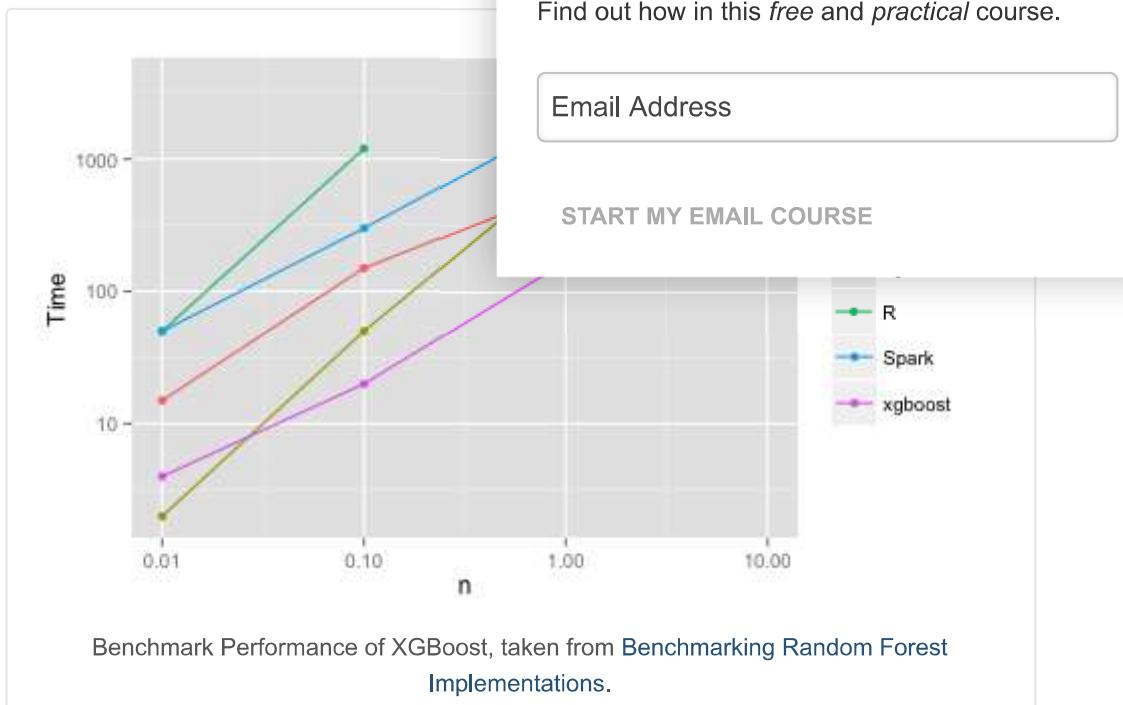
1. Execution Speed.
2. Model Performance.

1. XGBoost Execution Speed

Generally, XGBoost is fast. Really fast when compared to other implementations of gradient boosting.

Szilard Pafka performed some objective benchmarks comparing implementations of gradient boosting and bagged random forests in the blog post titled “[Benchmarking Random Forest Implementations](#)”.

He also provides all the code on [GitHub](#) and a more detailed write-up on [his blog](#).



His results showed that XGBoost was almost always faster than the other benchmarked implementations from R, Python Spark and H2O.

From his experiment, he commented:

 I also tried xgboost, a popular library for boosting which is capable to build random forests as well. It is fast, memory efficient and of high accuracy

— Szilard Pafka, [Benchmarking Random Forest Implementations](#).

2. XGBoost Model Performance

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XGBoost dominates structured or tabular datasets on classification and regression predictive modeling problems.

The evidence is that it is the go-to algorithm for competition winners on the Kaggle competitive data science platform.

For example, there is an incomplete list of first, second and third place competition winners that used titled: [XGBoost: Machine Learning Challenge Winning Solutions](#).

To make this point more tangible, below are some insightful quotes from Kaggle competition winners:

-  As the winner of an increasing amount of Kaggle competitions, XGBoost showed us again to be a great all-round algorithm worth having.
- Dato Winners' Interview: 1st place, Mad Professor
-  When in doubt, use xgboost.
- Avito Winner's Interview: 1st place, Owen Zhang
-  I love single models that do well, and my best one was XGBoost, which got me to the 10th place by itself.
- Caterpillar Winners' Interview: 1st place
-  I only used XGBoost.
- Liberty Mutual Property Inspection, Winner's Interview: 1st place, Qingchen Wang
-  The only supervised learning method I used was gradient boosting, as implemented in the excellent xgboost package.
- Recruit Coupon Purchase Winner's Interview: 2nd place, Halla Yang

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Gradient boosting is an approach where new models are created that predict the residuals or errors of prior models and then added together to make the final prediction. It is called gradient boosting because it uses a gradient descent algorithm to minimize the loss when adding new models.

This approach supports both regression and classification predictive modeling problems.

For more on boosting and gradient boosting, see Trevor Hastie's talk on [Gradient Boosting Machine Learning](#).

Trevor Hastie - Gradient Boosting Machine Learning



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Official XGBoost Resources

The best source of information on XGBoost is the [official GitHub repository](#) for the project.

From there you can get access to the [Issue Tracker](#) and the [User Group](#) that can be used for asking questions and reporting bugs.

A great source of links with example code and help is the [Awesome XGBoost page](#).

There is also an [official documentation page](#) that includes a getting started guide for a range of different languages, tutorials, how-to guides and more.

There are some more formal papers on XGBoost that are worth a read for more background on the library:

- [Higgs Boson Discovery with Boosted Trees, 2014.](#)
- [XGBoost: A Scalable Tree Boosting System, 2016.](#)

Talks on XGBoost

When getting started with a new tool like XGBoost, it can be helpful to review a few talks on the topic before diving into the code.

XGBoost: A Scalable Tree Boosting System

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Tianqi Chen, the creator of the library gave a talk to the LA Data Science group in June 2016 titled “XGBoost: A Scalable Tree Boosting System“.

XGBoost A Scalable Tree Boosting System June 02,...



You can review the slides from his talk here:



[Tianqi Chen - XGBoost: Overview and Latest News](#)
by [Data Science LA](#)

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There is more information on the [DataScience LA blog](#).

XGBoost: eXtreme Gradient Boosting

Tong He, a contributor to XGBoost for the R interface gave a talk at the NYC Data Science Academy in December 2015 titled “XGBoost: eXtreme Gradient Boosting“.

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Kaggle Winning Solution Xgboost Algorithm - Learn...



You can review the slides from his talk here:

XGBoost
eXtreme Gradient Boosting
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Xgboost from Vivian S. Zhang

There is more information about this talk on the [NYC Data Science Academy blog](#).

Installing XGBoost

There is a comprehensive installation guide on the [XGBoost documentation website](#).

It covers installation for Linux, Mac OS X and Windows.

It also covers installation on platforms such as R and Python.

XGBoost in R

If you are an R user, the best place to get started is

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From this page you can access the [R vignette Package ‘xgboost’ \[pdf\]](#).

There are also some excellent R tutorials linked from this page to get you started:

- [Discover Your Data](#)
- [XGBoost Presentation](#)
- [xgboost: eXtreme Gradient Boosting \[pdf\]](#)

There is also the official [XGBoost R Tutorial](#) and [Understand your dataset with XGBoost](#) tutorial.

XGBoost in Python

Installation instructions are available on the [Python Package Index](#).

The official [Python Package Introduction](#) is the best place to start learning XGBoost in Python.

To get started quickly, you can type:

```
1 sudo pip install xgboost
```

There is also an excellent list of sample source code and [Walkthrough](#).

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Summary

In this post you discovered the XGBoost algorithm for applied machine learning.

You learned:

- That XGBoost is a library for developing fast and high performance gradient boosting tree models.
- That XGBoost is achieving the best performance on a range of difficult machine learning tasks.
- That you can use this library from the command line, Python and R and how to get started.

Have you used XGBoost? Share your experiences in the comments below.

Do you have any questions about XGBoost or about this post? Ask your question in the comments below and I will do my best to answer them.

Discover The Algorithm Winning Competitions!

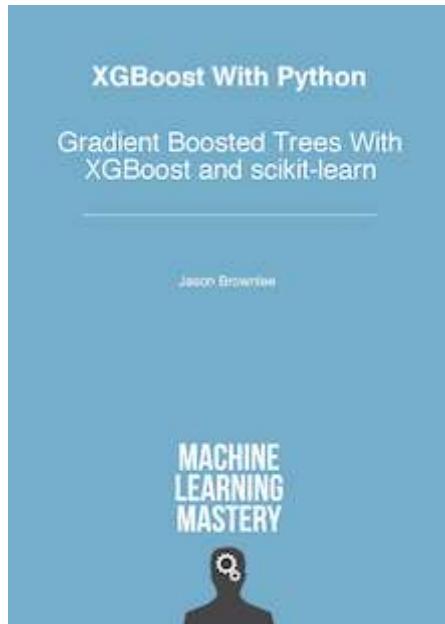
Develop Your Own XGBoost Models in Minutes

...with just a few lines of Python

Discover how in my new Ebook:

[XGBoost](#)

[Your Start in Machine Learning](#)



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Jason Brownlee, PhD is a machine learning researcher with modern machine learning methods.

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It covers **self-study tutorials** like:
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48 Responses to A Gentle Introduction to XGBoost for Applied Machine Learning

Seo Young Jae July 10, 2017 at 6:25 pm #

[REPLY ↗](#)

Good information, thank you. Just one question.

Biggest difference from the gbm is normalization?

Does gbm not normalize, but does xgboost automatically normalize variables and automatically handle missing values? Did I get it right?



Jason Brownlee July 11, 2017 at 10:28 am #

[REPLY ↗](#)

The biggest difference is performance not normalization

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Seo Young Jae July 10, 2017 at 7:46 pm #

REPLY ↗

I ran xgboost on R.

However, I found that input values can not be performed in the form of factors.

In case of gbm, it is possible to use factor type variable.

In that respect, xgboost seems to have some disadvantages.



Jason Brownlee July 11, 2017 at 10:29 am #

You must transform your categorical v



Seo Young Jae July 11, 2017 at 2:32 pm #

Is it ok to force a categorical vari



Jason Brownlee July 12, 2017

It depends on the variable. It might make sense if the variable is ordinal. If not, a one hot encoding would be the preferred approach.



sapan September 18, 2018 at 3:44 am #

REPLY ↗

this seems to be a limitation of the xgboost implementation you're using, not of the algorithm itself.



dksahu September 6, 2017 at 5:53 pm #

REPLY ↗

reference for monotonocity constraint for decision trees in xgboost?



Jason Brownlee September 7, 2017 at 12:50 pm #

REPLY ↗

Sorry, I do not.



Aman Garg September 13, 2017 at 5:44 am #

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Could you please tell that if XGBoost can also be used for unsupervised learning – clustering of large datasets?

If yes, does XGBoost provides an edge over other unsupervised algorithms – like K means clustering, DBSCAN etc. ?



Jason Brownlee September 13, 2017 at 12:37 pm #

REPLY ↗

Not as far as I know. Gradient boosting is a supervised learning algorithm.



Petros Koulouris September 20, 2017 at 5:14 pm #

Jason, I would love to see how to perform model parameters. I used the caret package and it types ie ranger, gbm, glmnet on the same German

Its been touted as extremely fast which I haven't ob



Jason Brownlee September 21, 2017 at 10:08 am #

Thanks for the suggestion Petros.



Sasikanth September 23, 2017 at 10:08 am #

REPLY ↗

Hello Jason,

Have you tried to install and use LightGBM from Microsoft. It is said to be better and faster than XGboost.



Jason Brownlee September 24, 2017 at 5:11 am #

REPLY ↗

I have not, perhaps in the future.



Norbert November 10, 2017 at 6:57 pm #

REPLY ↗

Yep, XGboost rocks. One year ago I have created a quick free online course how to use it efficiently in Python – <http://education.parrotprediction.teachable.com/p/practical-xgboost-in-python>

Jason Brownlee November 11, 2017 at 9:00 pm #

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Cool, thanks for the ref Norbert. That is also about the time I released my book on the topic.



Frank Ludeña January 18, 2018 at 8:44 am #

REPLY ↗

Hello good afternoon, with respect to the fact that xgboost does not support categorical variables, I trained the following model in caret with a factor variable with xgbtree and I had no problem, (a single variable to exemplify). I am doing something wrong?

```
pase0.xgbTree_x=train(as.factor(PASE)~TIPO_CLIENTE,data=pase0,trControl=trainControl(method='repeatedcv',number=5,repeats=10,verboseIter = TRUE),method='xgbTree',allowParallel=TRUE,tuneGrid=xbab.tuning)
```

The categorical variable is TIPO_CLIENTE



Jason Brownlee January 18, 2018 at 10:10 am #

Sorry, I cannot help you with xgboost



Abhilash Menon April 5, 2018 at 2:02 am #

Hi Dr. Brownlee, Is there a way to get all the predictions of our model as a column in the test dataset. I am concerned about how the order of instances will be preserved in this case (as in, the prediction corresponding to an instance should be in the same row as the instance). Could you please shed some light on this issue?

Thanks!

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Jason Brownlee April 5, 2018 at 6:14 am #

REPLY ↗

The order of the inputs will match the order of the outputs.



Brett April 8, 2018 at 5:00 am #

REPLY ↗

Not sure if this is the place for it, feel free to delete if not... but I just wanted to drop you a note to say thank you for the site... whenever it pops up in a search (which is often) I know I'm going to get some quality info.



Jason Brownlee April 8, 2018 at 6:30 am #

REPLY ↗

Thanks Brett, I really appreciate the ki

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**IanDz** April 17, 2018 at 7:14 pm #

REPLY ↗

Jason, just wanted to thank you for all the amazing stuff you do! Your articles are some of the best online!

**Jason Brownlee** April 18, 2018 at 8:02 am #

REPLY ↗

Thanks IanDz, I really appreciate your support!

**GopalKrishna** June 3, 2018 at 12:47 pm #

Jason,

Xgb Importance output includes Split, RealCover and Frequency when you pass add. parameters – train

While Split value is understood, could you help understand what appear against specific features only.

Also, in such expanded output what meaning should be given to importance table?

Thanks

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**Jason Brownlee** June 4, 2018 at 6:22 am #

REPLY ↗

This documentation better explains the table:

<http://xgboost.readthedocs.io/en/latest/R-package/discoverYourData.html#feature-importance>

**Purvi Prajapati** December 4, 2018 at 10:09 pm #

REPLY ↗

Could we apply XGBoost for Multi-Label Classification Problem?

Kindly reply me. I am working on Tree based approach for Multi-label classification.

**Jason Brownlee** December 5, 2018 at 6:16 am #

REPLY ↗

Perhaps. Sorry, I don't have any examples of multi-label prediction. I hope to cover it in the future.

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Purvi Prajapati December 5, 2018 at 3:51 pm #

REPLY ↗

Let me know is it applicable to Multi-Label Classification or not.



Jason Brownlee December 6, 2018 at 5:50 am #

REPLY ↗

Maybe, I don't know.



Apoorv January 23, 2019 at 2:50 am #

I think you can do by setting the objective requirements (from xgboost documentation:

<https://xgboost.readthedocs.io/en/latest/parameters.html>

multi:softmax: set XGBoost to do multiclass classification to set num_class(number of classes)

multi:softprob: same as softmax, but output a probability reshaped to ndata * nclass matrix. The result contains probability belonging to each class.

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Mak Wai Keong December 15, 2018 at 7:17 pm #

REPLY ↗

Hi all

I am very keen to know how Xgb can be used in the context of Learning (such as intelligent tutoring – to pick right context of knowledge for user).

I am new in this area, but is very keen to apply AI to learning.

One way I saw was the use of Dialogs to know what is known and what is not known, and what is to be known.

Looking forward for you experts for tips and advice



Jason Brownlee December 16, 2018 at 5:22 am #

REPLY ↗

Start with a strong definition of your problem as a supervised learning problem then apply xgboost. This framework will help:

<http://machinelearningmastery.com/how-to-define-your-machine-learning-problem/>



Monchy January 15, 2019 at 12:48 am #

REPLY ↗

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I see that one-hot encoding of factor variables is required. However, in my R implementation XGBoost performs without any error or warning messages when I include factors. Does the algorithm ignore these variables?



Jason Brownlee January 15, 2019 at 5:53 am #

REPLY ↗

I think R handles the factors automatically.

No, they are not ignored.



Amal January 22, 2019 at 8:59 pm #

Hello

I need to know what it the best to use in case of bir
gradient discent and why
thank you so much



Jason Brownlee January 23, 2019 at 8:4

It is not knowable. You must test a su
specific dataset.

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Thomas March 22, 2019 at 5:58 am #

REPLY ↗

All the bells and whistles are there but the meat of the algorithm is extremely poorly presented.
Can't believe this is listed second on Google.



Jason Brownlee March 22, 2019 at 8:42 am #

REPLY ↗

Sorry to hear that Thomas.

What do you think was missing exactly? What would you like to see?



Soroosh June 13, 2019 at 12:23 pm #

REPLY ↗

Two main points:

1) Comparing XGBoost and Spark Gradient Boosted Trees using a single node is not the right comparison. Spark GBT is designed for multi-computer processing, if you add more nodes, the processing time dramatically drops while Spark ma
distributed cluster, but on a Hadoop cluster.

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2) XGBoost and Gradient Boosted Trees are bias-based. They reduce variance too, but not as good as variance-based models like Random Forest), so when you are dealing with Kaggle datasets XGBoost works well, but when you are dealing with the real world and data streaming problem, Random Forest is a more stable model (stability in terms of handling high variance data which happens a lot in streaming data)



Jason Brownlee June 13, 2019 at 2:36 pm #

REPLY ↗

Thanks.



Abdallah Elbohy July 22, 2019 at 12:50

Thanks for adding information. But are
And which datasets will be more stable with ran



Jason Brownlee July 22, 2019 at 2:

I think so.

Tabular data is often best solved with xgbo

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Mrudhula September 6, 2019 at 4:39 am #

REPLY ↗

may i know the disadvantages of xgboost sir???



Jason Brownlee September 6, 2019 at 5:06 am #

REPLY ↗

Good question.

It can be slow.

It can create a complex model.

...



ralph September 8, 2019 at 8:03 pm #

REPLY ↗

Hi, and thanks for this very clear post!

Just to make sure I understand properly: if speed is not a concern, xgboost will bring nothing more than a classical random forest, right?

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**Jason Brownlee** September 9, 2019 at 5:14 am #

REPLY ↗

No, it is a different algorithm called stochastic gradient boosting, and it offers both performance (skill) and speed improvements over other implementations.

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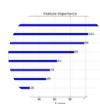


Welcome! I'm **Jason Brownlee** PhD and I help developers get results with machine learning.
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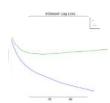
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[How to Develop Your First XGBoost Model in Python with scikit-learn](#)



[Feature Importance and Feature Selection With XGBoost in Python](#)



[Avoid Overfitting By Early Stopping With XGBoost In Python](#)

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How to Visualize Gradient Boosting Decision Trees With XGBoost in Python



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