

Yggdrasil Decision Forests: A Fast and Extensible Decision Forests Library

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ABSTRACT

Yggdrasil Decision Forests is a library for the training, serving and interpretation of decision forest models, targeted both at research and production work, implemented in C++, and available in C++, command line interface, Python (under the name TensorFlow Decision Forests), JavaScript, Go, and Google Sheets (under the name Simple ML for Sheets). The library has been developed organically since 2018 following a set of four design principles applicable to machine learning libraries and frameworks: simplicity of use, safety of use, modularity and high-level abstraction, and integration with other machine learning libraries. In this paper, we describe those principles in detail and present how they have been used to guide the design of the library. We then showcase the use of our library on a set of classical machine learning problems. Finally, we report a benchmark comparing our library to related solutions.

CCS CONCEPTS

• **Computing methodologies** → **Classification and regression trees; Supervised learning; Boosting; Bagging.**

KEYWORDS

machine learning, decision forests, random forest, gradient boosted trees, library, yggdrasil decision forests, tensorflow

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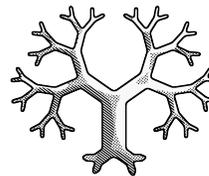
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1 INTRODUCTION

This work introduces Yggdrasil Decision Forests (YDF), a library for the training, serving, and interpretation of decision forests[†]. Decision forests are a rich class of Machine Learning (ML) models that utilize decision trees as weak learners to learn powerful functions. Decision forests stand out for their ease of use due to the relatively small number of hyper-parameters that enjoy intuitive default values and stability; their competitive and often superior performance on tabular data; their native support for numerical and categorical features without the need for preprocessing; their robustness to noisy data; their sample efficiency; and, their lightweight training and fast inference. Popular decision forests learning algorithms include Random Forests [3], Gradient Boosted Decision Trees [9], AdaBoost [25], and popular decision tree learning algorithms include C4.5 [23], and CART [4].



Yggdrasil
Decision Forests

Figure 1: Logo of the YDF library. Yggdrasil is a mythological holy tree in the Nordic culture. While not as ambitious as the Yggdrasil tree, our library aims to reach and support all relevant domains of machine learning.

In spite of the advances in other areas of ML and the growth of neural networks in particular over the past decade, decision forests remain competitive solutions to many real-world problems and, as a technology, are integral to many production systems to date, as evidenced by the many open-source libraries [7, 13]. As such, software libraries that facilitate the use of decision forests are central to software engineering in industry as well as academic

[†]Yggdrasil Decision Forests, whose logo is illustrated in Figure 1, is available at <https://github.com/google/yggdrasil-decision-forests>.

research, with the design choices behind them having significant ramifications for research and development. While we acknowledge that this is a challenge faced by software libraries in general, it is particularly more acute in ML due to its many moving parts and the sheer volume of novel methods and algorithms that make up a training or inference algorithm. If the library proves rigid and hard to extend in the face of rapid and often unforeseen developments in the literature, by continually building atop that stack, developers and researchers alike run the risk of creating overly complex and hard-to-maintain software which may ultimately constrain product quality and the scope of research.

With that in mind, we developed YDF based on four design principles: simplicity of use; safety of use; modularity and high-level abstraction; and compatibility and integration with other ML libraries. These guidelines have proved consequential for the development of YDF, which is what motivated us to share them with the community for the benefit of software engineers and researchers. We discuss the four pillars of YDF in Section 2. To explain how these guidelines determined the design choices in the development of YDF, we discuss its architecture in detail in Section 3.1. In Section 4, we present an application of YDF to classical ML problems, followed by a complete benchmark to compare YDF with existing solutions in Section 5. Section 6 concludes this work.

YDF is used in several internal products with an estimated number of predictions in the tens of millions per second. YDF is integrated with TensorFlow [1], making it easy for users to integrate it and compare it to other machine learning algorithms, such as neural networks. This is particularly helpful as YDF is integrated in our internal AutoML systems, and has proven to be successful compared to deep models on certain tasks: YDF is the preferred solution in approximately a quarter of real-world use cases, with tens of thousands of models trained every day.

2 FOUR DESIGN PRINCIPLES

2.1 Simplicity of use

Simplicity of use refers to the ease and efficiency with which a typical user of the library can deploy and maintain a solution. This is an increasingly difficult objective because, with the democratization of ML, the users of ML libraries now include not just researchers and experienced software engineers, but also a diverse population of non-ML researchers, students, and hobbyists among others. In addition to standard software library development best practices, therefore, simplicity in the context of an ML library entails the following properties:

High-level interactions and messages: The API, documentation, error messages, and results (such as model evaluation reports), should communicate with enough abstraction that is easily digested by the user but that nonetheless provides enough context for troubleshooting. This often means communicating ideas at a high and intuitive level with as much detail as necessary to allow the user to build a mental model of the library and its workflows. In addition, error messages must provide directions and guidelines to resolve the underlying issues. To illustrate this point, we write in Table 1 two messages that describe the same underlying error from a supervised binary classification pipeline.

Sensible default values and behavior: The library should rely on meaningful and documented default parameters and behaviors. Those default values and behaviors should be explicit to and adjustable by the user so that they can be tailored to their specific use case. For instance, while the quality of a model can often be improved by optimizing the hyper-parameters of the learning algorithm, some hyper-parameter values give sufficiently satisfactory results in most cases (e.g., a shrinkage rate of 0.1 is reasonable for most cases in gradient boosted trees learning). As another example, YDF can automatically determine the characteristics and semantic (e.g., numerical vs. categorical) of an input feature—as detailed in Section 3.4. The output of this automated system is then presented to the user, which gives the user an opportunity to rectify an incorrectly determined type or to modify it arbitrarily.

In practice, YDF takes this rule one step further by adopting the following philosophy: Any operation that can be automated should be automated, the user should be made aware of the automation, and should be given control over it. This is summarized in YDF’s motto: *“With only five lines of configuration, you can produce a functional, competitive, trained and tuned, fully evaluated and analysed machine learning model. With four more lines of configuration, you can compare this model to any other machine learning model. With three more lines, you can deploy your model in production.”*

Clarity and transparency: The user should have an accurate mental model of what the library does. To that end, the library must concretely define its concepts and terminology, and must accurately document metrics and algorithms with citations to the literature where appropriate. The library should explicitly note any heuristic or approximation that it uses for efficiency reasons on large datasets (e.g., evaluation on a random subset of the dataset). Reports should be self-contained, readable, and exhaustive.

2.2 Safety of use

Applied ML is rather unusual in that errors can lead to suboptimal yet entirely functional models! As an obvious example, tuning the hyper-parameters of a model on a held-out test dataset can lead to great offline but poor live model performance. This effect can be hard to distinguish from the impact of a distributional shift. Other common ML mishaps include modeling features according to an incorrect semantic (e.g., numerical features interpreted as categorical, thereby preventing the model from using order and scale information), or comparing trained models without accounting for the training and evaluation uncertainties.

The *safety of use* principle aims to reduce the likelihood for both experienced and inexperienced users to introduce such errors and increase the chances of catching them during development. For an ML library this entails the following:

Warning and error messages : Just as a compiler warns the user of potential mistakes, an ML library should look for possible errors and alert the user accordingly. When error seems likely or the impact of a potential error catastrophic, the error should interrupt the operation by default, with an

Table 1: Example of (a) poor and (b) well-written messages for an error.

(a) Invalid tensor shape name="internal_tensor_1" shape=[None, 4], dtype=int64, [large stack...]
(b) Binary classification training (task=BINARY_CLASSIFICATION) requires a training dataset with a label having 2 classes, however, 4 classe(s) were found in the label column "color". Those 4 classe(s) are [blue, red, green, yellow]. Possible solutions: (1) Use a training dataset with two classes, or (2) use a learning algorithm that supports single-class or multi-class classification e.g. learner='RANDOM_FOREST'

option to ignore it explicitly. When error seems less likely, a non-interrupting warning will do instead.

Furthermore, the note on *high-level interactions and messages* stated in the previous section applies to these warnings as well. For instance, the training of a multi-class classification model on a label that looks like a numerical value (i.e., with a large number of unique values), the error could state that: The classification label column "revenue" looks like a regression column (4,123 unique values or 50,000 examples, 99% of the values look like numbers). Solutions: (1) Configure the training as a regression with task=REGRESSION, or (2) disable the error with `disable_error.classification_look_like_regression=true`.

Easily accessible, correct methods : The library should make it easy to (automatically) execute what is considered ML best practices. Explanations of those practices should be well documented and easily available to the user. For example, model evaluation should contain confidence bounds with a sufficiently detailed description of how they are computed (e.g., bootstrapping, closed form solution, approximation) and how they may be used. Similarly, model comparison should include the results of appropriate statistical tests.

2.3 Modularity and high level abstraction

Modularity is a well-understood but informal blueprint for providing adaptability in software design [27]. In YDF, modularity implies that any sufficiently-complex part of the code may be understood as an independent module, with the interface between the various modules relying on clearly and concretely defined high-level concepts that do not expose their internals, and that are extensible and interchangeable. The initial version of every module can be as simple and generic as possible, even at the expense of execution efficiency, to facilitate readability.

At the start of development, modularity incurs a development cost and may therefore seem unwarranted. In fact, overly generic and slow code can be counterproductive. In YDF, however, we observed that modularity brought about many advantages as we elaborate shortly. As the library grows with newly published techniques, some modules become overly complex or inefficient. In cases like that, modularity allows for the re-writing of a specific module in isolation without having to understand the library in its entirety. It also allows recycling unit- and integration-tests of the previous version of the module. A re-write may often involve breaking up a single module into sub-modular parts.

Consider, as an example, the *splitter* routines that are at the core of every decision tree learning algorithm and are responsible for selecting split conditions for an intermediate node in the tree.

In YDF, the initial splitter implementation was a single module handling only numerical features on classification labels. The splitter was implemented using an "in-sorting" approach (i.e., sorting feature values for each node) making it simple to implement and test, usable for both deep and shallow trees, but slower than more advanced or specialized splitters. A few other splitters supporting other common feature types were later added as separate modules.

As support for other types of features (e.g., categorical, pre-sorted numerical, categorical-set [10], with or without missing values), other types of labels (e.g., regression, ranking), parameters (e.g., divide and conquer growth, global growth [26], oblique splits [29]), and shape of trees (e.g., shallow, deep) became necessary, the splitters were refactored and sub-modularized. YDF splitter code is now organized into three types of modules responsible for label type, feature type, and the specific splitting logic, with the resulting organization favoring code reuse and reducing the cost of extension and maintenance. For example, the module handling binary classification (label type) is used for all feature types, and the module handling categorical features (feature type) is used for all label types. This new design incorporated the engineering experience acquired during the implementation of the first generation of splitters.

Modularity also allows for the cohabitation of both generic-and-slow and specialized-and-fast code, where the initial simple modules serve as the ground truth in unit testing of specialized or optimized modules. For example, as mentioned above, the first YDF splitters used a simple in-sorting approach. Later, more efficient but complex splitters (e.g., pre-sorting approach, distributed approach) used the in-sorting approach as unit tests. In the case of deep trees (e.g., trees trained by the Random Forest learning algorithm), in-sorting is sometimes more efficient than pre-sorting. The modularity thus allows YDF to dynamically choose the most efficient splitter implementation for each node.

2.4 Integration with other ML libraries

ML libraries and frameworks should easily interact with each other and allow compositions. The possibility of *interaction* between libraries reduces the risk of the "framework trapping effect," in which the user is limited to the methods available in the library they are most familiar with, or on which the project relies, possibly missing some more suitable methods available in other libraries, resulting in sub-optimal solutions. For example, while R [24] contains a rich variety of data mining and decision forest libraries, it is not trivial for TensorFlow [1] users to use them.

Composability is important for both research and advanced production work. For example, the composition of decision forests and neural networks can lead to improvements in model quality [5, 10, 14, 16]. But neural network libraries often show poor

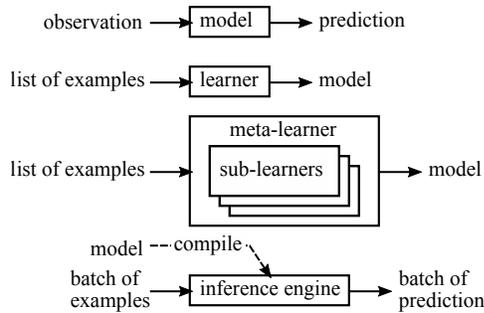


Figure 2: High level modules in YDF.

efficiency when executing the branching algorithms used to train decision forests, making the composability of neural networks and decision forests libraries a prerequisite for such hybrid research.

3 STRUCTURE OF YDF

In this section, we present the design decisions behind YDF and show the role the principles of Section 2 played in the formation of these decisions. Figure 2 depicts the high-level structure of YDF. We explain each of the components in this figure in the remainder of this section.

3.1 LEARNER-MODEL abstraction

YDF’s inter-module communication and user API relies on two model-agnostic ML concepts: `LEARNERS` and `MODELS`. A `MODEL` is a function, in the mathematical sense, that takes an observation as input, and returns a prediction. A `LEARNER` is a function that takes a list of examples as input and returns a `MODEL`. An `EXAMPLE` is a couple `{OBSERVATION, LABEL}`.

The `LEARNER-MODEL` abstraction is simple but generic enough for the integration of any new learning algorithm because it makes few assumptions about how the learning algorithm or model work internally. `LEARNERS`, for example, are not required to rely on stochastic gradient descent for optimization.

The `LEARNER-MODEL` abstraction is commonly used in the non-parametric learning R [24] packages [17, 28, 32]. In contrast, in Python ML libraries, we more routinely encounter the `ESTIMATOR-PREDICTOR` paradigm. For example, in scikit-learn [6] both the training and inference logic are encoded into the same object using the `model.fit` and `model.predict` functions. A similar design choice exists in XGBoost [7] and TensorFlow [1]. Note that, for consistency, the port of YDF in TensorFlow, called *TensorFlow Decision Forests*, uses the `ESTIMATOR-PREDICTOR` abstraction.

We argue that the distinction between `LEARNERS` and `MODELS` allows for the separation of training and inference logic (the inference logic is generally simpler than training) as well as code reuse (i.e., different `LEARNERS` can train the same type of `MODEL`, and a given `LEARNER` can produce different types of `MODELS`). For example, Breiman et al. [4] and Guillaume-Bert and Teytaud [11] are two algorithms to train Random Forest models. While the algorithms are different in the way they learn random forests, the models they produce have a similar structure, and the same post-training

Random Forest-specific tools are applicable to both `LEARNER`’s outputs. Finally, the separation of the learning and inference logic facilitates the development of technology-agnostic tools such as hyper-parameter tuners, cross-validation learner evaluators, model ensemblers, feature selection algorithms, and model agnostic interpreters.

To illustrate the benefit of separating the learning and inference logic for library integration and efficiency, consider the following example. Suppose a `LEARNER` trains a linear and a decision tree `MODEL` using two separate external libraries and returns the best performing one. The `MODEL` returned by the learner is either a linear model or a decision tree, compatible with the tooling and the respective external library. Deploying the model to a production service so as to generate predictions only requires loading the inference logic of one of the models. By comparison, if the learning and inference logic are packed into the same object, this object is not directly compatible with the external libraries. Finally, loading the model in a production setting to generate predictions requires loading (or at least making accessible) the inference and training logic of both models and the model selection logic.

In YDF, `MODELS` and `LEARNERS` are implemented by deriving abstract model and learner C++ classes respectively. This abstraction is independent of the task at hand: YDF includes `LEARNERS` with support for classification, regression, ranking, and uplifting tasks. The abstract classes expose various additional functionality common to many learners and models, such as (de-)serialization, determining variable importance, and human-readable summary.

A new `LEARNER` can be integrated into YDF using a C++ registration mechanism (e.g., `REGISTER_AbstractLearner(MyLearner)`)—see Section 3.5 for details on the YDF registration mechanism. YDF comes with a few built-in `LEARNERS` such as `CART` [15], `Random Forest` [3] and `Gradient Boosted Trees` [9], as well as `meta-learners` that we will describe in Section 3.2. Additionally, YDF offers learners that are effectively wrappers to other ML libraries.

3.2 Meta-learners

One of the interesting properties of the `LEARNER-MODEL` abstraction is that it allows for the composition of algorithms. To illustrate this point, consider a hyper-parameter tuner which is code that is responsible for finding the optimal hyper-parameters of a learner. It turns out that a hyper-parameter tuner can itself also be thought of as a `LEARNER`: It returns a model trained with a base `LEARNER` but using the optimal hyper-parameter values. To make matters more interesting, the method used by the hyper-parameter tuner to assess the optimality of candidate hyper-parameters (e.g., cross-validation, train-validation) is itself a hyper-parameter of the hyper-parameter tuner! We call all such `LEARNERS` that use another or multiple other `LEARNERS`, `META-LEARNERS`.

Other `META-LEARNERS` include: the “calibrator” which calibrates the predictions of a `MODEL`; the “ensembler” which ensembles a set of `MODELS`; and the “feature selector” which determines the optimal subset of input features for a `LEARNER` on a given dataset.

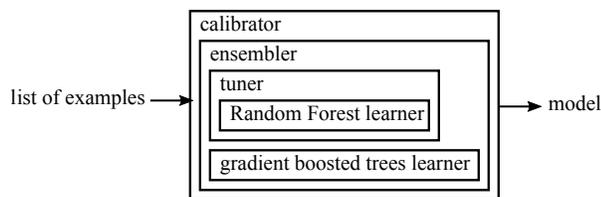


Figure 3: Representation of the three imbricated META-LEARNERS.

META-LEARNERS too can be composed together. Figure 3 shows an example of a calibrator META-LEARNER containing an ensembler, which itself contains both a hyper-parameter tuner optimizing a Random Forest LEARNER, and a vanilla (i.e., without hyper-parameter tuning) Gradient Boosted Tree LEARNER.

3.3 Model validation

By default, YDF LEARNERS do not take validation datasets as input. Instead, if the learning algorithm requires a validation dataset (e.g., for early-stopping), it is extracted once (for train-validation) or multiple times (for cross-validation) from the training dataset by the LEARNER implementation itself. The amount of examples to extract is a hyper-parameter of the LEARNER. For applications where distribution shift is a potential issue, YDF LEARNERS support an optional validation dataset as input. Each LEARNER can use this validation dataset as desired.

3.4 Automated feature ingestion

One of the more important facets of an input feature is its semantic, which directly determines its mathematical properties. Using the appropriate feature semantics is critical to train good models. YDF defines several model agnostic feature semantics: *Numerical features* (i.e., features with numerical semantics) are values in a continuous or discrete space with total ordering and scale significance. These generally represent quantities or counts, such as the age of a person, or the number of items in a bag. *Categorical features* are values in a discrete space without order. They are generally used to represent types such as the color *red* in the set $\{red, blue, green\}$. Other semantics include structural information like *categorical sets* (i.e., where a value is a set of categories), *categorical lists*, *numerical lists*, *numerical sets*, *text*, *boolean*, and *hashes*.

It is worth noting that the value of a feature may be *missing* or *unavailable* and that, for multi-valued features such as categorical sets in particular, a missing value is semantically different from the empty set. Algorithms take great care in handling missing values and different algorithms can handle missing values differently, which is referred to as imputation strategy. The decision tree learning algorithm used in decision forest LEARNERS, for example, supports *global* and *local* imputation where missing values are replaced by the mean (numerical features) or most frequent (categorical feature) value estimated on the whole dataset (global) or the examples in the same tree node.

Generally speaking, the semantics of an input feature cannot be determined reliably from values or its representation. For example, the string “2” in a CSV file could be a numerical value, a categorical

value, free text, or a numerical list with only one element. YDF uses a number of heuristics to assist the user in automatically determining feature semantics and build auxiliary data structures and metadata as required for the given feature type (such as dictionaries for categorical features). As we noted previously, while basic heuristics often yield reasonable results, YDF insists that the user validate and optionally modify the automatically determined feature semantics.

3.5 Modularity

YDF is organized into interchangeable modules. Most modules are implemented with object-oriented programming inheritance, that is, by deriving and registering an abstract class. The LEARNERS and MODELS, “inference engines”, and “distributed computation backend” modules are presented respectively in Sections 3.1, 3.7, and 3.9. Here, we describe other noteworthy modules.

READERS read a stream of examples. Different dataset readers support different file formats.

WRITERS write a stream of examples as a dataset with support for many file formats.

Decision tree IO imports and exports a decision tree from and to a file stored on disk. This module is used by all models made of trees.

SPLITTERS are algorithms that find the splitting conditions in a decision tree.

Official modules are directly part of the YDF code base. But custom modules can be hosted outside of the YDF code base using a Bazel [19] third-party dependency.

3.6 Model self evaluation

It is often essential to validate the quality of a model (i.e., to determine if quality is satisfactory) and use this information to direct model development (i.e., select the more performant model). A typical method to estimate model quality is by evaluating metrics of interest on held-out examples that are not seen by the learning algorithm. While simple, this method can be problematic and unstable in applications with a small amount of labeled data.

Other approaches to obtaining a fair estimate of model quality includes out-of-bag evaluation and cross-validation methods. In YDF, we abstract out all such model validation methods as a model SELF-EVALUATION module, leading to a powerful model-agnostic abstraction that can be utilized by LEARNERS and META-LEARNERS alike. For example, the feature-selector META-LEARNER can choose the optimal input features for a Random Forest MODEL using Out-of-bag SELF-EVALUATION.

3.7 Inference engine

The most naïve algorithm to compute the prediction of a decision tree is made up of a single *while* loop that iterates from the root node of the tree, taking the left or right branch according to the node condition, and terminating at one of the leaves. This is shown in Appendix A.

This simple algorithm is, however, inefficient on modern CPUs due to its slow and unpredictable random memory access pattern and branching mispredictions [2]. This observation inspired a line of research to optimize tree inference by using more complex but more efficient tree traversal logic. A prominent example of tree inference

algorithms is QuickScorer [18]. It can efficiently infer decision trees with up to 64 nodes on a 64-bit CPU, with the obvious caveat that it does not extend to larger trees such as those generated by the Random Forest algorithm [3].

In addition to the tree traversal algorithm, another factor that contributes to the latency of tree inference is the types of conditions in decision nodes. An inference algorithm that only supports one type of condition will inevitably be faster than an algorithm that supports many types. Additionally, instruction-level parallelism when available often has an outsize impact on latency. Finally, hardware accelerators (e.g. GPU, TPU, FPGA) allow for significant optimization as well.

To handle this diversity of solutions and to maximize model inference speed, but to shield the user from this complexity, YDF introduces the concept of *inference engine* or *engine* for short. An engine is the result of a possibly *lossy* compilation of a MODEL for a specific inference algorithm. In other words, we compile a MODEL into an engine, which is chosen based on the model structure and available hardware. In this way, space, complexity, and latency can be traded off depending on which factors are important to a particular production environment. For example, when the program size is important, such as on embedded devices like Internet-of-things, and when the model is known in advance, YDF can be compiled with only the required engine.

3.8 Splitters

Splitters are modules that find the optimal decision for a given node according to a splitting criteria. Their complexity, therefore, is tied to the number and type of features as well as the cardinality of their space of values. By default, YDF’s splitters are *exact* for numerical features, in the sense that numerical values are taken on face value and are in no way transformed (e.g., by discretization). This naturally leads to more candidate splits to be considered, an approach that could prove slow when the value of a feature cover a large range. This exact approach is similar to XGBoost [7] but different from LightGBM [13]. Like those libraries, YDF also supports *approximate* splitting but discretization, leading to a significant speed-up at the cost of a potential degradation to model quality.

In addition to numerical features, YDF natively supports categorical features with exact splitting [8] (similar to LightGBM), random categorical projection [3], and one-hot encoding (similar to XGBoost). Finally, YDF has special support for oblique numerical splits [29] and categorical-set splits [10].

3.9 Distributed training

Distributed training is essential for training on large datasets and computationally-intensive learning algorithms such as hyper-parameter tuners. To facilitate the development of distributed algorithms, YDF defines an API with the primitives necessary for decision forest distributed training, along with a distributed training framework for common META-LEARNERS, all with built-in fault-tolerance.

The implementation of this API are modifiable, with two particular implementations available based on gRPC and TensorFlow Parameter Server distribution strategies. But because the development and testing of distributed algorithms can be cumbersome,

YDF also contains a third implementation specialized for development, debugging, and unit-testing. This implementation simulates multi-worker computation in a single process, making it easy to use breakpoints or execute the distributed algorithm step by step. How the user selects which distributed implementation to use is a single piece of configuration.

The YDF implementation of decision forests distributed training relies on both “feature parallel” and “example parallel” distribution based on the work of Guillaume-Bert and Teytaud [11]. Each *training worker* is responsible for a subset of input features. Communication between workers is optimized with a delta-bit encoding and multi-round hierarchical synchronization so as to minimize the maximum network IO among workers. The type and number of features allocated to each worker is dynamically adjusted to handle fluctuation in worker availability due to concurrent execution. Workers evaluate the quality of the model on a validation dataset, and possibly trigger early stopping of the training.

3.10 Multi API and integration with other ML frameworks

C and C++ code is generally well supported by other languages. YDF is available in C++, on the web platform using JavaScript and WebAssembly, in Go, and Command line interface (CLI). YDF is also available in Python through TensorFlow [1] under the name TensorFlow Decision Forests, making it compatible with the TensorFlow ecosystem. YDF supports NumPy [12] and Pandas [31] making it easy to use on small datasets in Python. YDF can read scikit-learn [6] decision forest models. YDF is also available as a Google Sheets add-on under the name Simple ML for Sheets [20]. This add-on makes standard modeling actions such as model training, evaluation and interpretation available without coding. It also exposes ML concepts to non-ML savvy users. For example, the task of “predicting missing values” is implemented using model training+inference, while the task of “detecting abnormal values” is implemented using cross-validation.

It is worth noting that models and training configurations are cross-API compatible. For example, a model trained with the Python API can be run with the JavaScript API.

3.11 Backwards compatibility and default values

YDF models are fully backwards compatible—as an anecdote, models trained in 2018 are still usable today. Additionally, the YDF training logic is deterministic: The same LEARNER on the same dataset always returns the same MODEL. This last rule may only be violated by changes in the underlying pseudo-random number generator implementation.

An important property of YDF, and a constraint we impose on the development of the library, is that hyper-parameters are backwards compatible: Running a LEARNER configured with a given set of hyper-parameters always returns the same MODEL—modulo changes to the pseudo-random number generators. This implies that default hyper-parameters cannot change and that all newer methods of learning are disabled by default. By construction, the default values of all hyper-parameters are set to the values recommended in the paper that introduces the algorithm or in the

authors' implementation of it. For example, by default, classification Random Forest uses an attribute sampling ratio of the square root of the total number of features as recommended by Breiman [3].

To simplify the use of the library, particularly for users who would like to use the latest algorithms in YDF but who are not well-versed in the literature and may not understand fully the hyper-parameters involved, YDF offers a hyper-parameter template system. For example, a learner configured with the `benchmark_rank1` parameter template will be trained with the best hyper-parameters according to our benchmark on a large number of real-world datasets. The `benchmark_rank1@v1` template for the gradient boosted trees learner [9] uses global tree growth [26] (i.e., best first or leaf-wise growth), sparse oblique splits [29], and random categorical splits [3]. As new versions of YDF are released, those hyper-parameters can change but YDF retains version information. For example, a learner configured with the `benchmark_rank1@v1` will be trained on the best hyper-parameters in version 1 of this template.

4 USAGE EXAMPLES

This section demonstrates a use case where we apply YDF for binary classification on the Adult dataset (also known as the Census Income dataset). This dataset is stored in two CSV files containing the training and test examples. Input features are either numerical or categorical, with some feature values missing.

We first highlight how one may use YDF with the CLI API to train, evaluate and analyse a classical gradient boosted trees model. This API is similar (but less verbose) than the C++ interface. We then show how to use the TensorFlow Decision Forests API and the Simple ML for Sheets tool to do the same task. In all three cases, the hyper-parameters of the learner are left to their default values. In addition, the input features are not explicitly fed to YDF; instead, YDF will use all available features (excluding labels) with automated semantic detection.

4.1 The CLI API

The following is the CLI usage example. The resulting artefacts—dataspec, model information, model evaluation report, and model inference benchmark report—are included in Appendix B for completeness.

```
# Detect feature semantics, producing dataspec
infer_dataspec --dataset=csv:train.csv
  --output=dataspec.pbtxt

# Print details of the inferred semantics
show_dataspec --dataspec=dataspec.pbtxt

# Configure the learner
cat <<EOF > learner.pbtxt
  task: CLASSIFICATION
  label: "income"
  learner: "GRADIENT_BOOSTED_TREES"
EOF

# Train the model
train --dataset=csv:train.csv \
  --dataspec=dataspec.pbtxt \
  --config=learner.pbtxt \
  --output=model_path
```

```
# Display information about the model
show_model --model=model_path

# Evaluate the model
evaluate --dataset=csv:test.csv \
  --model=model_path

# Generate model predictions
predict --dataset=csv:test.csv \
  --model=model_path \
  --output=csv:predictions.csv

# Benchmark the model inference speed
benchmark_inference --dataset=csv:test.csv \
  --model=model_path
```

4.2 The Python and Tensorflow API

In this section, we showcase the TensorFlow Decision Forests API.

The port of YDF in TensorFlow does not use the YDF model evaluation logic demonstrated in Section 4.1. Instead, TensorFlow native metric implementations are used for evaluation.

```
import tensorflow_decision_forests as tfdf
import pandas as pd

# Load datasets as Pandas dataframes
train_df = pd.read_csv("train.csv")
test_df = pd.read_csv("test.csv")

# Convert the datasets to TensorFlow format
train_ds = tfdf.keras
    .pd_dataframe_to_tf_dataset(train_df,
    label="income")
test_ds = tfdf.keras
    .pd_dataframe_to_tf_dataset(test_df,
    label="income")

# Train a model
model = tfdf.keras
    .GradientBoostedTreesModel()
model.fit(train_ds)

# Summary of the model structure.
model.summary()

# Evaluate the model.
model.compile(metrics=["accuracy"])
print(model.evaluate(test_ds,
    return_dict=True))
```

4.3 Simple ML for Sheets

In this section, we showcase the Simple ML for Sheets tool. The dataset is provided as a training and testing sheets of data as shown in fig. 4. The user open the training sheet, selects the “train a model” task and clicks on “Train” (fig. 5). After a few seconds, a model is trained with default hyper-parameters. The user then runs the “evaluate a model” task and obtain an evaluation report similar to the one shown in sec. B.3. Finally, the user runs the “Understand a model” task and a details model report similar to the one presented in sec. B.1, sec. B.2 and fig. 7.

5 EXPERIMENTS

We compare the accuracy of YDF v0.2.5 to four popular decision forests learning libraries: XGBoost v1.5.1 (XGB) [7], scikit-learn

K	L	M	N	O
age	workclass	education	occupation	income
44	Private	7th-8th	Machine-op-inspct	<=50K
20	Private	Some-college	Other-service	<=50K
40	Private	HS-grad	Adm-clerical	<=50K
30	Private	Some-college	Exec-managerial	<=50K
67	Self-emp-inc	HS-grad	Prof-specialty	>50K
18	Private	Some-college	Sales	<=50K
51	Private	Bachelors	Prof-specialty	<=50K
32	Private	Bachelors	Exec-managerial	>50K
33	Private	10th	Handlers-cleaners	<=50K
46	Private	HS-grad	Handlers-cleaners	<=50K
56	Private	HS-grad	Other-service	<=50K
44	Private	Masters	Exec-managerial	>50K
41	Private	Assoc-voc	Prof-specialty	<=50K
19	Private	HS-grad	Sales	<=50K
27	Private	Some-college	Prof-specialty	>50K

Figure 4: Example of training data presented in a spreadsheet in Simple ML for Sheets.

The screenshot shows the 'Simple ML for Sheets' interface. At the top, there is a title bar with a close button. Below it, the question 'What do you want to do?' is followed by a dropdown menu set to 'Train a model'. A link 'Learn how to use this task' is provided. The 'Name of the model' field contains 'my model'. The 'Label' dropdown is set to 'income'. There are expandable sections for 'Source columns' and 'Advanced options'. A prominent blue 'Train' button is at the bottom.

Figure 5: Configuration of the “Train a model” task in Simple ML for Sheets.

v1.0.2 (SKLearn) [6], LightGBM v3.0.0.99 (LGBM) [13], and TensorFlow BoostedTrees Estimators v2.9.1 (TF BTE) [21]). We also include a linear classifier (TF Linear) on 70 small tabular (binary and multi-class) classification datasets from the OpenML repository [30]. The list of datasets used in our evaluation appears in Appendix C.7. The number of examples ranges from 150 to 96,320, with a mean of 8,647 examples per dataset. The number of features ranges from 5 to 1,777, with a mean of 119 input features per dataset.

5.1 Learners

For each library, we evaluate learners using both their default hyper-parameters as well as hyper-parameter values tuned using an automated tuner. The default hyper-parameters of each library might differ, except for the “number of trees” which is universally fixed to 500. Learners that use the default hyper-parameter values are tagged with “(default hp)”

As noted in Section 3.11, YDF sets the default values for all hyper-parameters to reflect the configurations in the original publication. To complement these results, we also evaluate a setting in which hyper-parameters are drawn from our benchmark configuration benchmark_rank1@v1, and tag these learners with “(benchmark hp)”. The definition of the default and benchmark_rank1@v1 hyper-parameters are presented in appendix C.1.

Tuned learners are tagged with *Autotuned*. We conduct hyper-parameter tuning by aggregating results from 300 unique random trials. Trials are scored either by log loss (noted (*opt loss*)) or accuracy (noted (*opt acc*)). For Random Forest models we use out-of-bag evaluation for validation, whereas for Gradient Boosted models we set aside 10% of the training data for validation. The hyper-parameters tuned by each library are listed in Appendix C.2.

Finally, we note that Scikit-learn, XGBoost and TensorFlow BoostedTrees Estimators libraries do not offer native support for categorical features. As such, for these learners, we encode all categorical features using one-hot encoding.

5.2 Metrics

We evaluate all pairs of dataset and learner using a 10-fold cross-validation protocol, where fold splits are consistent across learners to facilitate a fair comparison. Note that, the hyper-parameter tuning is applied independently on each of the 10 folds for each library.

We measure accuracy, AUC (for binary classification), training time, and inference latency of each model. We further report the overall mean and median rank of each learner across all datasets, the number of wins or losses between pairs of learners, and the mean training and inference time of each learner.

5.3 Computing resources

We train each model on a single machine without using distributed training and with a 20 threads limit. The inference of the model is evaluated with a single thread for YDF, and a number of threads selected by the library for other learners. The reported training and inference times exclude dataset reading. In aggregate, we trained a total of 1.3 million models consisting of 840 million trees.

5.4 Results

Due to space constraints, we have included the mean cross-validation accuracy of all learners on every dataset in Appendix C.4, and a pairwise comparison of learners Appendix C.3. Here, we present a summary of these results in Figure 6 where we render the *mean rank* of each learner—equivalent to the “mean rank” column in the table reported in Appendix C.4. The mean rank is the average, over all datasets, of the rank of the learner (between 1 and 16) compared to other learners. We also show in Table 2 the average training and inference duration for each learner.

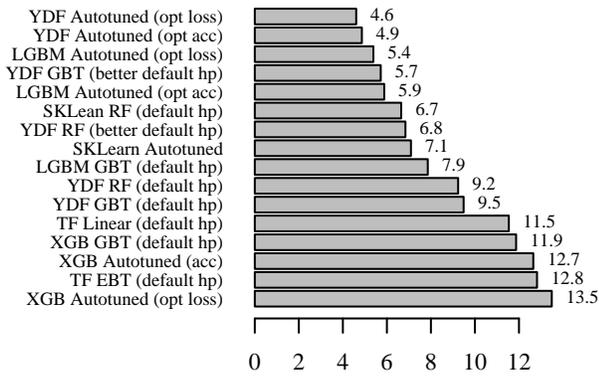


Figure 6: Mean learner ranks: The rank of the 16 learners averaged over the 70 datasets. The smaller, the better.

Table 2: Training and inference duration in seconds of (untuned) learners, using the default hyper-parameters of the respective libraries, averaged over 10 cross-validation folds and 70 datasets. Learners are ordered according to their quality rank reported in Figure 6. Individual measures for each dataset and learners are given in Appendix C.5 and C.6.

Learner	training (s)	inference (s)
YDF GBT (benchmark hp)	39.99	0.108
SKLearn RF (default)	7.01	0.250
YDF RF (benchmark hp)	29.86	0.598
LGBM GBT (default)	4.91	0.061
YDF RF (default)	4.41	0.326
YDF GBT (default)	34.79	0.044
TF Linear (default)	55.59	8.050
XGB GBT (default)	20.72	0.015
TF EBT (default)	212.06	1.949

5.5 Observations

On the mean accuracy computed over 70 datasets, we make the following observations:

- No one learner is always better than another learner. The largest difference is between auto-tuned YDF and XGBoost with 612 wins and 88 losses. The effective difference of quality between closely-ranked learners is rather small. For example, the average difference in accuracy between auto-tuned YDF and LightGBM is about 0.5% for a standard deviation of 1.9%—see Appendix C.4.
- YDF performs better than other candidate libraries both with and without automatically tuned hyper-parameters. The YDF setting where the tuner optimizes for loss has rank 1, and YDF with benchmark hyper-parameters has rank 4, standing above all other non-tuned learners.
- Automatically tuned LightGBM comes in close second place with respect to mean rank, but ranks first in terms of the number of pairwise wins and losses.

- For Random Forests and Gradient Boosted Trees learners, YDF with all its features enabled—see Section 3.11—performs significantly better than YDF with the default hyper-parameters.
- Tuning the hyper-parameters increases the quality of YDF and LightGBM learners significantly (+4 and +6 rank change respectively).
- Surprisingly, scikit-learn and XGBoost without hyper-parameter tuning offer slightly better (respectively +2 and +1 rank change) results than with hyper-parameter tuning. We believe that is due to the relatively small size of the datasets and the one-hot encoding of categorical features, tuning the hyper-parameters makes the model more prone to overfitting. Note that the same hyper-parameter tuning library is used for all the learners.
- XGBoost and TF Boosted Trees on average yield a lower accuracy than a linear model. Gradient Boosted Trees models perform better than Random Forest models in terms of accuracy.

Moving on to the training speed of the models, we observe that LightGBM is significantly faster to train than YDF and XGBoost models for the GBT algorithm. This comparative performance can be explained by the difference in the configuration of the splitter algorithms in the three libraries. See Section 3.8. YDF is slightly faster than scikit-learn for the RF algorithm but much faster than TensorFlow based models.

On the inference speed of the models, we observe that:

- Ignoring the different number of threads used, the inference speed of gradient boosted tree models trained default hyper-parameters is the fastest with XGBoost, followed by YDF, followed by LightGBM. Gradient Boosted Trees models trained with TF Estimator Boosted Trees are two orders of magnitude slower.
- As expected, the much larger Random Forest models are slower than Gradient Boosted Trees models. However, YDF Random Forest inference is slightly slower than scikit-learn.
- YDF with “benchmark hp”, which notably includes oblique splits, are significantly slower to train and to infer than the “default” version.
- The algorithmic complexity of inference of the linear model is significantly less than that of the decision forest models. Surprisingly, the inference of linear models executed through TensorFlow are slowest.

6 CONCLUSION

We presented a new library for the training, inference, and interpretation of decision forest models called Yggdrasil decision forests. The library is designed around four principles to ensure extensibility to new methods and efficient usage. While designed for this library, we believe these principles carry over to other machine learning libraries. We showed how to use the CLI and Python APIs of Yggdrasil and empirically compared its quality and speed with existing libraries.

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A NAÏVE DECISION TREE INFERENCE

Algorithm 1: Simple tree inference algorithm

```

Input: example  $x$ 
 $c \leftarrow$  root node of the tree
while  $c$  is not a leaf do
   $e \leftarrow$  evaluate the condition of  $c$  on  $x$ 
  if  $e$  is TRUE then
     $c \leftarrow$  POSITIVE CHILD OF  $c$ 
  else
     $c \leftarrow$  NEGATIVE CHILD OF  $c$ 
  end if
end while
return  $c$ 's value

```

B ARTEFACTS FROM THE CLI USAGE EXAMPLE

B.1 Column information

Sample from the column information (dataspec) returned by `show_dataspec`.

Number of records: 22792

Number of columns: 15

Number of columns by type:

CATEGORICAL: 9 (60%)

NUMERICAL: 6 (40%)

Columns:

CATEGORICAL: 9 (60%)

3: "education" CATEGORICAL has-dict vocab-size:17 zero-ood-items most-frequent:"HS-grad" 7340 (32.2043%)

14: "income" CATEGORICAL has-dict vocab-size:3 zero-ood-items most-frequent:"<=50K" 17308 (75.9389%)

5: "marital_status" CATEGORICAL has-dict vocab-size:8 zero-ood-items most-frequent:"Married-civ-spouse" 10431 (45.7661%)

...

NUMERICAL: 6 (40%)
0: "age" NUMERICAL mean:38.6153 min:17 max:90 sd:13.661
10: "capital_gain" NUMERICAL mean:1081.9 min:0 max:9999
sd:7509.48
11: "capital_loss" NUMERICAL mean:87.2806 min:0 max:4356
sd:403.01
...

Terminology:

nas: Number of non-available (i.e. missing) values.
ood: Out of dictionary.
manually-defined: Attribute which type is manually defined
by the user i.e. the type was not automatically inferred.
tokenized: The attribute value is obtained through
tokenization.
has-dict: The attribute is attached to a string dictionary
e.g. a categorical attribute stored as a string.
vocab-size: Number of unique values.

B.2 Model information

Sample from the result returned by *show_model*.

Type: "GRADIENT_BOOSTED_TREES"
Task: CLASSIFICATION
Label: "income"

Input Features (14):

age
workclass
fnlwgt
...
hours_per_week
native_country

Variable Importance: NUM_AS_ROOT:

1. "age" 37 #####
2. "capital_gain" 24 #####
3. "marital_status" 22 #####
4. "hours_per_week" 21 #####
...

Variable Importance: NUM_NODES:

1. "occupation" 703 #####
2. "fnlwgt" 659 #####
3. "education" 614 #####
4. "age" 557 #####
...

Loss: BINOMIAL_LOG_LIKELIHOOD
Validation loss value: 0.578763
Number of trees per iteration: 1
Number of trees: 186
Total number of nodes: 9898

Number of nodes by tree:
Count: 186 Average: 53.2151 StdDev: 7.25844
Min: 23 Max: 63 Ignored: 0

[23, 25) 1 0.54% 0.54%
[25, 27) 0 0.00% 0.54%
[27, 29) 0 0.00% 0.54%

...
[57, 59) 25 13.44% 70.97% #####
[59, 61) 23 12.37% 83.33% #####
[61, 63] 31 16.67% 100.00% #####

Depth by leafs:
Count: 5042 Average: 4.86573 StdDev: 0.443584
Min: 2 Max: 5 Ignored: 0

[2, 3) 30 0.60% 0.60%
[3, 4) 113 2.24% 2.84%
[4, 5) 361 7.16% 10.00% #
[5, 5] 4538 90.00% 100.00% #####

Number of training obs by leaf:
Count: 5042 Average: 757.465 StdDev: 2542.45
Min: 5 Max: 20094 Ignored: 0

[5, 1009) 4426 87.78% 87.78% ####
[1009, 2014) 192 3.81% 91.59%
...
[8041, 9045) 11 0.22% 97.42%
[9045, 10050) 11 0.22% 97.64%

Attribute in nodes:

703 : occupation [CATEGORICAL]
659 : fnlwgt [NUMERICAL]
614 : education [CATEGORICAL]
...
47 : sex [CATEGORICAL]
34 : race [CATEGORICAL]

Attribute in nodes with depth <= 0:

37 : age [NUMERICAL]
24 : capital_gain [NUMERICAL]
22 : marital_status [CATEGORICAL]
...
3 : workclass [CATEGORICAL]
2 : occupation [CATEGORICAL]

Attribute in nodes with depth <= 1:

80 : fnlwgt [NUMERICAL]
77 : capital_gain [NUMERICAL]
73 : age [NUMERICAL]
...
33 : hours_per_week [NUMERICAL]
29 : relationship [CATEGORICAL]

Condition type in nodes:

2509 : ContainsBitmapCondition
2342 : HigherCondition
5 : ContainsCondition
...

B.3 Model evaluation report

The evaluation report is composed of both text and plots (fig.7). The dataset was evaluated on 9769 examples for an accurate of 0.8734, and with a 95% confidence boundaries of [0.8678 0.8789] computed with bootstrapping (W). Other common binary classification metrics are reported (AUC, PR-AUC, AP, logloss, error rate).

Evaluation:

Number of predictions (without weights): 9769
 Number of predictions (with weights): 9769
 Task: CLASSIFICATION
 Label: income

Accuracy: 0.873477 CI95[W][0.867811 0.878978]
 LogLoss: 0.277841
 ErrorRate: 0.126523

Default Accuracy: 0.758727
 Default LogLoss: 0.552543
 Default ErrorRate: 0.241273

Confusion Table:

truth\prediction	<00D>	<=50K	>50K
<00D>	0	0	0
<=50K	0	6962	450
>50K	0	786	1571
Total: 9769			

One vs other classes:

"<=50K" vs. the others

auc: 0.929051 CI95[H][0.92419 0.93390]
 CI95[B][0.92355 0.93420]
 p/r-auc: 0.9756 CI95[L][0.97184 0.97888]
 CI95[B][0.97323 0.97791]
 ap: 0.975609 CI95[B][0.97323 0.97790]

">50K" vs. the others

auc: 0.929051 CI95[H][0.92170 0.9364]
 CI95[B][0.92369 0.93454]
 p/r-auc: 0.83002 CI95[L][0.81431 0.8446]
 CI95[B][0.81766 0.8431]
 ap: 0.829984 CI95[B][0.8175 0.84308]

B.4 Model inference benchmark report

Following is the inference benchmark report. The model was run 20 times over the whole dataset. Three engines have been found compatible with the model. The fastest one, called GradientBoostedTreesQuickScorer shows an average inference time of 1.066 μ s per examples on a single CPU:

```
batch_size : 100 num_runs : 20
time/example(us) time/batch(us) method
-----
1.066 106.6 GradientBoostedTreesQuickScorer
6.7385 673.85 GradientBoostedTreesGeneric
15.829 1582.9 Generic slow engine
-----
```

C EXPERIMENTS**C.1 Default and benchmark_rank1@v1 hyper-parameters**

The following hyper-parameters have been used for non-hyper-parameter tuned learners.

Random Forest default hyper-parameters

- categorical_algorithm: CART
- growing_strategy: LOCAL

- max_depth: 16
- min_examples: 5
- num_candidate_attributes: Breiman rule of thumb
- split_axis: AXIS_ALIGNED

Random Forest rank1@v1 hyper-parameters

Same as the default hyper-parameters with the following changes.

- categorical_algorithm: RANDOM
- split_axis: SPARSE_OBLIQUE
- sparse_oblique_normalization: MIN_MAX
- sparse_oblique_num_projections_exponent: 1

Gradient Boosted Trees hyper-parameters

- early_stopping: LOSS_INCREASE
- l1_regularization: 0
- l2_regularization: 0
- max_depth: 6
- num_candidate_attributes: -1 i.e. all
- shrinkage: 0.1
- sampling_method: NONE
- use_hessian_gain: false
- growing_strategy: LOCAL
- categorical_algorithm: CART
- split_axis: AXIS_ALIGNED

Gradient Boosted rank1@v1 hyper-parameters

Same as the default hyper-parameters with the following changes.

- growing_strategy: BEST_FIRST_GLOBAL
- categorical_algorithm: RANDOM
- split_axis: SPARSE_OBLIQUE
- sparse_oblique_normalization: MIN_MAX
- sparse_oblique_num_projections_exponent: 1

C.2 Hyper-parameter space for hyper-parameter tuning

The following hyper-parameter were considered during automatic hyper-parameter optimization.

Yggdrasil Decision Forests : Min sample per leaf: 2 to 10. Categorical splitting algorithm: CART or Random. Splits: Axis aligned or Sparse. Random Forest: Max depth: 12 to 30. Gradient Boosted Trees: Hessian splits: Yes or No. Shrinkage: 0.02 to 0.15. Num candidate attribute ratio: 0.2 to 1.0. Growing strategy: divide-and-conquer (with max depth in 3 to 8) or global (with max num nodes in 16 to 256).

LightGBM : We use similar hyper-parameters as for YDF as well as remarks regarding parameter tuning from the LightGBM documentation. Gradient Boosted Trees: Num leaves: 16 to 256. Min data in leaf: 2 to 10. Max depth: 3 to 8. Learning rate: 0.02 to 0.15. Bagging fraction: 0.5 to 1.0. Feature fraction: 0.2 to 1.0.

XGBoost : We use similar hyper-parameters as used in [22] as well as remarks regarding parameter tuning on the XGBoost documentation. Gradient Boosted Trees: Eta (shrinkage): 0.002 to 0.015. Max depth: 2 to 9. Subsample: 0.5 to 1.0. ColSample by tree: 0.2 to 1.0. Min child weight: 2 to 10.

Scikit-learn : Random Forest: Max depth: 12 to 30. Min sample per leaf: 1 to 40.

C.3 Pair wise learner comparison

Tab. 3 shows the pairwise comparison between each learners regarding accuracy.

C.4 Accuracies

Tab. 4 shows the accuracy for each learner on each dataset. The reported values are the average over the 10 cross-validation rounds. Learners are sorted by average global rank (the first learners are the better).

C.5 Training time

Tab. 6 shows the training time of each learner on each dataset. The reported values are the average over the 10 cross-validation rounds.

C.6 Inference time

Tab. 7 shows the inference time of each learner on each dataset. The reported values are the average over the 10 cross-validation rounds.

C.7 Datasets

Tab. 5 shows statistics about each dataset. The reported values are the average over the 10 cross-validation rounds.

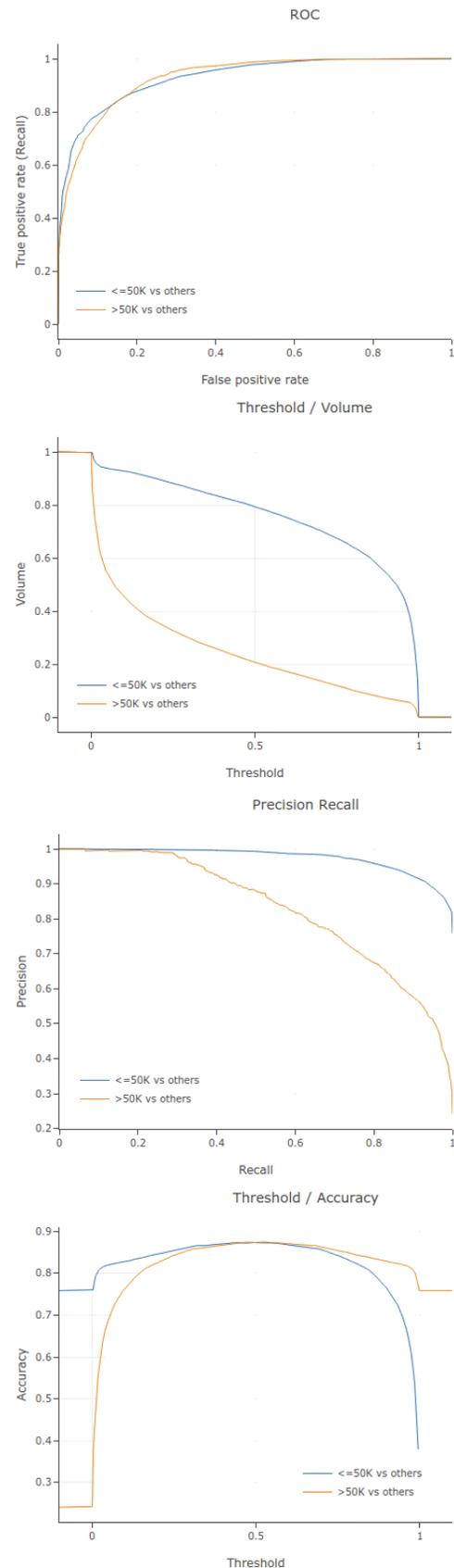


Figure 7: Example of model evaluation report plots

Table 3: Pairwise comparison between each learners regarding accuracy. Each cell contains the “number of wins / number of losses (average accuracy difference)” of the row learner compared to the column learner over all the datasets and all the cross-validation folds. The number of comparisons (sum of wins and losses) is ‘number of datasets x number folds’. Ties are counted as 0.5 win / 0.5 loss. For example, a large number of wins and a large positive mean metric difference indicates that the row learner is better than the column learner. Learners are sorted by average global rank (the first learners are the better). The cell is green iff. more than half of the pairwise comparisons are won. Note that the number of wins and the cell color does not take into account the amount of metric difference (only which one is better).

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1 YDF Autotuned (opt loss)		341/359	377/323	396/305	394/306	428/273	457/243	442/258	465/235	524/177	498/202	563/138	585/116	605/95	600/100	612/88
2 YDF Autotuned (opt acc)	359/341		385/315	402/298	406/294	432/269	458/243	435/265	465/235	499/201	508/192	554/147	580/120	596/105	594/107	602/98
3 LGBM Autotuned (opt loss)	323/377	315/385		345/355	372/328	392/308	419/281	407/294	442/258	485/215	498/202	538/163	565/136	589/111	569/131	608/92
4 YDF GBT (benchmark hp)	305/396	298/402	355/345		374/327	406/294	435/266	418/282	415/286	492/209	490/211	542/159	564/137	578/123	574/126	591/109
5 LGBM Autotuned (opt acc)	306/394	294/406	328/372	327/374		386/315	418/283	401/300	435/265	469/231	485/215	538/163	563/137	584/116	560/140	600/100
6 SKLearn RF (default hp)	273/428	269/432	308/392	294/406	315/386		383/318	343/358	354/346	453/247	405/295	518/182	493/207	547/153	539/162	556/144
7 YDF RF (benchmark hp)	243/457	243/438	281/419	266/435	283/418	318/383		332/368	347/354	451/249	421/279	521/180	503/197	589/112	588/112	593/107
8 SKLearn Autotuned	258/442	265/435	294/407	282/418	300/401	358/343	368/332		356/344	466/235	408/293	525/176	503/198	570/131	555/145	575/126
9 LGBM GBT (default hp)	235/465	235/465	258/442	286/415	265/435	346/354	354/347	344/356		426/275	447/254	505/196	547/154	561/140	555/145	582/118
10 YDF RF (default hp)	177/524	201/499	215/485	209/492	231/469	247/453	249/431	293/466	275/426		340/360	495/205	440/261	540/161	537/163	554/146
11 YDF GBT (default hp)	202/498	192/508	202/498	211/490	215/485	279/405	279/421	293/408	254/447	360/340		471/229	473/227	521/179	520/181	535/166
12 TF Linear (default hp)	138/563	147/554	163/538	159/542	163/538	182/518	180/521	176/525	196/505	205/495	229/471		258/442	276/424	283/417	297/404
13 XGB GBT (default hp)	116/585	120/580	136/565	137/564	137/563	207/493	197/503	198/503	154/547	261/440	227/473	442/258		449/252	444/257	461/240
14 XGB Autotuned (opt acc)	95/605	105/596	111/589	123/578	116/584	153/547	112/589	131/570	140/561	161/540	179/521	424/276	252/449		414/286	376/324
15 TF EBT (default hp)	100/600	107/594	131/569	126/574	140/560	162/539	112/588	145/555	163/537	181/520	417/283	257/444	286/414			305/396
16 XGB Autotuned (opt loss)	88/612	98/602	92/608	109/591	100/600	144/556	107/593	126/575	118/582	146/554	166/535	404/297	240/461	324/376	396/305	

Table 4: Accuracy of each learner on each datasets. Datasets are indexed from 1 to 70 as follow: (1) MFeatFou, (2) Adult, (3) Vehicle, (4) Dressess, (5) MFeat, (6) SteelPlatesF, (7) Adult, (8) BloodTrans, (9) IntAds, (10) PC1, (11) Nomao, (12) Cylinder, (13) GestureSeg, (14) Madelon, (15) Numerai 28.6, (16) RobotNav, (17) BankMark, (18) CNAE9, (19) KC1, (20) Phishing, (21) CMC, (22) Pen Digits, (23) JChess2PCs, (24) Segment, (25) DNA, (26) MFeatK, (27) OzoneL8, (28) Splice, (29) Wilt, (30) Letter, (31) Semeion, (32) Churn, (33) CreditG, (34) FOTTheorem, (35) Mice Protein, (36) Vowel, (37) Balance Scale, (38) ClimateC, (39) JMI, (40) PC4, (41) Spambase, (42) Phoneme, (43) Diabetes, (44) MFeatF, (45) Bioresponce, (46) ILPD, (47) KRvsKP, (48) Satimage, (49) Car, (50) CreditA, (51) AnalcatdataD, (52) Eucalyptus, (53) MFeat Zernike, (54) TicTacToe, (55) Analcatdata, (56) Electricity, (57) MFeat Pixel, (58) Texture, (59) Iris, (60) Beast W, (61) Isolet, (62) PC3, (63) Sick, (64) Opt Digits, (65) WDBC, (66) Banknote, (67) Har, (68) Connect4, (69) KC2, (70) GSarBD.

Learner	Med.Rank	Avg.Rank	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30			
YDF Autotuned (opt loss)	4	4.6	.842	.870	.797	.618	.729	.796	.868	.778	.975	.938	.968	.772	.705	.828	.520	.997	.907	.925	.868	.971	.543	.994	.947	.982	.961	.970	.946	.967	.985	.975			
YDF Autotuned (opt acc)	4	4.9	.834	.873	.804	.604	.717	.798	.872	.779	.979	.941	.973	.772	.701	.835	.519	.997	.909	.929	.869	.971	.543	.995	.954	.986	.963	.967	.943	.966	.984	.973			
LGBM Autotuned (opt loss)	5	5.4	.834	.876	.770	.592	.724	.801	.874	.761	.977	.939	.974	.773	.668	.851	.519	.996	.910	.945	.856	.972	.559	.992	.941	.986	.964	.961	.942	.964	.984	.970			
YDF GBT (benchmark hp)	5	5.7	.843	.874	.792	.564	.711	.803	.872	.777	.977	.938	.972	.776	.692	.806	.519	.996	.908	.932	.860	.972	.554	.991	.981	.985	.962	.965	.944	.965	.985	.973			
LGBM Autotuned (opt acc)	5/5	5.9	.832	.875	.773	.582	.723	.803	.874	.767	.977	.940	.973	.791	.676	.841	.519	.996	.908	.946	.836	.971	.553	.992	.941	.987	.963	.961	.944	.964	.984	.970			
SKLearn RF (default hp)	6	6.7	.834	.854	.748	.606	.701	.795	.854	.739	.979	.940	.970	.802	.683	.737	.513	.995	.906	.933	.867	.974	.526	.992	.973	.981	.957	.966	.944	.969	.983	.969			
YDF RF (benchmark hp)	7.5	6.8	.844	.871	.764	.618	.709	.803	.869	.769	.974	.938	.968	.774	.669	.823	.520	.995	.907	.939	.871	.965	.552	.994	.988	.980	.946	.953	.944	.967	.985	.964			
SKLearn Autotuned	7	7.1	.833	.865	.747	.606	.701	.787	.864	.790	.977	.934	.970	.800	.682	.737	.519	.995	.905	.927	.864	.974	.533	.992	.928	.981	.956	.967	.943	.968	.982	.968			
LGBM GBT (default hp)	8	7.9	.833	.874	.760	.588	.706	.798	.873	.765	.976	.941	.972	.789	.662	.821	.517	.996	.909	.850	.857	.971	.555	.990	.873	.986	.961	.960	.940	.964	.984	.966			
YDF RF (default hp)	10	9.2	.839	.867	.752	.598	.703	.782	.866	.779	.970	.935	.967	.706	.652	.732	.518	.995	.908	.847	.869	.964	.550	.989	.823	.978	.955	.957	.941	.969	.984	.953			
YDF GBT (default hp)	10	9.5	.808	.874	.760	.572	.697	.786	.873	.767	.974	.941	.972	.737	.645	.809	.520	.997	.909	.912	.836	.971	.545	.989	.869	.981	.962	.936	.941	.963	.984	.957			
TF Linear (default hp)	14	11.5	.814	.852	.765	.588	.729	.697	.857	.777	.949	.931	.936	.774	.473	.558	.519	.701	.887	.902	.856	.928	.514	.945	.674	.924	.936	.939	.942	.942	.946	.768			
XGB GBT (default hp)	12	11.9	.810	.869	.760	.602	.714	.768	.867	.770	.967	.939	.966	.806	.613	.810	.516	.994	.904	.907	.853	.954	.551	.985	.861	.972	.947	.929	.937	.954	.981	.955			
XGB Autotuned (acc)	14	12.7	.806	.862	.719	.566	.703	.753	.859	.786	.965	.926	.958	.748	.601	.819	.518	.988	.903	.866	.852	.949	.547	.976	.831	.966	.949	.927	.935	.956	.977	.910			
TF EBT (default hp)	13.25	12.8	.799	.859	.739	.580	.714	.751	.857	.775	.967	.932	.937	.528	.738	.519	.991	.900	.839	.859	.940	.553	.966	.669	.943	.900	.937	.955	.982	.803					
XGB Autotuned (opt loss)	14	13.5	.816	.862	.734	.606	.698	.752	.859	.767	.960	.932	.959	.730	.605	.818	.518	.987	.900	.864	.852	.947	.559	.977	.834	.967	.947	.925	.935	.952	.974	.916			
Learner	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60					
YDF Autotuned (opt loss)			.946	.960	.763	.619	1.000	.975	.966	.944	.818	.914	.954	.910	.758	.970	.804	.696	.994	.918	.997	.878	.202	.601	.810	.995	.994	.917	.976	.995	.940	.954			
YDF Autotuned (opt acc)			.942	.962	.750	.620	1.000	.976	.954	.933	.816	.914	.954	.908	.776	.967	.797	.698	.994	.913	.994	.861	.202	.626	.798	.999	.993	.944	.973	.994	.953	.956			
LGBM Autotuned (opt loss)			.948	.958	.740	.617	1.000	.948	.862	.941	.816	.910	.955	.900	.744	.972	.807	.678	.996	.916	.995	.857	.208	.621	.783	.997	.993	.934	.975	.987	.940	.961			
YDF GBT (benchmark hp)			.946	.964	.746	.603	1.000	.969	.947	.943	.816	.912	.958	.899	.767	.969	.792	.678	.995	.917	.996	.845	.201	.560	.797	1.000	.991	.904	.974	.993	.947	.963			
LGBM Autotuned (opt acc)			.946	.958	.727	.614	1.000	.938	.856	.935	.813	.906	.955	.897	.724	.973	.800	.683	.995	.917	.997	.859	.210	.626	.783	.990	.993	.935	.974	.986	.940	.957			
SKLearn RF (default hp)			.946	.959	.769	.635	1.000	.981	.816	.920	.819	.911	.955	.916	.759	.969	.810	.696	.993	.920	.964	.862	.210	.616	.785	.991	.992	.914	.980	.979	.953	.969			
YDF RF (benchmark hp)			.912	.960	.772	.626	1.000	.958	.904	.935	.819	.911	.951	.900	.763	.968	.808	.695	.991	.914	.968	.852	.198	.644	.781	.985	.979	.897	.968	.989	.953	.969			
SKLearn Autotuned			.944	.959	.768	.632	1.000	.982	.862	.919	.818	.909	.955	.917	.758	.970	.810	.683	.993	.919	.964	.855	.197	.605	.783	.991	.992	.914	.979	.980	.940	.964			
LGBM GBT (default hp)			.930	.960	.745	.607	1.000	.939	.858	.946	.813	.907	.954	.892	.753	.961	.800	.686	.992	.916	.990	.852	.174	.617	.775	.993	.982	.924	.966	.985	.947	.954			
YDF RF (default hp)			.927	.959	.767	.619	1.000	.948	.846	.932	.816	.907	.949	.898	.754	.962	.807	.686	.991	.911	.969	.855	.210	.617	.771	.985	.987	.900	.974	.973	.940	.959			
YDF GBT (default hp)			.909	.957	.750	.598	.999	.898	.830	.935	.805	.901	.954	.883	.759	.952	.794	.688	.995	.908	.990	.844	.203	.579	.767	.989	.980	.915	.956	.981	.967	.960			
TF Linear (default hp)			.915	.865	.751	.673	.996	.668	.866	.950	.805	.908	.971	.751	.772	.969	.748	.715	.958	.853	.910	.868	.206	.576	.826	.841	.995	.753	.961	.984	.913	.957			
XGB GBT (default hp)			.895	.954	.750	.603	.973	.872	.816	.926	.809	.900	.940	.873	.750	.935	.778	.666	.981	.905	.954	.846	.193	.598	.747	.957	.960	.907	.944	.940	.944				
XGB Autotuned (acc)			.893	.948	.725	.586	.982	.783	.840	.922	.810	.899	.932	.864	.742	.954	.783	.708	.979	.894	.944	.854	.201	.565	.747	.945	.964	.846	.955	.958	.953	.961			
TF EBT (default hp)			.843	.955	.735	.536	1.000	.834	.854	.937	.812	.903	.936	.860	.734	.935	.779	.688	.972	.879	.953	.864	.188	.580	.740	.971	.966	.785	.937	.942	.920	.960			
XGB Autotuned (opt loss)			.882	.939	.714	.586	.979	.815	.837	.917	.807	.889	.931	.866	.751	.952	.777	.698	.973	.894	.935	.858	.190	.556	.740	.936	.955	.846	.957	.887	.949				
Learner	61	62	63	64	65	66	67	68	69	70																									
YDF Autotuned (opt loss)			.963	.900	.975	.985	.972	1.000	.993	.861	.839	.861																							
YDF Autotuned (opt acc)			.961	.895	.978	.983	.970	.999	.993	.860	.833	.865																							
LGBM Autotuned (opt loss)			.960	.894	.972	.985	.967	.993	.993	.859	.843	.865																							
YDF GBT (benchmark hp)			.959	.891	.980	.983	.977	.999	.992	.847	.826	.870																							
LGBM Autotuned (opt acc)			.960	.897	.971	.985	.961	.994	.993	.860	.841	.866</																							

Table 5: Name and size of the datasets.

Dataset	Examples	Features	Categorical features	Numerical features
Adult	48842	14	8	6
Adult v2	32561	14	8	6
Analcatdata_Authorship	841	70	0	70
AnalcatData_Dmft	797	4	2	2
Balance_Scale	625	4	0	4
Bank_Marketing	45211	16	9	7
Banknote_Authentication	1372	4	0	4
Beast_W	699	9	1	8
Bioresponce	3751	1776	0	1776
Blood_Transfusion_Service_Center	748	4	0	4
Car	1728	6	6	0
Churn	5000	20	0	20
Climate_Model_Simulation_Crashes	540	20	0	20
CMC	1473	9	0	9
CNAE9	1080	856	0	856
Connect4	67557	42	0	42
Credit_Approval	690	15	11	4
Credit_G.	1000	20	13	7
Cylinder_Bands	540	39	35	4
Diabetes	768	8	0	8
DNA	3186	180	0	180
Dresses_Sales	500	12	11	1
Eletricity	45312	8	0	8
Eucalyptus	736	19	14	5
First_Order_Theorem_Proving	6118	51	0	51
Gesture_Phase_Segmentation_Preprocessed	9873	32	0	32
GSar_Bio_Deg	1055	41	0	41
Har	10299	561	0	561
ILPD	583	10	1	9
Internet_Advertisements	3279	1558	0	1558
Iris	150	4	0	4
Isolet	7797	617	0	617
JM1	10885	21	5	16
Jungle_Chess_2PCs	44819	6	0	6
KC1	2109	21	0	21
KC2	522	21	0	21
KR_vs_KP	3196	36	36	0
Letter	20000	16	0	16
Madelon	2600	500	0	500
MFeat_Factors	2000	216	0	216
MFeat_Fourier	2000	76	0	76
MFeat_Karhunen	2000	64	0	64
MFeat_Morphological	2000	6	0	6
MFeat_Pixel	2000	240	0	240
MFeat_Zernike	2000	47	0	47
Mice_Protein	1080	81	53	28
Nomao	34465	118	0	118
Numerai_28.6	96320	21	0	21
Opt_Digits	5620	64	0	64
Ozone_Level_8h	2534	72	0	72
PC1	1109	21	0	21
PC3	1563	37	0	37
PC4	1458	37	0	37
Pen_Digits	10992	16	0	16
Phishing_Websites	11055	30	0	30
Phoneme	5404	5	0	5
Satimage	6430	36	0	36
Segment	2310	19	0	19
Semeion	1593	256	0	256
Sick	3772	29	29	0
Spambase	4601	57	0	57
Splice	3190	61	61	0
Steel_Plates_Fault	1941	27	0	27
Texture	5500	40	0	40
Tic_Tac_Toe	958	9	9	0
Vehicle	846	18	0	18
Vowel	990	12	2	10
Wall_Robot_Navigation	5456	24	0	24
WDBC	569	30	0	30
Wilt	4839	5	0	5

Table 6: Training time in seconds, averaged over the 10 fold cross-validation, for each learner and each dataset. Datasets are indexed similarly as tab. 4.

Learner	Avg.	1	2	2	3	3	4	4	5	5	6	6	8	8	9	9	10	10	11	11	12	12	13	13	14	14	15	15	16	16	17	17	18	18	19	19	20	20	22	22	23	23	24	24	25	25
YDF GBT (benchmark hp)	28.74	28.13	31.69	3.92	6.29	2.95	9.60	8.75	4.79	56.94	5.25	57.92	3.42	83.13	31.61	25.96	27.95	22.84	60.24	3.58	22.45	34.49	128.10	7.76	22.06																					
SKLearn RF (default)	8.26	6.49	16.50	4.66	3.68	3.72	4.71	2.77	3.92	11.78	3.69	14.56	4.79	7.19	9.06	44.38	3.97	12.52	4.08	3.76	4.36	7.93	11.82	2.74	5.25																					
YDF TRF (benchmark hp)	19.81	12.22	10.63	2.73	2.76	2.57	3.05	5.31	2.52	112.10	2.77	69.26	2.70	26.74	43.90	93.70	6.86	13.08	27.63	3.19	4.75	6.15	7.80	3.47	9.51																					
LGBM GBT (default)	1.22	3.78	0.94	0.05	0.12	0.04	0.15	0.65	0.03	0.27	0.06	4.01	0.05	5.45	1.50	0.92	1.06	0.83	0.16	0.07	0.43	1.66	5.74	0.79	0.47																					
YDF RF (default)	4.60	3.88	5.27	2.46	2.46	2.33	2.70	2.83	2.37	2.72	2.52	8.65	2.49	8.44	4.68	19.46	3.17	5.11	4.99	2.52	3.17	3.40	5.92	2.68	3.66																					
YDF GBT (default)	20.61	32.99	13.56	3.40	4.91	4.03	7.87	8.94	2.77	39.38	3.29	72.21	3.25	56.64	30.01	9.47	14.79	23.50	50.79	3.33	17.98	29.24	34.34	8.01	19.97																					
TF Linear (default)	68.15	23.10	55.12	6.93	8.52	9.01	6.40	12.84	5.94	564.50	11.76	118.00	15.94	27.34	176.10	107.40	14.46	60.73	210.20	14.61	23.14	18.15	53.38	12.65	79.39																					
XGB GBT (default)	6.70	7.89	17.26	0.07	0.23	0.03	0.37	1.56	0.01	10.13	0.09	23.99	0.34	35.00	2.76	1.95	2.43	6.71	16.55	0.10	2.28	8.89	17.49	1.23	3.34																					
TF EBT (default)	91.45	112.40	62.17	12.62	11.73	7.05	24.03	31.00	7.62	216.70	7.50	96.24	13.08	68.11	77.72	136.70	26.35	62.48	857.40	10.06	21.87	131.40	81.73	35.04	83.15																					
YDF GBT (benchmark hp)	24.47	4.88	7.54	4.56	251.00	38.31	7.27	3.44	21.27	29.97	8.93	5.02	3.42	8.63	4.89	9.55	7.10	2.98	37.83	53.99	3.00	10.53	21.36	14.59																						
SKLearn RF (default)	4.92	3.81	5.08	3.74	9.33	3.51	4.46	5.00	5.50	3.22	4.03	2.90	2.31	9.55	4.94	4.96	5.45	2.58	4.66	11.80	3.44	3.38	3.49	4.82																						
YDF TRF (benchmark hp)	10.03	4.53	4.35	2.79	13.93	13.00	4.63	2.70	21.33	3.54	3.20	2.41	2.60	25.21	3.08	4.99	4.99	2.58	17.40	370.80	2.46	2.62	11.58	2.40																						
LGBM GBT (default)	5.36	0.28	0.59	0.07	8.82	1.35	0.18	0.04	2.38	1.36	0.96	0.06	0.06	0.19	0.09	0.33	0.13	0.03	8.97	2.17	0.03	0.15	0.99	0.23																						
YDF RF (default)	3.55	2.76	2.78	2.47	4.75	3.64	2.89	2.42	5.27	2.83	2.70	2.32	2.47	3.51	2.42	3.15	2.77	2.53	3.59	12.27	2.33	2.56	3.28	2.30																						
YDF GBT (default)	28.73	4.04	6.76	3.21	75.54	53.58	4.09	3.33	24.85	52.74	8.72	5.58	3.00	3.50	4.84	11.27	4.54	2.89	31.44	30.98	3.37	5.44	24.83	9.59																						
TF Linear (default)	24.08	33.50	24.81	11.31	28.38	76.31	16.39	11.85	27.16	14.12	7.21	6.15	9.80	23.58	18.33	37.45	11.03	6.03	73.92	610.40	7.70	20.07	20.03	6.68																						
XGB GBT (default)	8.11	0.42	5.92	0.17	73.57	11.92	0.32	0.12	12.57	2.08	1.52	0.07	0.05	7.84	0.14	0.83	0.31	0.02	12.75	9.85	0.02	1.64	4.68	0.70																						
TF EBT (default)	102.80	20.86	22.34	10.84	1350.00	462.00	12.55	8.46	101.20	31.27	29.06	7.31	8.62	43.20	12.28	19.50	14.19	6.69	340.40	345.00	6.02	13.11	76.87	7.85																						
YDF GBT (benchmark hp)	3.45	3.35	5.83	17.24	4.80	21.61	75.14	42.23	53.75	3.74	697.50	3.59	2.93	34.22	6.12	6.37	238.80	216.00	3.01	5.28																										
SKLearn RF (default)	3.12	4.82	3.18	6.49	2.53	3.60	13.17	1.96	7.91	5.38	21.67	3.01	7.06	8.23	4.40	3.62	28.78	23.97	5.50	2.80																										
YDF TRF (benchmark hp)	2.54	2.42	3.77	8.92	2.47	3.17	12.62	9.28	10.17	2.40	631.90	3.35	11.83	7.83	2.47	2.43	255.80	39.40	2.39	2.96																										
LGBM GBT (default)	0.05	0.04	0.08	2.26	0.07	0.43	3.11	2.56	4.86	0.04	184.60	0.08	0.08	1.23	0.11	0.11	55.75	14.18	0.03	0.09																										
YDF RF (default)	2.40	2.40	2.47	5.38	2.34	2.45	5.99	3.29	4.08	2.39	27.40	2.51	2.40	3.40	2.40	2.34	16.45	13.06	2.37	2.45																										
YDF GBT (default)	3.06	3.09	4.35	10.84	6.57	10.63	27.73	32.52	36.55	3.15	872.40	5.02	3.17	19.32	3.37	8.72	267.00	139.70	2.70	4.66																										
TF Linear (default)	9.29	5.22	8.91	16.38	6.87	23.69	47.12	71.48	22.76	8.26	307.40	13.79	24.14	35.80	10.88	6.83	280.90	92.53	10.89	15.16																										
XGB GBT (default)	0.09	0.06	1.49	5.28	0.14	0.51	11.52	10.74	12.93	0.05	627.10	0.13	6.17	10.07	0.11	0.10	245.00	161.00	0.03	0.11																										
TF EBT (default)	8.30	9.99	13.05	91.09	6.81	30.65	48.43	477.90	141.30	7.51	6862.00	10.88	24.71	181.00	8.35	7.26	988.70	236.90	7.63	10.20																										

