Tribuo: Machine Learning with Provenance in Java

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Abstract

Machine Learning models are deployed across a wide range of industries, performing a wide range of tasks. Tracking these models and ensuring they behave appropriately is becoming increasingly difficult as the number of deployed models increases. There are also new regulatory burdens for ML systems which affect human lives, requiring a link between a model and its training data in high-risk situations. Current ML monitoring systems often provide provenance and experiment tracking as a layer on top of an ML library, allowing room for imperfect tracking and skew between the tracked object and the metadata. In this paper we introduce Tribuo, a Java ML library that integrates model training, inference, strong typesafety, runtime checking, and automatic provenance recording into a single framework. All Tribuo's models and evaluations record the full processing pipeline for input data, along with the training algorithms, hyperparameters and data transformation steps automatically. The provenance lives inside the model object and can be persisted separately using common markup formats. Tribuo implements many popular ML algorithms for classification, regression, clustering, multi-label classification and anomaly detection, along with interfaces to XGBoost, TensorFlow and ONNX Runtime. Tribuo's source code is available at https://github.com/oracle/tribuo under an Apache 2.0 license with documentation and tutorials available at https://tribuo.org.

Keywords: Provenance, Classification, Regression, Java

1. Introduction

Machine Learning models are increasingly deployed across industries to improve computer systems and integrate with large existing software systems. There has been an explosion of tools to help companies and individuals train, monitor and deploy ML models. Several of these tools provide provenance and reproducibility support to existing libraries (*e.g.*, TF Extended (Karmarkar et al., 2020), Weights & Biases (Biewald, 2020)), though most of them provide this tracking by modifying or parsing existing scripts rather than direct integration with the libraries performing the ML computations. As a consequence they may not capture all the interactions between a script and data and may increase the overhead of building ML systems, both for the data scientist and computationally. In contrast, Tribuo provides a comfortable type-safe ML library that integrates *provenance* as a core feature built into *every* model and evaluation with no additional overhead. To facilitate integration with large software systems we've implemented Tribuo in Java, as the JVM is the most popular platform for building enterprise software (Cloud Foundry Inc, 2018).

Tribuo's design has four core elements: features and output dimensions are *named* rather than indexed, feature spaces are sparse by default, objects in Tribuo are strongly typed with runtime validation checks, and all operations that result in datasets, models or evaluations

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Рососк

are tracked in provenance objects. Consequently Tribuo's data points are objects containing sparse arrays of features, where each feature has a name and a numeric value, along with an output object which represents the ground truth value for the prediction task (*e.g.*, for classification, a label string; for regression, a numeric value). The first two elements emerged from an initial focus on Natural Language Processing, but have proved widely useful for inference time feature space validation and working with complex tabular datasets. The latter two elements follow from our experience deploying ML systems in large enterprise codebases, where compile time checking is important, and provenance allows us to trace and debug models in production.

2. System design

Machine Learning systems have a variety of constraints that must be satisfied for reliable deployment of models, however these constraints are often hidden by the model interface which accepts a multidimensional array as input and produces a multidimensional array as output. For example, classification models cannot be directly applied to regression tasks, models must receive features from the space they have been trained on, many models must be trained before they can be applied. As machine learning becomes more prevalent, mismatches in these properties cause issues with deployed ML systems which can be hard to diagnose such as asking a NLP system to make a prediction when it was not trained on any of the input words. In Tribuo, we prevent several classes of user error through a mixture of compile-time and runtime checks. We use Java's type system to enforce that models are trained before they are applied, and that classification models are only trained and applied on classification tasks. At runtime, we check that the features present in the input data have the correct names, dropping features that the model hasn't seen and raising an exception if there is no feature overlap between the input data and the model. We also capture feature metadata that can be used to raise additional warnings if, for example, the input data is outside the range of the features which the model was trained on.

The nature of these checks means that Tribuo requires stronger contracts between its data sources, model trainers and the models themselves. This contrasts with many ML libraries that follow scikit-learn's (Pedregosa et al., 2011) lead in expecting a minimal interface of two functions (fit and predict) that accept anything "array-like". Tribuo's model trainers (which implement the Trainer interface) only accept Tribuo's Dataset objects as inputs for model training. This allows them to enforce that the type of the dataset (*e.g.*, Classification, Regression) matches the type of the trainer and that the dataset contains the necessary provenance information to describe itself. Similarly Tribuo's Model objects can only make predictions on examples that have the correct output type, enforcing that when loading an unknown model from disk you get an error message rather than silently using a regression model to make predictions on a classification task. While these type restrictions, along with the provenance requirements, make it more complicated to extend Tribuo with new models or data loaders, they provide stronger guarantees for code built on top of Tribuo and do not increase the complexity of *using* Tribuo. We think this trade-off is acceptable as users of Tribuo outnumber the number of people developing Tribuo itself.

Tribuo has Java implementations of CART (Friedman et al., 2009), Classifier Chains (Read et al., 2011), Factorization Machines (Rendle, 2010), Linear Chain Conditional Ran-

dom Fields (Lafferty et al., 2001), linear & logistic regressions trained using SGD (Bottou, 2010), multinomial Naive Bayes and sparse linear regressions using the Lasso and Elastic Net penalties (Friedman et al., 2009). There are a variety of SGD algorithms implemented, including popular ones from the neural network literature such as Adam (Kingma and Ba, 2014) and AdaGrad (Duchi et al., 2011), which can be applied to the factorization machines, CRFs and linear models. It also has Java implementations of multi-class Adaboost, Bagging, Random Forests (Friedman et al., 2009) and extremely randomized trees (Geurts et al., 2006), where Adaboost and Bagging can use any other trainer as the base learner. In addition to the native Tribuo implementations it also wraps the Java implementations of LibSVM and LibLinear (Fan et al., 2008) (the latter via the liblinear-java implementation (Waldvogel, 2021)), and it uses the Java interfaces to the C implementations of TensorFlow (Abadi et al., 2016), ONNX Runtime (developers, 2021) and XGBoost (Chen and Guestrin, 2016). Tribuo runs on Java 8 and newer versions, while the native libraries (ONNX Runtime, TensorFlow and XGBoost) are available for x86_64 platforms running on Windows, macOS and Linux. ONNX Runtime and XGBoost also work on ARM64 platforms, though users will need to compile these dependencies themselves. Many Tribuo models can be exported in the ONNX model format¹ for deployment in other languages, on accelerator hardware, and on cloud platforms.

3. Provenance for data, models and evaluation

The history or creation path of an object or piece of data is referred to in the academic literature as its *provenance* or *lineage*. Tracking the provenance of Machine Learning datasets, models and evaluations is an active area of research, which principally focuses on monitoring the behaviour of the system to record how data flows into a model (Namaki et al., 2020; Phani et al., 2021), both training data and other information such as hyperparameter values and algorithm choices. Such systems imply some overhead in the tracking (*e.g.*, Vamsa reparses Python scripts to extract provenance) and a potential lack of fidelity if the system did not understand some part of the computation. Tracking the training data used by any given model is increasingly important for GDPR compliance and regulations like the EU's proposed AI regulatory framework² which require that all "high-risk" models can be traced back to their training data, meaning that data provenance will likely be further integrated into Machine Learning Systems.

In Tribuo, we chose to build provenance into the core of the system, each object (such as a data source, data transformation, training algorithm or model) knows exactly how it was created and the provenance of all elements that were used to construct/train it. It is a necessary part of implementing Tribuo's API that the provenance methods return useful values, and code which does not appropriately use the provenance does not pass our continuous integration tests. This means that when working inside Tribuo, everything the user does is tracked and transcribed into the provenance objects automatically, and those objects are themselves fields of the host object that is the subject of the provenance. As a result, the Tribuo provenance objects is fast and cheap). Tribuo's provenance can be conceptually

^{1.} https://onnx.ai/

 $^{2. \ {\}tt https://digital-strategy.ec.europa.eu/en/policies/regulatory-framework-ai}$

Рососк

split into two kinds, configuration and instance information. Configuration describes information statically known before the computation begins, *e.g.*, model hyper-parameters, the path to training data files, training algorithm choice. Instance information is derived from the computation as it is executed, *e.g.*, SHA-256 hashes of the training data, user supplied information, OS and machine architecture. The configuration aspects can be separated out of a provenance object and stored separately as a configuration file in a variety of formats (currently xml, json, protocol buffers and edn) for running reproducible experiments.

The central provenance object is ModelProvenance. It contains a DataProvenance. which is extracted from the training dataset, and a TrainerProvenance, which is extracted from the training algorithm. If the model is an ensemble then it also contains a list of ModelProvenance objects, one per ensemble member. The DataProvenance object tracks the number of features, the number of examples, any transformations applied both at a per feature and global level (e.g., zero mean unit variance rescaling), and the original DataSourceProvenance. The DataSourceProvenance tracks the location the data was loaded from, whether a file on disk, a DB connection, or created in memory, along with a hash of the data and other relevant information such as the feature extraction procedure and the mapping between columns and features. The TrainerProvenance includes the training algorithm (along with any nested algorithms in the case of an ensemble), the algorithm's hyperparameters (e.q., learning rate, tree depth), and any RNG seeds to ensure reproducibility. When evaluating models, the ModelProvenance is stored inside the evaluation alongside the DataProvenance for the test data. To prevent the provenance from becoming stale and to avoid having to figure out which provenance applies to which model, we store these provenance objects *inside the model object*. If necessary to maintain confidentiality the provenance can be redacted and replaced with a hash which can be linked to the provenance in an external database, similar to other model tracking systems.

4. Uses of model and data provenance

We have two main uses for provenance information in Tribuo's models and evaluations. The first is simply tracking models via their metadata. As the provenance is stored in the model object both in memory and on disk, it is guaranteed to be present with the model and so is hard to confuse with the provenance for a different model. When there are hundreds of models in production, this makes it simple to understand what data a specific model was trained on and what the training algorithm was without resorting to a potentially inaccurate external system. The models are *self-describing*, they know properties of their training data like the input feature distributions, the output label distributions and the number of training examples, in addition to a full description of the training algorithm used, along with any feature transformations applied to the data before training.

The second use is as a way of storing the input pipeline in a recoverable fashion inside the model object. This is most useful when using Tribuo's columnar data system to featurise inputs. The columnar package can extract features of different kinds from input strings, either by converting them directly into numeric feature values, binarising categorical variables, or applying a full text processing pipeline among other options. The processing infrastructure has its provenance recorded as part of the training data provenance, stored inside the model object. Using the configuration extractor the columnar provenance can be converted into configuration for the columnar processor and the processing object can be re-instantiated, ready to process new inputs after the model has been loaded. This system is not specific to Tribuo's columnar processor, *any* Tribuo data loader can be reconstructed from the provenance, and the system is not closed world, it can be extended by implementing the appropriate interfaces in user classes outside of Tribuo's namespace.

Over time we plan to expand Tribuo's use of provenance information, first to add full automatic reproducibility of Tribuo trained models and evaluations and then to use the reproducibility framework as a basis for an experimental tracking system that integrates hyperparameter optimization.

5. Conclusion

In this paper we presented Tribuo, a ML library for the Java platform, that has a strong focus on type-safety, runtime checks, and metadata tracking via provenance objects. The focus on provenance makes Tribuo well suited for use in systems where any data and algorithms used in model creation must be tracked for compliance or regulatory reasons. Tribuo's source code is available at https://github.com/oracle/tribuo under an Apache 2.0 license with documentation and tutorials available at https://tribuo.org.

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