Vamsa: Tracking Provenance in Data Science Scripts

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ABSTRACT

Machine learning (ML) which was initially adopted for search ranking and recommendation systems has firmly moved into the realm of core enterprise operations like sales optimization and preventative healthcare. For such ML applications, often deployed in regulated environments, the standards for user privacy, security, and data governance are substantially higher. This imposes the need for tracking provenance end-to-end, from the data sources used for training ML models to the predictions of the deployed models.

In this work, we take a first step towards this direction by introducing the ML provenance tracking problem in the context of data science scripts. The fundamental idea is to automatically identify the relationships between data and ML models and in particular, to track which columns in a dataset have been used to derive the features of a ML model. We discuss the challenges in capturing such provenance information in the context of Python, the most common language used by data scientists. We then, present Vamsa, a modular system that extracts provenance from Python scripts without requiring any changes to the users’ code. Using up to 450K real-world data science scripts from Kaggle and publicly available Python notebooks, we verify the effectiveness of Vamsa in terms of coverage, and performance. We also evaluate Vamsa’s accuracy on a smaller subset of manually labeled data. Our analysis shows that Vamsa’s precision and recall range from 87.5% to 98.3% and its latency is typically in the order of milliseconds for scripts of average size.

1. INTRODUCTION

Machine learning (ML) has proven itself in multiple consumer applications such as web ranking and recommendation systems. In the context of enterprise scenarios, ML is emerging as a compelling tool in a broad range of applications such as marketing/sales optimization, process automation, preventative healthcare, and automotive predictive maintenance, among others.

For such enterprise-grade ML applications, often deployed in regulated environments, the standards for user privacy, security, and explainability are substantially higher. which now has to be extended to ML models. Consider the following scenarios:

Compliance. The protection of personal data is crucial for organizations due to relatively recent compliance regulations such as HIPAA [3] and GDPR [4]. As more emerging applications rely on ML, it is critical to ensure effective ongoing compliance in the various pipelines deployed in an organization is preserved. Thus, developing techniques that automatically verify whether the developer’s data science code is compliant (e.g., tools that determine if the features used to build a machine learning model are derived from sensitive data such as personally identifiable information (PII) [57]) is an immediate priority in the enterprise context.

Reacting to data changes. Avoiding staleness in the ML models deployed in production is a crucial concern for many applications. To this end, detecting which models are affected because data has become unreliable or data patterns have changed, by tracking the dependencies between data and models becomes critical. For example, it is possible that the code used to populate the data had some bug which was later discovered by an engineer. In this case, one would like to know which ML models were built based on this data and take appropriate action. Similarly, one might want to investigate whether the feature set of a ML model should be updated, once new dimensions have been added in the data.

Model debugging. Diagnosis and debugging of ML models deployed in production remain an open challenge. An important aspect of model debugging is to understand whether the decreased model quality can be attributed to the original data sources. For example, a data scientist while debugging her code might eventually find that the ML model is affected by a subset of the data which contains 0 values for a particular feature. In such scenarios, one needs to automatically track the original data sources used to produce this model and evaluate whether they also contain 0 values.

The aforementioned scenarios motivate the need for tracking provenance end-to-end, from the data sources used for training ML models to the predictions of the deployed ML models. In this paper, we take a first step towards this direction by introducing the ML provenance tracking problem. The core idea is to automatically identify the relationships between data and ML models in a data science script and in particular, to track which columns in a dataset have been used to derive the features (and optionally labels) used to train a ML model. To address this problem, we design Vamsa [3] a system that automatically tracks coarse-grained

1Vamsa is a Sanskrit word that means lineage.
provenance from scripts written in Python (the most common language used by data scientists) using a variety of static analysis techniques.

Consider the Python script presented in Figure 1 that was created in the context of the Kaggle Heart Disease competition. The script trains a ML model using a patient dataset from a U.S. hospital. The model takes as input a set of features such as Age, Blood pressure, and Cholesterol, and predicts whether a patient might have a heart disease in the future. After performing static analysis on the script, Vamsa not only detects that this script trains a ML model but also that the columns Target and SSN from the heart_disease.csv dataset are not used to derive the model’s features.

Building a system that captures such provenance information is challenging: (1) As opposed to data provenance in SQL, scripting languages are not declarative and thus may not specify the logical operations that were applied to the data. This is exacerbated in dynamically typed languages, such as Python. (2) Data science is still an emerging field as exemplified by popular libraries like scikit-learn still evolving their APIs and growth of newly available frameworks like PyTorch. (3) Scripts encode various phases of the data science lifecycle including exploratory analysis, visualizations, data preprocessing, training, and inference. Hence, it is nontrivial to identify the relevant fraction of the scripts that contribute to the answer of a specific provenance query.

Vamsa is specifically designed to address the aforementioned challenges without requiring any modifications to the users code by solely relying on a modular architecture and a knowledge base of APIs of various ML libraries. Vamsa does not make any assumption about the ML libraries/frameworks used to train the models and is able to operate on all kinds of Python libraries as long as the appropriate APIs are included in the knowledge base. Additionally, Vamsa’s design allows users to improve coverage by simply adding more ML APIs in the knowledge base without any further code changes.

This paper makes the following contributions:

1. Motivated by the requirements of enterprise-grade ML applications, we formally introduce the problem of ML provenance tracking in data science scripts that train ML models. To the best of our knowledge, this is the first work that addresses this problem.

2. We present Vamsa, a modular system that tackles the ML provenance tracking problem in data science scripts written in Python without requiring any modifications to the users’ code. We thoroughly discuss the static analysis techniques used by Vamsa to identify variable dependencies in a script, perform semantic annotation and finally extract the provenance information.

3. Using real-world data science scripts from Kaggle and publicly available Python notebooks, we perform experiments using up to 450K scripts and verify the effectiveness of Vamsa in terms of coverage, and performance. We also evaluate Vamsa’s accuracy on a smaller subset of manually labeled data. Our analysis shows that Vamsa’s precision and recall range from 87.5% to 98.3% and its latency is typically in the order of milliseconds for scripts of average size.

```python
# importing libraries and modules
1. import catboost as cb
2. from sklearn.model_selection import train_test_split
3. import pandas as pd

# reading from a data source
4. train_df = pd.read_csv('heart_disease.csv')

5. selecting a set of features and specifying the ground truth
6. train_df = train_df.drop(['SSN', 'Target'], axis=1)
7. train_x = train_df.drop(['SSN', 'Target'])
8. train_y = train_df['Target']

# splitting the training data to train and validation sets
9. train_x, val_x1, train_y_val, val_y = train_test_split(
   train_x, train_y, test_size=0.20)

# initializing a model
10. clf = cb.CatBoostClassifier(eval_metric="AUC", iterations=40)

# training the model
11. clf.fit(train_x1, train_y1, eval_set=(val_x1, val_y))
```

Figure 1: A data science script written in Python

The rest of the paper is organized as follows: in Section 2 we formally define the problem of ML provenance tracking and in Section 3 we give an overview of Vamsa’s architecture. Sections 4, 5, and 6 provide a detailed description of Vamsa’s major components and their corresponding algorithms. Section 7 presents our experimental evaluation and Section 8 discusses related work. We conclude the paper and discuss directions for future work in Section 9.

2. PROBLEM STATEMENT

We start by defining the concepts used by Vamsa, followed by the problem of ML provenance tracking in data science scripts that Vamsa targets.

A Data Source $D$ can be a database table/view, a spreadsheet, or any other external files that is typically used in Python scripts to access the input data e.g., hdf5, npy.

A common ML pipeline accesses data source $D$ and learns a ML model $M$ with two steps. First, feature engineering is conducted to extract a set of training samples from $D$ to be used to train the model $M$. The training samples consist of features and labels that are both derived from selected columns in $D$ by e.g., transformation functions. The training process then derives the model $M$ by optimizing a learning objective function determined by the training samples and specific predictive or descriptive needs.

A Data Science Script reads from a set of data sources $D$ and trains a set of machine learning models $M$. In this work, we focus on scripts written in Python, as this is the major language currently used by data scientists.

We now formally define the problem of automated ML provenance tracking which Vamsa targets. The essence is to identify which columns in a dataset have been used to derive the features (and optionally labels in the context of

Note that there are also data science scripts that do not perform any model training but provide other functionality (e.g., visualization, optimization, etc.) In this work, we focus on data science scripts that include statements that train ML models as our goal is to capture the relationships between data sources and generated ML models.

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Figure 1: A data science script written in Python
supervised learning) of a particular ML model in a data science script, thus automatically capturing the relationships between data sources and models at a coarse grain level and during static analysis time.

**ML Provenance Tracking.** Given a data science script, find all triples \((M, D, C)\) where each \(M \in \mathcal{M}\) is a constructed machine learning model trained in the script using data source \(D\). In particular, the model is trained using features (and optionally labels) derived from a subset of columns of data source \(D\), denoted as \(C\). The goal is to identify each trained model \(M\) in the script, its data source \(D\), and the columns \(C\) that were used to train model \(M\).

**Example 1:** The input of Vamsa is a data science script such as the one in Figure 1. The script reads from `heart_disease.csv` as a data source \(D\) and trains an ensemble of decision trees using catboost library [49]. In this script, only a single model was trained. Note that not all the columns of the data source have been used to derive the model’s features and labels. To select the features, in the script, a range of columns \([3, +\infty)\) from \(D\) is explicitly extracted, followed by the drop of the columns \{SSN, Target\}. Similarly, only the Target column was used to derive the labels. Thus, the desired output is a triple \((M, D, C)\) where \(M = \text{clf}\) is the variable that contains the trained model, \(D = \text{heart_disease.csv}\) is the training dataset, and \(C\) is the set: \([3, +\infty)\) \(\setminus\{\text{SSN}\}\). Vamsa automatically parses the script and produces this output.

3. VAMSA ARCHITECTURE

Vamsa takes as input a script and produces the provenance information that captures the relationship between data sources accessed by the script and the ML models trained in the script. It follows a modular architecture (illustrated in Figure 2) that addresses all the above challenges without requiring manual modifications to the users’ code.

At a high-level, Vamsa performs static analysis on the Python script to derive the relationships between all variables in the script, followed by an annotation phase that assigns semantic information to the variables in the script. It then uses a generic provenance tracking algorithm that extracts the feature set for all the ML models trained in the script and stores this information in a central catalog that can be accessed by various provenance applications.

More specifically, Vamsa processes data science scripts with the following three major modules: the Derivation Extractor, the ML Analyzer, and the Provenance Tracker that we discuss in detail in the following sections:

1. **Derivation Extractor** generates a workflow intermediate representation (WIR) of the script. It extracts the major workflow elements including imported libraries, variables, and functions, as well as their dependencies (Section 4).

2. **ML Analyzer** annotates variables in WIR based on their roles in the script (e.g., features, labels, and models). To this end, it uses our proposed annotation algorithm and a knowledge base that contains information about the various APIs of different ML libraries (Section 5). Through the knowledge base, we are able to declaratively introduce semantic information to Python functions which in turn allows us to track provenance in data science scripts.

3. **Provenance Tracker** infers a set of columns that were explicitly included in or excluded from the features/labels by using the annotated WIR and consulting the knowledge base. We remark that acquiring labeled data is non-trivial or even infeasible [59] in real-world settings. The Provenance Tracker is able to operate in both supervised and unsupervised learning settings (in the latter by tracking provenance only at the features level).

Vamsa does not make any assumption about the ML libraries/frameworks used to train the models. By utilizing a modular architecture combined with a knowledge base of APIs for various ML libraries, Vamsa is able to operate on all kinds of Python libraries as long as the appropriate APIs are included in the knowledge base. Additionally, this design allows users to improve coverage by simply adding more ML APIs in the knowledge base, without having to modify their code or Vamsa’s other components.

To evaluation Vamsa, we have populated our knowledge base with APIs from four well-established data science libraries: scikit-learn [46], XGBoost [2], LightGBM [3], and Pandas [37]. Nevertheless, Vamsa can operate on top of any other library such as CatBoost [49], StatsModels [58], and Graphlab [1], among others.

4. DERIVATION EXTRACTOR

In the first phase, Vamsa parses the Python script and by performing static analysis, builds a workflow model which captures the dependencies among the elements of the script including imported libraries, input arguments, operations that change the state of the program, and the derived output variables. This model is captured in a workflow intermediate representation (WIR) (Section 3). Section 4.2 describes how Vamsa automatically generates the model instances.

4.1 Workflow Model

To formally define the WIR model, we introduce the notions of variables, operations, and provenance relationships (PRs). We then discuss how Derivation Extractor component generates the WIR for a given script.

**Variable.** In programming languages, variables are containers for storing data values. We denote the set of all variables in the data science script as \(V\). For instance, `catboost`, `cb`, `train_df` are a few examples of variables in the script of Figure 1.
**Operation.** An operation \( p \in P \) operates on an ordered set of input variables \( I \) to change the state of the program and/or to derive an ordered set of output variables \( O \). An operation may be called by a variable, denoted as caller \( c \). While an operation may have multiple inputs/outputs, it has at most one caller.

**Example 2:** In Figure 1, the import statements, `read_csv()` in line 4, `attribute_values` in line 5, `CatBoostClassifier()` in line 9, and `fit()` in line 10 are examples of operations. Consider the `fit()` operation: it is invoked by the `clf` variable and takes three arguments namely, features and labels, and an evaluation set. While `fit()` does not explicitly produce an output variable, it changes the state of the variable `clf` from model to trained model.

**Provenance relationship.** An invocation of an operation \( p \) (by an optional caller \( c \)) depicts a provenance relationship (PR). A PR is represented as a quadruple \( (I, c, p, O) \), where \( I \) is an ordered set of input variables, (optional) variable \( c \) refers to the caller object, \( p \) is the operation, and \( O \) is an ordered set of output variables that was derived from this process. A PR can be represented as a labeled directed graph, which includes (1) a set of input edges (labeled as ‘input_edge’), where there is an input edge \( (v, p) \) for each \( v \in I \), (2) a caller edge (labeled as ‘caller_edge’) \( (c, p) \) if \( p \) is called by \( c \), and (3) a set of output edges (labeled as ‘output_edge’), where there is an output edge \( (p, v) \) for each \( v \in O \). For consistency, we create a temporary output variable for the operations that do not explicitly generate one.

**Example 3:** Consider line 4 of the script in Figure 1 where the CSV file is read. The corresponding PR is depicted in Figure 3 (dashed rectangle) and corresponds to the quadruple \( (I, c, p, O) \) where \( I = \{ \text{'heart\_disease.csv'} \} \), \( c = \text{pd} \), and \( p = \text{read\_csv} \). We create a temporary variable and set \( O = \{ \text{tmp\_csv} \} \) to be used as the input by another PR.

**Workflow Intermediate Representation.** PRs are composed together to form a WIR \( G \), which is a directed graph that represents the sequence and dependencies among the extracted PRs. The WIR is useful to answer queries such as: “Which variables were derived from other variables?”, “What type of libraries and modules were used?”, and “What operations were applied to each variable?”. More formally, a WIR is a directed bipartite graph \( G = (V \cup P, E) \) with vertices \( V \cup P \) and edges \( E \subseteq (V \times P) \cup (P \times V) \). Each edge has an associated type from the following set: \{input_edge, output_edge, caller_edge\}.

**Example 4:** Figure 3 illustrates a fraction of a WIR that was generated from the script of Figure 1. The variables and operations are represented by rectangles and ovals, respectively. The caller, input, and output edges are marked in blue, red, and black color, respectively. Consider the operation `fit()`: one can tell from the following: 1) it is called by variable `clf`; 2) it has two ordered input variables `train_x2` and `train_y2`; and 3) a temporary variable, denoted as `tmp_fit`, was created as its output.

### 4.2 WIR Generation

Vamsa generates workflows with the following three-step process. First, its Derivation Extractor component parses the script to obtain a corresponding abstract syntax tree (AST) representation. It then identifies the relationships between the nodes of the AST to generate the PRs. Finally, it composes the generated PRs into a directed graph.

Figure 4 shows a fraction of an AST that was generated from line 4 of the script in Figure 1. The AST is a collection of nodes that are linked together based on the grammar of the Python language. Informally, by traversing the AST from left-to-right and top-to-bottom, we can visit the Python statements in the order presented in the script.

Due to the recursive nature of AST node definitions, the WIR generation algorithm is naturally recursive. The algorithm, denoted as `GenWIR` and illustrated in Figure 5, takes as input the root of the AST tree and traverses its children from left-to-right. For each visited AST node, in order to generate PRs, it invokes a recursive procedure `GenPR` (Figure 5). Each invocation of `GenPR` in line 3 of `GenWIR` may create multiple PRs. All the PRs are accumulated (line 4) and a graph \( G \) is constructed by connecting the inputs/caller/outputs of PRs.

The procedure `GenPR` is illustrated in Figure 5 and takes as input an AST node and a set of already generated PRs. It returns a set of WIR variables and the updated PRs. The

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**References:**

https://github.com/python/cpython/blob/master/Lib/ast.py
Algorithm GenWIR
Input: AST root node $r$.
Output: WIR $G$.
1. $\text{PRs} := \emptyset$.
2. for each $v$ in children($r$) do
3. $(\emptyset, \text{PRs}') := \text{GenPR}(v, \text{PRs})$;
4. $\text{PRs} := \text{PRs} \cup \text{PRs}'$.
5. Construct $G$ by connecting PRs.
6. return $G$;

Procedure GenPR($v$, PRs)
Input: AST node $v$ and PRs generated so far.
Output: a set of WIR variables and updated PRs.
1. $c := \emptyset$; $p := \text{extract from node}(v, \text{‘operation’})$;
2. if $v \in \{$Str, Num, Name, NameConstant$\}$ then
3. return $(\{v\}, \text{PRs})$;
4. $(I, \text{PRs}) := \text{GenPR}(\text{extract from node}(v, \text{‘input’}), \text{PRs})$;
5. $(c, \text{PRs}) := \text{GenPR}(\text{extract from node}(v, \text{‘caller’}), \text{PRs})$;
6. $(O, \text{PRs}) := \text{GenPR}(\text{extract from node}(v, \text{‘output’}), \text{PRs})$;
7. $\text{PRs} := \text{PRs} \cup \text{PR}(I, c, p, O)$;
8. return $(O, \text{PRs})$;

Figure 5: WIR generation algorithm

The returned WIR variables may be used as input/caller/output of other PRs. To this end, GenPR initially obtains the operation from the attributes of the AST node (line 1). If the AST node is a literal or constant, it returns the current PRs (line 3). Otherwise, to obtain each of input variables $I$, potential caller $c$, and potential derived variables $O$, GenPR recursively calls itself (lines 4-6). Once all the required variables for a PR are found, a new PR is constructed and added to the set of so far generated PRs (line 7). It finally returns the output of the last generated PR as well as the updated set of PRs (line 8).

During this process, the procedure GenPR extracts the input and output set and a potential caller variable for each PR (see definition of PR in Section 4.1). To this end, it investigates the AST node attributes to instantiate these variables by invoking the extract from node procedure which we summarize next. The procedure takes as input an AST node and a literal parameter denoting the information requested (input, output, caller, operation), and consults the abstract grammar of AST nodes to return the requested information for the given node. For example, when processing the Assign node of the AST in Figure 4, the procedure identifies Assign.value as input, Assign as operation, and Assign.targets as output. It also sets the caller as $\emptyset$, as the procedure does not return a caller for the AST node type Assign.

Complexity. Each AST edge is visited at most once during the WIR generation. Thus, for a Python script whose corresponding AST contains $N$ edges, GenWIR has $O(N)$ complexity. More specifically, the extract from node procedure requires constant time since for each visited AST node, it only traverses a bounded number of neighbors (see the Python grammar). In addition, the number of nodes/edges in a WIR is also bounded by the number of nodes/edges in its corresponding AST since for each node/edge in the AST, we may generate a corresponding node/edge in WIR.

5. MACHINE LEARNING ANALYZER

The generated WIRs capture the dependencies among the variables and operations in a script. Nevertheless, WIRs alone do not provide semantic information such as the role of a variable in the script (e.g., ML model, features) or the type of each object (e.g., CSV file, DataFrame). To support provenance queries, semantic information about variables should be associated to the WIRs. Such information, in turn, identifies critical variables such as hyperparameters, models, and metrics for ML applications.

Finding the role of each variable in a WIR is a challenging task for multiple reasons: (1) One cannot accurately deduce the role/type of input and output of each operation by only looking at the name of the operation as different ML libraries may use the same name for different tasks; (2) Even in the same library, an operation may accept different numbers of inputs or provide different outputs. For example, in the sklearn library, the function fit accepts a single input when creating a clustering model but two inputs when generating a classification/regression model; (3) The type of the caller object might also affect the behavior of the operation. For instance, in sklearn, invocation of the fit function by a Random Forest classifier creates a model but calling it via LabelEncoder does not; (4) The APIs of many libraries are not yet stable and change as these evolve; (5) Some variables are even harder to semantically annotate because of lack of concrete APIs associated with them. For example, identifying when a variable represents features is challenging since typically there is no specific API to load the training dataset. Instead, the common practice is to use generic functions such as read_csv to load training data similarly to other data sources.

A semantic annotation framework to be usable across various data science scripts must be: (1) compatible with the various ML libraries (sklearn, xgboost), version, and modules (e.g., ensemble, svm). For each unique API in a library, the KB captures the corresponding library, module, caller type, and the operation name (e.g., train_test_split from the model_selection module of the sklearn library or read_csv from the Pandas library). For each potential input of an operation, the KB stores its role (features, labels, hyperparameter, and metric) and its data type (DataFrame, array, CSV file). Similarly, the KB contains semantic information about the outputs of the various operations.

Example 5: Table 1 shows three tuples in our KB. These are a subset of tuples that are utilized by the annotation algorithm to identify the variables that correspond to models and features in the script of Figure 1. The second tuple shows that when the operation fit is called via a model constructed by catboost library, its first and second input are features and labels, respectively. It also accepts the valida-
Table 1: Example of facts in Vamsa knowledge base

| Library | Module           | Caller | API_Name          | Inputs                  | Outputs              |
|---------|------------------|--------|-------------------|-------------------------|----------------------|
| catboost| NULL             | NULL   | CatBoostClassifier| eval_metrics: hyperparameter | model               |
| catboost| NULL             | model  | fit               | features, labels         | trained model        |
| sklearn | model_selection  | NULL   | train_test_split  | features, labels         | validation features  |

Algorithm Annotation

Input: WIR $G$ and knowledge base $KB$.
Output: Annotated WIR $G^+$.
1. Find the import process nodes in $G$ as the seed set $S$.
2. for each $v_i \in S$ do
3. Extract library $L$ and module $L'$.
4. Starting from $v_i$, follow a DFS forward traversal on PRs:
   1. for each seen $PR = (I, c, p, O)$ do
      1. Obtain annotation of $v_i \in I$ and $v_o \in O$
         by invoking $KB(L, L', c, p)$
   7. for each annotated $v_i \in I$ do
   8. Starting from $v_i$, follow a DFS backward traversal on PRs:
      1. for each seen $PR = (I, c, p, O)$ do
         1. Obtain annotation of $v_i \in I$
         by invoking $KB(O, p)$
   11. return $G^+$;

Figure 6: Annotation algorithm
A core component of the algorithm is the traversal set. There are various operations that take features (or labels) and an operation parameter. As an example, the function drop in the Pandas library is used to remove rows when the parameter axis is set to 0, and remove columns when the value of the parameter is 1. The parameters of the operations are also captured in the WIR, and thus we can easily verify their values. The condition that needs to be checked to verify whether a particular invocation of an operation is used to remove columns is also added into the KB along with the operation.

We query this table by invoking \( \text{KB}_C(p) \) where \( p \) is the name of the operation. The query returns \( \emptyset \) if there is no matching entry in the KB. However, if the operation matches to one of the entries in the table, the query returns the following output: (1) condition: the condition associated with the operation as mentioned above (if any); 2) column exclusion: whether the operation can be used for column exclusion; and 3) traversal rule: a description on how to start a backward traversal from the node’s input edges in order to identify a set/range of indices/column names.

Example 7: Figure 7 is another fraction of WIR that was generated from line 5 of the script in Figure 1 that includes a Subscript operation. The statement in line 5 keeps all the rows but only includes the columns from index 3 to the last index in the dataset. One can find the set of included columns by traversing backward the nodes following the input edge of the Subscript operation and reaching the constant values connected with the Slice operations. The traversal rule associated with the Subscript operation shows that the input edge of this node must be followed in a backward manner to eventually reach the selected columns. Note that this is the case for all WIRs that contain this operation.

Similarly, consider the drop operation in Figure 3. This operation is related to feature selection since its caller (train_df) was annotated as features and it operates at the level of columns (the condition axis = 1 is satisfied by this invocation of the operation). To find the columns that were dropped, we again need to follow the input edge of drop backwards until we reach the constants ‘Target’ and ‘SSN’.

Our provenance tracking algorithm is illustrated in Figure 8. The algorithm takes as input the annotated WIR \( G^+ \) and the KB, and returns two column sets: the columns that from which features/labels were explicitly derived (inclusion set \( C^+ \)) and (2) the columns that are explicitly excluded from the set of features/labels (exclusion set \( C^- \)). The algorithm scans each PR to find the ones with a variable that has been annotated as features (or labels) and an operation which can potentially be used for feature (or label) selection based on the information stored in the KB (line 2-3).

A core component of the algorithm is the GuideEval operator (shown in Figure 5) that starts a guided traversal of the WIR based on the information in the KB.

For each of the selected PR, the GuideEval operator queries the KB and obtains the corresponding condition.
**Algorithm PTracker**

*Input:* Annotated WIR $G^+$, knowledge base KB.
*Output:* Column inclusion set $C^+$, column exclusion set $C^−$.
1. $C^+ := φ; C^− := φ$
2. for each PR in PRs do
3. if it has a variable that was annotated as features or labels
and KB$_C$(p) ≠ φ
4. GuideEval(PR, $G^+$, KB, $C^+$, $C^−$);
5. return $C^+$, $C^−$;

**Operator GuideEval(PR, $G^+$, KB, $C^+$, $C^−$)**

*Input:* Visited PR, annotated WIR $G^+$, knowledge base KB, column inclusion set $C^+$, column exclusion set $C^−$.
*Output:* Updated $C^+$, $C^−$.
1. condition, column_exclusion, traversal_rule = KB$_C$(p);
2. if exists condition and it is False then return φ
3. if PR has constant inputs cnst then
4. if column_exclusion = True then
5. $C^− := C^− ∪ cnst$;
6. else $C^+ := C^+ ∪ cnst$;
7. return $C^+$, $C^−$;
8. Obtain new PR on $G^+$ based on traversal_rule;
9. GuideEval(PR, $G^+$, KB, $C^+$, $C^−$);

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**Figure 8: Provenance tracking algorithm**

column_exclusion flag, and traversal_rule (line 1). If a condition exists but it is not matched by the particular operation, we can deduce that the operation was not used for feature (or label) selection and return without further action (line 2). Otherwise, the operator checks if this PR contains constant values in its input set (line 3). If so, it incorporates the discovered constant values/range of column indices into the inclusion/exclusion sets based on the column_exclusion flag. In case the PR does not directly contain the columns, the GuideEval operator follows the traversal_rule to obtain a new PR on $G^+$ (line 8) that needs to be evaluated. It then calls the GuideEval operator again for this PR (line 9).

**Example 8:** Continuing example [1], the provenance tracking algorithm finds the drop operation with a caller that was annotated as features (Figure [3]) and thus invokes the GuideEval operator. Since the corresponding path query is satisfied (aka, axis = 1), we know that the operation is used for feature selection and in particular feature exclusion (based on the information in the KB). Thus, the algorithm follows the traversal rule to perform a backward traversal from its the operation’s input edge until it finds the constants ‘Target’, and ‘SSN’. These two columns are then added to the exclusion set.

When the feature tracking algorithm finds the Subscript operation (Figure [7]) in the annotated WIR, it invokes the GuideEval operator again. Note that the Subscript operation does not have an associated path query in KB. Thus, the GuideEval operator only obtains the corresponding traversal rule from the KB and initiates a backward traversal starting from the input edge of the Subscript operation. A similar process is performed when the GuideEval operator visits ExtSlice and Slice nodes. Using the traversal rule associated with the Slice operation in the KB, the algorithm looks for a range of columns with lower bound (respectively upper bound) that can be found by traversing the appropriate input edges of the Slice node (see Figure [7]).

**Complexity Analysis.** Let $V_T \subseteq V$ be the set of variables that were annotated as features or labels. Let $|P_m|$ be the maximum number of operations that are directly connected to a variable in $V_T$. The provenance tracker algorithm scans all the PRs to find the set $V_T$ and evaluates, in constant time, whether the corresponding operations are related to feature/label selection. If an operation is indeed related to feature selection, the algorithm follows the traversal rule which in the worst case, visits all the edges of $G^+$. The algorithm, thus, has $O(|V_T| |P_m| |E|)$ complexity. Note that in practice $|V_T| \ll |V|$.

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**Table 2: Output of pre-processing pipeline**

| Dataset | Error-free & Python 3 compatible NTBK$_2$/Kaggle$_2$ | Scripts with selected ML libraries NTBK$_3$/Kaggle$_3$ |
|---------|-----------------------------------------------------|-------------------------------------------------|
| NTBK (807K) | 447K | 28.9K |
| Kaggle (4.8K) | 4.2K | 1.2K |

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**7. EXPERIMENTAL EVALUATION**

In this section, we evaluate Vamsa on a large set of Python scripts and provide an analysis of our experimental results. Our experiments are designed to answer the following questions: (1) What is the accuracy of Vamsa in identifying the features used to train ML models?; (2) How often is Vamsa able to extract provenance information (coverage) from a data science script?; (3) What is the latency of Vamsa?

### 7.1 Experimental Settings

**Datasets.** To evaluate Vamsa on a variety of data science scripts, we downloaded a large set of publicly available Python scripts from two different data sources: (1) a large-scale corpus that consists of 1.2M Python notebooks published in 2017 that was crawled from Github [5] (NTBK dataset). From this corpus, we excluded the notebooks that do not include any import statement resulting in a corpus of 807K scripts, (2) a set of 4.8K Python scripts that we downloaded via the public Kaggle API[7](Kaggle dataset).

**Dataset pre-processing pipeline.** Real-world scripts may have syntax errors or may not be compatible with Python 3 (which is the version of Python that Vamsa’s implementation currently targets). Moreover, not all of them train machine learning models. For these reasons, we created a data pre-processing pipeline that applies various filters to the scripts in order to capture only those that are relevant to the ML provenance tracking problem. The pipeline is invoked on both the NTBK and Kaggle dataset.

We now show how the pipeline works using the NTBK dataset as an example. The pipeline takes as input the 807K Python scripts and prunes the scripts for which we cannot generate the corresponding abstract syntax tree due to syntax errors, exceptions triggered by Python’s AST generation module or incompatibility with Python 3. The resulting dataset is denoted as NTBK$_2$. The pipeline then prunes the scripts that are not importing any of the following ML frameworks: scikit-learn, XGBoost [2], and LightGBM as well as the scripts that do not invoke any training-related operations from these frameworks (e.g., fit, create, and train).

[7]https://github.com/Kaggle/kaggle-api
Table 3: Accuracy of Vamsa on the labeled datasets

| Dataset | Column Exclusion | Column Inclusion | Annotation Precision |
|---------|------------------|------------------|----------------------|
|         | Precision | Recall | Jaccard Coeff. | Precision | Recall | Jaccard Coeff. | Model | Train Dataset |
| Kaggle5 | 93.82%   | 94.97%   | 92.78% | 87.37%   | 89.22%   | 87.49% | 100% | 99.33% |
| NTBK5   | 98.59%   | 98.25%   | 97.94% | 90.21%   | 95.24%   | 90.14% | 100% | 98.66% |

Table 4: Vamsa coverage in large-scale evaluation

| Dataset | ML Analyzer Coverage | Prov. Tracker Coverage |
|---------|----------------------|------------------------|
| Kaggle5 | 94.92% | 94.92% |
| NTBK5   | 88.52% | 77.81% |

Table 2 shows more information about the NTBK and Kaggle dataset after the pipeline has been applied to them.

**Experimental methodology.** A challenge when evaluating Vamsa with such large-scale corpora is to determine the correctness of the output. Unfortunately, due to the novel nature of ML provenance tracking, there is no public benchmark available. The brute force approach would be to manually go over the corpus and determine the relationships between ML models and data sources so that we can evaluate Vamsa’s output. Since this is not feasible at the scale we are operating, we decided to perform two classes of experiments. First, we select a small subset of scripts for which we manually extract the provenance information (ground truth) and evaluate the accuracy of Vamsa on those. The second class of experiments is performed on the large corpus. The goal is to evaluate the coverage of the system, defined as how often Vamsa extracts the provenance information. We also evaluate both component-level and end-to-end system performance.

**Hardware and software configuration.** We conducted our experiments on a Linux machine powered by an Intel 2.30 GHz CPU with 8 GB of memory. For all the experiments we used Python 3.7.2. We manually populated our knowledge base with the APIs from scikit-learn, XGBoost, LightGBM, and Pandas.

7.2 Experiments with Labeled Datasets

These experiments evaluate the accuracy of Vamsa on a set of Python scripts for which we have manually extracted the relationship between data sources and ML models. From each of the Kaggle and NTBK5 datasets, we randomly selected 150 scripts, ensuring that Vamsa can produce output for all the selected scripts. We evaluate the accuracy of Vamsa on both column exclusion and column inclusion using three metrics: precision, recall and Jaccard coefficient. The precision shows the proportion of discovered included/excluded columns that were truly included/excluded in the feature selection process. The recall shows the proportion of the true included/excluded columns that were discovered by Vamsa. The Jaccard coefficient evaluates the similarity of the two sets. The higher the values of these metrics are, the better the accuracy of Vamsa is. Given a script, the ground truth consists of two sets, namely the included columns $C^+_T$ and excluded columns $C^-_T$. The metrics for column exclusion are defined as follows:

\[
\text{Precision} = \frac{|C^- \cap C^+_T|}{|C^-|} \quad (1)
\]

\[
\text{Recall} = \frac{|C^- \cap C^+_T|}{|C^-_T|} \quad (2)
\]

\[
\text{Jaccard Coefficient} = \frac{|C^- \cap C^+_T|}{|C^- \cup C^+_T|} \quad (3)
\]

The metrics for column inclusion are similar but take into account the column inclusion set that Vamsa produces as well as the included columns in the ground truth.

Additionally, we investigate in more detail, how often Vamsa correctly identifies which variables correspond to ML models and which to training datasets as this is a prerequisite for correctly identifying the features/labels. To this end, we also report results that show the precision of the annotation phase (for both models and training datasets). The annotation precision shows the proportion of discovered models/training datasets that were true models/training datasets according to the manual labeling we did on the two datasets. Table 2 shows the results on the two datasets. For each metric, we report the average values obtained over the 150 scripts of the dataset. As shown in the table, Vamsa achieves high precision and recall values for all the tasks evaluated. Overall, we can make the following observations:

1. When Vamsa identifies a model, its training dataset, and the corresponding features, the output is highly reliable.

2. Vamsa reported models 100% accurately and made a few mistakes in detecting their training datasets. We further investigated these scripts and found that the data scientists appended the testing data to the training data in order to perform global value transformations. The merged test data then got separated via a slicing operation immediately before training. Vamsa’s annotation algorithm was not able to follow this operation, i.e. merge followed by split, and mistakenly identified the testing dataset as the training dataset.

3. Vamsa detects column exclusion sets slightly better than column inclusion ones. This is because, for column exclusion, data scientists typically use a set of specific APIs such as drop and pop from Pandas, or del keyword, which can be tracked more easily.
7.3 Large-scale Experiments

In these experiments, we use a large corpus of Python scripts both from the NTBK and Kaggle datasets extracted from the pre-processing pipeline. The goal is to evaluate the coverage of various components of Vamsa (Derivation Extractor, ML Analyzer, Provenance Tracker) as well as the performance/efficiency of the system. We also present a detailed analysis of the cases where Vamsa was not able to produce an answer.

Derivation Extractor. First, we evaluate the coverage of Vamsa on generating the workflow intermediate representation for our scripts. Note that the Derivation Extractor is a standalone component that does not rely on the KB to produce the WIR. For this reason, we perform our experiment using two large datasets NTBK2 (447K scripts) and Kaggle2 (4.2K scripts) that import multiple ML libraries.

Our results show that Vamsa successfully generates the WIR for 95.70% of the scripts in the Kaggle2 dataset and 89.27% of the scripts in the NTBK2 dataset. The few cases where Vamsa is not able to produce a WIR are mainly due to Vamsa’s current implementation. In particular, we have not yet covered certain constructs in the Python grammar such as DictComp, SetComp, and JoinedStr. However, we’d like to note that incorporating these constructs in Vamsa is solely a matter of extending the implementation and does not require any change in Vamsa’s design or architecture.

ML Analyzer. The goal of this experiment is to investigate the coverage of the ML Analyzer and in particular, how often the annotation algorithm identifies ML models and training datasets. In this evaluation, we use the NTBK3 (28.9K scripts) and Kaggle3 (1.2K scripts) datasets.

Table 4 shows the percentage of the cases where the ML Analyzer can annotate at least one variable as a model and one other variable as a training dataset. As shown in the table, Vamsa can report model and training datasets for 94.62% and 82.91% of the scripts in the Kaggle3 dataset.

The coverage is a bit lower for the NTBK3 dataset.

To better understand the cases where Vamsa was not able to perform the annotation, we first investigated the cases that the ML Analyzer could not find a model. We identified the following reasons for the failure: 1) Some scripts called APIs commonly used for training models, such as e.g., fit, to perform other operations such as feature extraction. In these cases, the ML Analyzer correctly did not report any model. 2) In a few scripts, the statements used to train a model were commented out. This was not detected by our pre-processing pipeline and thus these scripts were falsely included in the final dataset. 3) Some scripts imported modules using the * notation. In these cases, Vamsa could not relate the import statement to the API calls. 4) In a few other scripts, the data scientist imported a module with an alias name and used the alias when invoking the APIs. Vamsa’s implementation does not currently cover such cases. We are continuously investigating these issues and improving Vamsa’s implementation.

We have also explored the cases where the ML Analyzer could not find a training dataset. We found that: 1) In some scripts, hard-coded data e.g., a large numpy array was used as the training data, and 2) Some APIs are not presented in our KB and thus the annotation algorithm is not able to perform back propagation. However, we’d like to point out that these cases would be covered by extending out KB to include more APIs. We note that allowing users to increase coverage by enhancing the KB as needed was one of the major requirements behind Vamsa’s design.

Provenance Tracker. We evaluate the Provenance Tracker component on the NTBK3 and Kaggle3 datasets. Table 4 shows the percentage of the cases where the Provenance Tracker can identify at least one set of features. Note that the Provenance Tracker is invoked only if the ML Analyzer can identify a model and its corresponding training dataset. We thus expect the coverage of this component to be bounded by the coverage of the ML Analyzer.

As shown in Table 4, Vamsa reports a non-empty column set for 80.61% of the scripts in Kaggle3 dataset and 70.20% of the scripts in the NTBK3 dataset. We have also analyzed the cases that Vamsa could find both a ML model and a training dataset but did not discover the column set. The main reasons for this behavior are the following: 1) In some scripts, the columns have not been selected explicitly but based on a condition on their values (e.g., a column is in the feature set if it contains at least N non-zero values.). (2) Similar to the ML Analyzer, some scripts required new rules to be added into the KB for the Provenance Tracker to operate correctly, and (3) Some scripts did not include any feature selection operations and thus Vamsa did not produce any output.

7.4 Performance Experiments

In this experiment, we evaluate the efficiency of each component of Vamsa as well as the end-to-end latency. To this end, we use a subset of the datasets on which Vamsa operates end-to-end successfully. We call these datasets NTBK4 (26.3K scripts) and Kaggle4 (1K scripts).

Breaking down the latency. We now evaluate the performance of the Derivation Extraction, ML Analyzer, and Provenance Tracker, as well as the end-to-end latency. Figure 9 shows the results. We observe that the time spent by each component is negligible on both datasets and on average is in the order of milliseconds. Furthermore, the most time is spent on derivation extraction in comparison to the other components. Breaking down the derivation extractor tasks to AST generation, PR generation, and WIR composition, we observed that most of the time is spent in AST generation and WIR composition. In particular, our analysis shows that for the Kaggle4 dataset, AST generation takes 106 milliseconds (msecs), PR generation takes 13 msecs and WIR composition takes 121 msecs. The corresponding numbers for the NTBK4 dataset are: 112 msecs, 11 msecs and 129 msecs.
Performance of Vamsa varying the lines of code. We further evaluate the performance of each component and the end-to-end performance as the lines of code in the script vary. Figure 10(a) and Figure 10(b) show the average latency of the components as the script size varies for both our datasets. We see that increasing the number of lines of code in a Python script naturally increases the latency of all Vamsa components. However, Vamsa can produce output within 9 seconds on a script consisting of 850 lines of code (see Figure 10(a)). Similarly, Vamsa requires 64 seconds to collect the provenance information on a script with 1.5K lines of code (see Figure 10(b)).

Size of intermediate representation. To gain more insight about the datasets, we evaluate the size of generated WIRs. Figure 11 shows the average size of WIR nodes and edges along with the average lines of code in the script. We see on average for each line of code, 8.70 nodes and 6.11 edges were created in a WIR.

8. RELATED WORK

We describe relevant related work from three areas: model management systems, provenance in databases, and workflow management systems.

Model management systems. There has been emerging interest in developing machine learning life-cycle management systems [55, 26, 64, 41, 56, 40, 63]. ModelDB [64] was one of the first open-sourced model management systems. It focused on storing trained models and their results to enable visual exploration and querying of metadata and artifacts (e.g., hyperparameters and accuracy metrics). ModelDB requires users to change their scripts to comply with their API for logging (e.g., adding “sync” to function calls), and it works for a specific set of libraries. ModelHub [41] aimed to store model weights across different versions with a focus on deep learning. It is a more fine-grained versioning system for the ML artifacts than other general-purpose systems such as Git. ModelHub enables querying on hyperparameters, accuracy, and information loss during training phases. Amazons ML experiments system [56] focuses on tracking metadata and provenance of ML experimentation data. This system automated the provenance extraction for SparkML [39] and scikit-learn [46] pipelines whenever a logical abstraction of operations (e.g., estimators/transformers) are available. ProvDB [40] proposed a graph data model and two graph query operators to store and query the provenance in data science projects. It works by ingesting the provenance via shell commands similar to versioning systems such as Git. The major focus of ProvDB is to efficiently store and query the ML provenance data. Finally, to enable the model diagnosis, Mistique [63] was developed to store model intermediates that are produced in different stages of traditional ML pipelines or hidden representations in deep learning (i.e., neuron activations produced by different layers in a neural network).

In contrast to this line of model management systems, (1) Vamsa does not require developers to modify their code, (2) Vamsa can operate on top of any library as long as it is included in the KB, (3) by focusing on the process of provenance extraction rather than efficiently storing the captured data, Vamsa is complementary to systems such as ProvDB [40] and Mistique [63], and (4) none of the previous systems aimed to track features that are used to train ML models.

Provenance in databases. Capturing lineage or provenance has been studied extensively for databases (e.g., surveys [60, 51, 20, 17]). Data provenance typically describes where data came from, why an output record was produced [18], and how it was derived [27]. Provenance can be captured at different granularities and in various levels of detail [40]. It can be as coarse-grain as datasets, files, and
their dependencies [14] or fine-grain including dependencies between input, intermediate, and output records [20, 35, 51]. The value of provenance is most exaggerated by the applications that can support including, but not limited to, explanations [44, 63, 24]; interactive visualizations [51, 50, 52, 30]; verification and recomputation when data sources are outdated or not reliable [32]; debugging [33, 36, 21]; data integration [22]; auditing and compliance [4]; and security [19, 35]. Finally, central to how provenance is utilized across domains is the task of provenance querying, a task complementary to the task of provenance capture. More specifically, provenance querying includes several subproblems involving the construction of provenance querying languages [35], provenance browsers [52, 30], and efficient indexing schemes for captured provenance to streamline provenance queries [33, 51, 53].

In contrast to this line of work, Vamsa is specifically designed to automatically capture provenance in data science scripts written in Python. Captured provenance in Vamsa can be used to answer queries such as “Which datasets were used to train/test a model?”, “What libraries have been used in this script?”, and “What type of ML model was trained?”. As such, the granularity of the provenance is at the level of variables and the operations that utilize them to derive output variables. The operations can be API calls (read_csv(·) from Pandas library), accessing objects properties (·.values), and user-defined functions including their implementation. In other terms, the way data science logic is specified in Python has little to no similarities with how queries are structured in databases. As such, the task of ML provenance tracking requires provenance capture techniques tailored to the intrinsic semantics of how data science logic is implemented in Python. Nevertheless, however, the identified provenance information from Vamsa can be stored and used by upstream applications, through provenance querying systems, in a similar fashion to how provenance is stored and used out of database workloads.

**Workflow management systems.** Workflows are widely used in scientific applications [17, 29, 28, 12, 20, 11] where scientists glue various tasks together and each task may take input data from previous tasks [25]. Workflow management systems aid in collecting, managing, and analyzing the provenance information to enable sharing of experiments and ensure their reproducibility [25]. Closer to our work are Starflow [16, 15], noWorkflow [43, 48], and YesWorkflow [35] systems. Starflow [16, 15] statically analyzes a Python program to build provenance traces at the level of functions for a Python script. However, it does not extract the dependencies inside of the functions. noWorkflow also transparently captures the control flow information and library dependencies in the scripts. It extracts the provenance in three levels of definition, deployment, and execution. In order to monitor the evolution of scripts, it also uses abstract syntax trees (AST) to discover user-defined functions and their arguments [45]. While Starflow [16] and YesWorkflow [35] require modifications to the users’ script, noWorkflow handles unmodified programs.

Our work differs from these works as follows: (1) By focusing on data science scripts, we are able to capture more relevant provenance information to our needs such as finding trained models, hyperparameters, datasets, and features; (2) noWorkflow systems also generate a dependency graph among the variables. However, the workflow is not statically generated and the program needs to be executed. This is not always possible due to external dependencies on both the datasets and the various imported libraries. Indeed, AST was not utilized to generate a workflow graph but to detect the user-defined functions and their arguments; (3) As opposed to YesWorkflow and Starflow, Vamsa does not require users to modify their code e.g., adding tags and decorators to the function and variable definitions. To this end, it uses the KB (Section 5.1) to automatically extract the relevant provenance information from the script.

### 9. CONCLUSIONS AND FUTURE WORK

ML has become a ubiquitous and integral technology across the stacks of enterprise-grade applications. Unfortunately, the management of machine learning logic is still in its infancy. In this direction, in this paper, we introduced the problem of ML provenance tracking with the goal to obtain connections between data sources and features of ML models—a fundamental type of provenance information that enables multiple upstream management applications including, but not limited to, compliance; security; model maintenance; and model debugging. Our proposed system, Vamsa, and our experimental evaluation show that it is indeed possible to recover this type of provenance with a very high precision and recall across large corpora of ML scripts authored imperatively in Python—even in the hard setting of static analysis time without availability of runtime information. Finally, we believe that the techniques and components of Vamsa (e.g., the KB and the framework for forward and backward traversals) are broadly applicable beyond the design of Vamsa and the scope of our work.

There are many areas for future work to explore both in the space of ML provenance tracking and the general space of automated management of ML pipelines. First, incorporating runtime information, if available, can better help us identify connections between data sources and ML models (e.g., access to data sources can let us provide the exact set of excluded features). Second, and in-line with the first line of future work, identifying finer-grained provenance information between data sources and ML models (e.g., which partitions of a data source were used for training a model) can better assist upstream applications (e.g., model debugging and compliance). Such type of information can be obtained either statically (e.g., identifying filters in Python scripts) or dynamically (e.g., tracing the inputs to ML models by inspecting program stacks and data flows at runtime). Finally, automatically populating or decreasing the manual effort for the population of the knowledge base (e.g., features that have not changed across library releases can share the same annotations) are technically challenging problems, yet provide an integral technology for the management of imperatively specified ML pipelines.

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