# A Static Analysis Framework for Data Science Notebooks

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## ABSTRACT

Notebooks provide an interactive environment for programmers to develop code, analyse data and inject interleaved visualisations in a single environment. Despite their flexibility, a major pitfall that data scientists encounter is unexpected behaviour caused by the unique out-of-order execution model of notebooks. As a result, data scientists face various challenges ranging from notebook correctness, reproducibility and cleaning. In this paper, we propose a framework that performs static analysis on notebooks, incorporating their unique execution semantics. Our framework is general in the sense that it accommodates a wide range of analyses, useful for various notebook use cases. We have instantiated our framework on a diverse set of analyses and have evaluated them on 2211 real world notebooks. Our evaluation demonstrates that the vast majority (98.7%) of notebooks can be analysed in less than a second, well within the time frame required by interactive notebook clients.

## CCS CONCEPTS

• **Theory of computation** → **Program analysis**; • **Software and its engineering** → **Integrated and visual development environments**.

## KEYWORDS

static analysis, notebooks, data science

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## 1 INTRODUCTION

Notebooks have become an increasingly popular development environment for data science. In 2020, JetBrains reported 10M notebooks on GitHub [1], an increase from 200K in 2015 [5]. Notebooks provide a dynamic read-eval-print-loop (REPL) experience where developers can rapidly prototype code while interleaving data visualizations including graphs, textual descriptions, tables etc. A notable peculiarity of notebooks is that the program i.e., notebook, is divided into non-scope inducing blocks of code called *cells*. Cells can be added, edited and deleted on demand by the user. Most importantly, cells, regardless of their order in the notebook, can be executed (and re-executed) by the user in *any given sequence*. This provides a level of incrementalism that improves productivity and flexibility. At the same time, such execution semantics make notebook behaviour notoriously difficult to predict and reproduce. This observation is highlight in [17]. Here the difficulty of reproducing notebook results is investigated, concluding that from a large set of notebooks, only 25% of notebooks could be executed without an error and less than 5% were trivially reproducible. Moreover, in [18] it was observed that there is an abundance of code smells and bugs in real world notebooks. Thus, the authors of this study argue for more code analysis tooling to improve the quality of notebooks. To understand the source of this phenomena, consider the example below.

*Example 1.1 (Motivating Example).* Consider the notebook in Figure 1 comprising of 5 cells. Each numbered from 1 to 5, indicated by the left hand side number in square brackets. In a script, the execution proceeds as if the cells were merged into a single cell and each statement is executed as dictated by the regular program control flow i.e., statements in *cell 1* are executed sequentially, followed by *cell 2*, *cell 3* and so on. However, in notebooks any given cell can be executed at any given time by the user. This produces a potentially infinite space of possible execution paths due to a lack of constraints on the order in which cells can be executed in. In the example notebook, *cell 1* and *cell 3* read data from a file into a data frame. In *cell 2* data in variable `d` is normalized and in *cell 4* the data is split into test and training segments. In *cell 5* the model is trained, tested and assessed for accuracy. It is apparent that several legitimate executions exist in this notebook. For example, one could start by executing *cell 3*, *cell 4* and *cell 5*. Another execution sequence is *cell 1*, followed by *cell 2*, *cell 4* and *cell 5*. Note, it is common to have several alternate executions in a notebook for reasons of experimentation etc.

Now consider the following scenario: suppose the user executes the sequence of cells 1, 2, 4, and 5. While this may not seem particularly ominous, it will in fact result in a data leak bug [12] as the function in *cell 2* normalizes the data and yet *cell 4* splits the data in to train and test data *after* the normalization, thus resulting in a what is know in data science as a data leak. Now, lets suppose the user, after some investigation, identifies this problem. They re-execute cell 1, skipping cell 2 (to avoid normalization) and execute *cell 4* and *cell 5*. The user may be perplexed as the same issue re-occurs. The problem is that the user executed *cell 4* which referred to variable $x$, which was previously computed by *cell 2*, resulting the using an old (or stale) value. One can see how a user can quickly get into a confusing situation, even for this relatively simple notebook[1].

Each of the bugs above demonstrate the ease at which a seemingly simple data science program can result in unforeseen behaviour in a notebook environment. Moreover, establishing the root cause is similarity difficult without engaging in time consuming post-mortem debugging that cannot prevent future bugs, or generalize the cause of the bug. On the other hand, if we were to restrict the notebook execution semantics, we would be removing precisely the flexibility that has made notebooks so popular in the last few years.

In this paper, we argue for the use of static analysis as an ante-mortem debugging mechanism. Our technique co-exists with the unique notebook execution flexibility, and yet reducing errors and debugging efforts by warning users *ahead of time* of hypothetical erroneous and safe actions. Due to the semantics of notebooks, standard static analysis tools cannot be directly applied, and to the best of our knowledge general static analyzers targeting notebooks have not been proposed in the literature. Moreover, the interactive nature of notebooks requires analyzers that are able to produce feedback within a second [4] to not disrupt the flow of the user experience. To this end, we propose NBLyzer, a static analysis framework that provides notebook users the ability to perform a *what-if* static analysis on given notebook actions. Notebook actions constitute opening a notebook, code changes, cell executions, cell creation, deletion etc. Our framework soundly reports potential issues that may occur for a given action within the time bounds required for users not to notice a disruption. For instance, consider the notebook in Example 1.1, as shown in Figure 1b, our framework will warn the user that the event of executing *cell 1* can lead to a data leakage by executing cells *2, 4* and *5* in milliseconds. Moreover, as shown in Figure 1c, it will warn in milliseconds that the event of executing *cell 1* can result in a stale state if *cell 4* is executed before *cell 2*. Conversely, our framework can recommend the execution of the sequence*cell 3, 4, 5* to be safe to execute after *cell 1* is executed. Our framework supports a wide range of static analyses[2]. In Section 4 we present several analyses implemented in NBLyzer, particularly targeting data science notebooks. Using these analyses, we facilitate the automation of several other important notebook development use cases including notebook correctness, notebook debugging, notebook reproducibility, notebook auditing, and notebook cleaning.

NBLyzer employs the theory of Abstract Interpretation [6] to perform intra-cell static analyses i.e., on individual cells, and thus in-cell termination is guaranteed for the price of an over-approximate analysis result. The key idea is to over-approximate the notebook semantics and computational state $\sigma$ and instead produce an abstract state $\sigma^\sharp$ which comprises of an element of an *abstract domain* that encodes the analysis property of interest. When analyses are triggered by an event, an inter-cell analysis is performed by propagating the analyses results (abstract state) to valid successor cells in the notebook. To select valid successors, we introduce the notion of *cell propagation dependencies*, which prunes away unnecessary sequences of cell executions on-the-fly, parametrized by the current abstract state. In this way, the abstract state is propagated efficiently while ensuring soundness and termination via both an intra and inter-cell termination criteria. We evaluate NBLyzer on 2211 real world notebooks and several instantiated analyses to demonstrate its utility and scalability. NBLyzer is able to analyze 98.7% of notebooks within a second. Overall, we claim the following contributions:

(1) A novel static analysis framework specifically for notebooks
(2) Several instantiated industrial static analyses implemented in NBLyzer, including a novel data leakage analysis that to the best of our knowledge, has not been presented before in the literature or implemented in any static analyzer.
(3) An extensive performance evaluation of NBLyzer that demonstrates its adequate performance based on [4] to perform only-the-fly static analysis within the notebook environment without degrading the user notebook experience.

## 2 OVERVIEW

In this section we give an overview of the NBLyzer static analysis framework for notebooks.

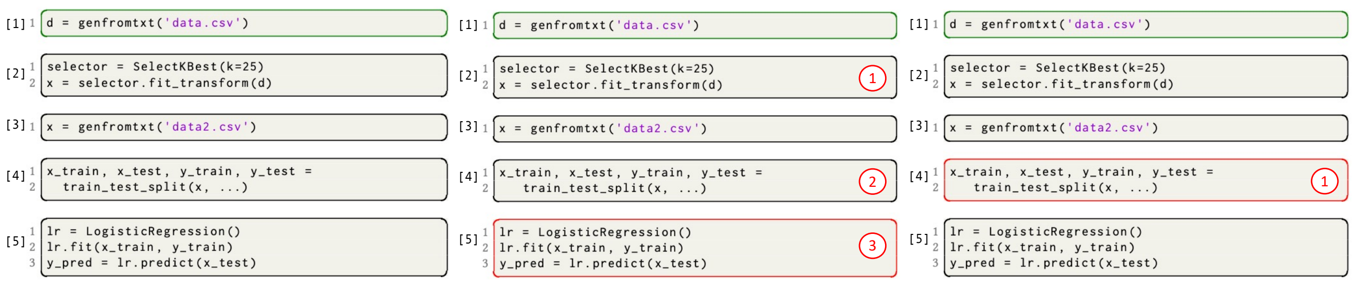
The high-level operation of the framework is depicted in Figure 2. A user performs actions on a notebook such as opening notebooks, adding cells, changing cells, executing cells, deleting cells among others. For each event, the user may want to initiate a what-if analysis, essentially asking NBLyzer *what can occur if I execute cell 1?* This allows the user to ahead of time avoid putting the notebook in a state that will lead to an error. Conversely, the user may ask NBLyzer *What executions are safe if I execute cell 1?* This allows the user to choose from a set of possible safe execution paths. Other examples of what-if questions include *Which cells will become isolated if I rename d to x cell 2?*, *Which cells will become redundant in the notebook I opened?* etc.

Each of these what-if questions can be useful for use cases including reproducibility, security auditing, notebook cleaning and simplification, debugging and education, among others.

From a systems perspective, a what-if analysis is a notebook event that is associated/configured to a set of analyses. For example, asking about notebook safety will entail a certain set of analyses, and asking about notebook cleanliness will entail a distinct set of analyses. NBLyzer therefore intercepts an event from the notebook client and determines the appropriate mode of operation. The modes of operation are described below.

***Maintenance mode.*** In the case that the event is a cell execution and the user has not attached analyses to this event, i.e., a what-if analysis is not triggered, then NBLyzer will perform cell maintenance for the executed cell. Since a cell execution will result in the concrete notebook state being updated, NBLyzer needs to ensure that the corresponding abstract state for all future invoked analyses is maintained. In addition, code summaries that enable faster analyses must also be updated. NBLyzer performs maintenance by updating (if the code has changed) all intermediate program representations including parsing the cell code into an abstract syntax tree (AST), converted the AST to a control flow graph (CFG) and producing use definition (U-D) chains. If the cell code has not changed, these are retrieved from a cache. Using the

[1]in fact this example is based on a real life notebook sourced from stackoverflow, where a user was experiencing a data leak
[2]that can be expressed as an abstract interpretation



```
[1] d = genfromtxt('data.csv')

[2] selector = SelectKBest(k=25)
    x = selector.fit_transform(d)

[3] x = genfromtxt('data2.csv')

[4] x_train, x_test, y_train, y_test =
      train_test_split(x, ...)

[5] lr = LogisticRegression()
    lr.fit(x_train, y_train)
    y_pred = lr.predict(x_test)
```

(a) Initial notebook

```
[1] d = genfromtxt('data.csv')

[2] selector = SelectKBest(k=25)
    x = selector.fit_transform(d)

[3] x = genfromtxt('data2.csv')

[4] x_train, x_test, y_train, y_test =
      train_test_split(x, ...)

[5] lr = LogisticRegression()
    lr.fit(x_train, y_train)
    y_pred = lr.predict(x_test)
```

(b) Data leak analysis

```
[1] d = genfromtxt('data.csv')

[2] selector = SelectKBest(k=25)
    x = selector.fit_transform(d)

[3] x = genfromtxt('data2.csv')

[4] x_train, x_test, y_train, y_test =
      train_test_split(x, ...)

[5] lr = LogisticRegression()
    lr.fit(x_train, y_train)
    y_pred = lr.predict(x_test)
```

(c) Stale state analysis

**Figure 1: Example Notebook**

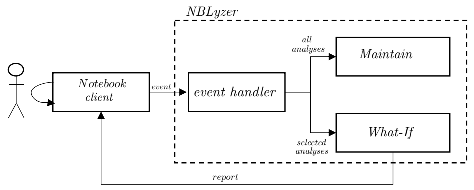


**Figure 2: Overview of NBLyzer**

CFG the static analyses are performed to update the notebook's abstract state, i.e., the resultant state from a static analysis required to perform future static analyses in the future. In the case the event is a non-execution event an abstract state may not need to be computed and only summary, AST, CFG and U-D information is updated. In Section 3.2.1 we provide a detailed account of the maintenance process.

***Propagation mode.*** In the case of a what-if analysis, i.e., an event with a subset of analyses associated with it, an inter-cell analysis is performed. Here starting from the global notebook abstract state, a set of possible abstract states are computed corresponding to the set of possible executions up to a limit $K$ depth or a fixpoint is reached on all branches. This process for each cell checks which other cells have a dependency and propagates the computed abstract state to the dependent cells, for which the incoming abstract state is treated as an initial state. For each cell, the abstract state is checked for correctness criteria, if an error is found a report is updated which serves as instruction for notebook clients to alert the user to the consequences of the event (e.g., by cell highlighting etc.). In Section 3.2.2 we provide a detailed account of the maintenance process.

## 3 TECHNICAL DESCRIPTION

In this section we provide a technical description of the NBLyzer framework.

### 3.1 Notebook Program Model

*3.1.1 Notebook.* A Notebook $N$ consists of a set of cells $c_i \in N$. A cell $c_i$ consists of a sequence of code statements $st^i_j(l, l')$ from a location $l$ to location $l'$ in a control flow graph (CFG) where $i$ refers to the cell number and $j$ the index of the statement in the cell. As an abuse of notation we allow $c_i$ to be also used as a label.

*3.1.2 Cell Execution.* An execution of a cell $c_i$ over a state space $\Sigma = V \longrightarrow D$ where $V$ is the set of notebook variables and $D$ is the concrete domain of execution, is denoted by $\sigma_{i+1} = [\![c_{i+1}]\!](\sigma_i)$, assuming the execution of $c_{i+1}$ terminates. Here $\sigma_{i+1} \in \Sigma$ is the output state and $\sigma_i \in \Sigma$ is the input state previously computed by a cell $c_i$ in the *execution sequence*. We denote access into a state as $\sigma(v)$ where $v \in V$ and we denote updating a state as $\sigma[v \mapsto d]$ where $v \in V$ and $d \in D$.

*3.1.3 Notebook Execution.* A notebook execution is a potentially infinite execution sequence $\sigma_0 \longrightarrow_{c_i} \sigma_1 \longrightarrow_{c_j} \ldots$ where $\forall k \geq 0, c_k \in N, \sigma_k \in \Sigma$ and $i = j \vee i \neq j$. The choice of the next cell in a execution sequence is determined by the user from the space of all cells in a notebook.

### 3.2 Analysis Framework

*3.2.1 Intra Cell Analysis.*

*Events and Analyses.* The inter-cell analysis is triggered by an event $e \in Event$. An event is attached to a set of analyses $A' \subset A$ by an mapping $\mathcal{M} : Event \longrightarrow \wp(A)$. An analysis $a$ is a tuple of a abstraction label $abs$ and condition $cond$. The condition $cond$ is an assertion on an abstract state of the analysis of type $abs$.

*Abstract state computation.* From the sequence of statements in a cell, we construct a control flow graph (CFG), a directed graph that encodes the control flow of the statements in a cell. We define a CFG as $\langle L, E \rangle$ where an edge $(l, st, l') \in E$ reflects the semantics of the cell statement $st$ associated with the CFG edge from locations $l$ to $l'$ in the cell.

A sound over-approximation $\sigma^\sharp$ of a state $\sigma$ is computed by iteratively solving the semantic fixed point equation $\sigma^\sharp = \sigma^\sharp_0 \sqcup [\![\bar{st}]\!]^\sharp(\sigma^\sharp)$ using the abstract semantics $[\![\bar{st}]\!]^\sharp$ for statements $\bar{st}$ in a cell and the initial abstract state $(\sigma^\sharp_0)$. At the cell level this computation is defined as $F_{c_i}$ which we refer to a *abstract cell transformer*. $F_{c_i}$ takes an abstract state and computes a fix-point solution [13, 14] in the abstract domain.

Since a what-if analysis may not be triggered on every event, and yet a cell is executed by the user, it is of small cost to maintain the abstract state along with the concrete state, as our analyses are designed to be faster than performing a concrete execution (See Section 6). We therefore maintain an abstract state $\sigma^\sharp$ which is updated each time a cell is executed, in parallel to the concrete executions of a notebook cell. At each execution, a cell transformer $F_{c_i}$ for a cell $c_i$ is applied with the current global state, returning an updated new global state i.e., $F_{c_i}(\sigma^\sharp) = \sigma^{\sharp\prime}$. We perform this maintenance for two reasons: Firstly, we may want to perform a static analysis just before cell execution, blocking execution if an error was found. Secondly, the global abstract state is needed to initiate a what-if analyses, once it's triggered by a user.

To analyze a cell, we reduce the static analysis problem to the computation of the least solution of a fix-point equation $\sigma^\sharp = F_{c_i}(\sigma^\sharp)$, $\sigma^\sharp \in \Sigma^\sharp$ where $\Sigma^\sharp$ is a domain of abstract properties, and $F_{c_i}$ is the abstract transformer for the cell, i.e., a composition of abstract statements transformers in the cell fix-point computation to solve the static analysis problem. We refer to [6] for a comprehensive background on abstract interpretation.

Within the abstract interpretation framework several analyses can co-exist by constructing an *independent product* of abstract domains. We denote executing several transformers in parallel for cell $c_i$ as $F^A_{c_i}$ where $A$ is a set of analyses. We refer the reader to [7] on literature on combining abstract domains with independent products.

*Cell summary computation.* Apart from computing the abstract state, we compute *pre-summaries*. Pre-summaries are intra-cell computed pre-conditions on a cell that are used to act as a pre-condition guard on if an abstract state should be propagated to that cell. We compute pre-summaries for each cell at notebook initialization time and during cell code changes.

In order to compute a pre-summary $pre_{c_i}$ for cell $c_i$ we construct use-def (U-D) structure using standard data-flow techniques [9]. U-Ds provide a mapping between variable usages and their definitions. A variable is a defined if it is used as a right-hand-side expression in a assignment statement or if it is a function $st$. A variable is used if it is in a left-hand-side of an assignment statement or in a function $st$. Thus, given a cell $c$ we can define the following sets of variables that define definitions and usages.

$$
\begin{aligned}
def(c) &= \{v \mid \forall\ st \in c \text{ s.t. } v \text{ is defined in } st\} \text{ and} \\
use(c) &= \{v \mid \forall\ st \in c \text{ s.t. } v \text{ is used in } st\}
\end{aligned}
$$

The U-D structure is computed using a reaching definitions dataflow analysis [9] and provides a mapping *use-def* for all symbols $v \in V$ in the cell. If a $v \in use(c)$ has no definition, it is mapped to $\bot$. Using the U-D structure we compute the set of all unbound variables in a cell:

$$pre_{c_i} = \{\ v \mid v \in use(c_i) \wedge use\text{-}def(v) = \bot\}$$

Depending on the analysis we may want to expand the definition of $pre_{c_i}$. For example, for access violation we may want to ignore variables in cells where no access patterns occur and a variable is never used to change and propagate information e.g., simply printing data.

### 3.2.2 Inter Cell Analysis.

*State propagation.* The inter-cell analysis computes a set of abstract states for the entire notebook up to a depth $K$ or to a global fixpoint solution (fixpoints on all active paths). The abstract state from a source cell is propagated to other cells if and only if there exists an edge that satisfies a cell propagation dependency. When the propagation occurs, an intra-cell analysis computation is performed that treats the incoming cell abstract state as the initial state.

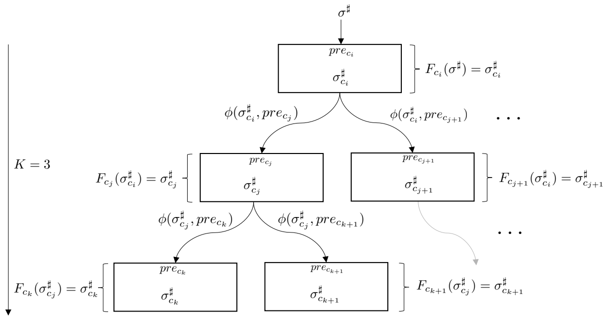

$\sigma^\sharp$
$pre_{c_i}$
$\sigma^\sharp_{c_i}$
$F_{c_i}(\sigma^\sharp) = \sigma^\sharp_{c_i}$
$\phi(\sigma^\sharp_{c_i}, pre_{c_j})$
$\phi(\sigma^\sharp_{c_i}, pre_{c_{j+1}})$
$\dots$
$K = 3$
$F_{c_j}(\sigma^\sharp_{c_i}) = \sigma^\sharp_{c_j}$
$pre_{c_j}$
$\sigma^\sharp_{c_j}$
$pre_{c_{j+1}}$
$\sigma^\sharp_{c_{j+1}}$
$F_{c_{j+1}}(\sigma^\sharp_{c_i}) = \sigma^\sharp_{c_{j+1}}$
$\phi(\sigma^\sharp_{c_j}, pre_{c_k})$
$\phi(\sigma^\sharp_{c_j}, pre_{c_{k+1}})$
$\dots$
$F_{c_k}(\sigma^\sharp_{c_j}) = \sigma^\sharp_{c_k}$
$pre_{c_k}$
$\sigma^\sharp_{c_k}$
$pre_{c_{k+1}}$
$\sigma^\sharp_{c_{k+1}}$
$F_{c_{k+1}}(\sigma^\sharp_{c_j}) = \sigma^\sharp_{c_{k+1}}$

**Figure 3: Inter Cell Analysis**

The inter-cell analysis propagation is depicted in Figure 3. Here the what-if analysis is triggered by an event $e$ for a source cell $c_i$. A pre-defined value of $K \in \{1, \dots, \infty\}$ is defined where $K = \infty$ means we compute until a fix-point, that determines the depth of the analysis. The dependency is defined by determining if the abstract state $\sigma'_{c_i}$ of the cell $c_i$ can be combined with the pre-summary $pre_{c_j}$ of another cell $c_j$ (which may be cell $c_i$ itself). If there is a dependency, the unbound variables in $c_j$ consume their values from $\sigma'_{c_i}$. This propagation is continued until all paths terminate either by reaching the $K$ limit, by achieving a fixpoint or by $\phi$ not holding for all cells in the notebook.

We formalise cell dependencies in the form of a graph definition. Note, in our technique the graph is constructed lazily during abstract state propagation phase.

*Definition 3.1 (Cell Propagation Dependency Graph).* We assume the sequence of cells form a directed dependency graph $\mathcal{G} = \langle N, D\rangle$ where $N$ is a finite set of cells, and $(c_i, R, c_j) \in \mathcal{R}$ defines an arc from cell $c_i \in N$ to $c_j \in N$ iff $\phi(\sigma^\sharp_{c_i}, pre_{c_j})$. How $\phi(\sigma^\sharp_{c_i}, pre_{c_j})$ is defined is analysis specific. In Section 4 we provide examples of how analyses can be defined to fit into the NBLyzer framework.

*Fixpoint pruning.* The control-flow from inter-cell execution can result in cycles. For example, a cell can be re-executed as the dependency $\phi$ repeatedly holds in a given sequence. For analyses with $K = \infty$ this can cause non-termination. Even, in the case for bounded $K$ values, ignoring fixpoints is a source of inefficiency. Firstly, by fixpoint we mean that the state $\sigma^\sharp_{c_i} = \sigma^{\sharp\prime}_{c_i}$, that is, in an analysis path (note many paths exist as shown in Figure 3), the state resulting from first execution of cell $c_i$ does not change after its next execution. There may or may not be execution of cells in between. Regardless, this implies that we can prune this execution path as other execution paths arising from the first execution of $c_i$ will subsume any further executions from the second execution of $c_i$. For analyses with high or infinite lattices, extrapolation operators are needed for force convergence. Therefore, we detect when we re-visit a cell and terminate the exploration on that path if a fixpoint is detected after the re-execution. In the case of high or infinite abstract domains, we extrapolate the fixpoint using standard widening techniques [6] for the given abstract domain.

Observation 3.1 (Fixpoint Subsumption). *Given a fixpoint on a cell execution path $p = \langle c_i, \ldots, c_{i+k} \rangle$ such that $c_i = c_{i+k}$ and $\sigma^\sharp_{c_i} = \sigma^\sharp_{c_{i+k}}$, any cell $c_j$ not in $p$ executed after $c_i$ will produce the same abstract state as being executed after $c_{i+k}$.*

Proof. Since the $c_i$ and $c_{i+k}$ are the same cell and since we have a fixpoint i.e., $\sigma^\sharp_{c_i} = \sigma^\sharp_{c_{i+k}}$, due to the monotonicity of the transformers no cell in $p$ changed the state, therefore executing any cell $c_j$ after $c_{i+k}$ will be the same as executing it after $c_i$ and therefore we can stop execution after $p$. □

**Algorithm 1** Event_Handler($code, c_i, e, K$)

```
1: global variables
2:     $\sigma^\sharp$ (global abstract state)
3:     $pre$ (cell to pre-summary mapping)
4:     $cfg$ (cell to cfg mapping)
5: end global variables
6: $A' = \mathcal{M}(e)$
7: if $A' = \emptyset \wedge e = execute$ then
8:     $\sigma^\sharp := Maintain(code, c_i, \sigma^\sharp, A)$
9: else
10:    $report := InterCell(\sigma^\sharp, c_i, K, [], A', \eta)$
11:    return $report$
```

*3.2.3 Algorithmic Implementation.* Our technique is described algorithmically, starting with Algorithm 1 which receives an event and determines if the computation should proceed in maintenance mode or what-if analysis mode. Given an event $e$ occurs, we obtain the source cell code *code*, identifier $c_i$, event $e$ and global abstract state. At line 6, we determine if there exist any analyses $A' \subseteq A$ that are attached to the event $e$. If not, we perform a maintenance in line 8 by calling $Maintain(code, c_i, \sigma^\sharp, A)$ and updating the global. Otherwise, we proceed with a what-if analysis by calling $InterCell(\sigma^\sharp, c_i, K, [], A', \eta)$ in line 10 and return the results of the analysis to the notebook. Here apart from the global state $\sigma^\sharp$, cell label $c_i$, and the analyses $A'$, the $K$ parameter is passed, along with a report which is initialized to an empty list [] (to simplify the algorithm description we represent the report as simply a list), and a mapping $\eta : N \rightarrow \Sigma^\sharp$ which maps each cell label to its last computed abstract state. This is required to detect fixpoints in the analysis paths.

In Algorithm 2 we describe intra-cell analysis, namely cell maintenance. The function *Maintain* first checks to see if a code change occurred. If so, the pre-summary $pre_{c_i}$ is re-built and an intra cell static analysis $F_{c_i}(cfg_{c_i}, \sigma^\sharp)$ is performed to produce a new abstract state $\sigma^\sharp$. If the code has not changed, since the abstract state may have changed in the meantime, we perform an intra-cell analysis i.e., $F^A_{c_i}(cfg_{c_i}, \sigma^\sharp)$ for all analyses in $A$. Note, that we cache CFGs, U-Ds, and pre-summaries to avoid unnecessary re-computation.

The *InterCell* algorithm described in Algorithm 3 performs the what-if analysis. Here analyses in $A'$ are executed on cells, starting

**Algorithm 2** Maintain($code, c_i, \sigma^\sharp, A$)

```
1: if $code$ not changed then
2:     $\sigma^{\sharp\prime} := F^A_{c_i}(cfg_{c_i}, \sigma^\sharp)$
3:     return $\sigma^{\sharp\prime}$
4: $ast := parse(code)$
5: $cfg_{c_i} := getCfg(ast)$
6: $ud := getUD(cfg)$
7: $pre_{c_i}$ := getPre(ud)
8: $\sigma^{\sharp\prime} := F^A_{c_i}(cfg_{c_i}, \sigma^\sharp)$
9: return $\sigma^{\sharp\prime}$
```

with the source cell $c_i$ in lines 2 and 5 and propagating the abstract state to cells that have a dependency i.e., satisfy $\phi(\sigma^{\sharp\prime}, pre_{c_j})$ as shown in lines 7 and 8. If $K = 0$ (line 1), meaning we have reached the required depth or a fixpoint is detected (line 3) we terminate. The algorithm worst case complexity is $O(n^K)$ in the number of cells $n$ for a given $K$.

**Algorithm 3** InterCell($\sigma^\sharp$, $c_i$, $K$, $report$, $A'$, $\eta$)

```
1: if $K = 0$ then return $report$
2: $\sigma^{\sharp\prime} := F^{A'}_{c_i}(cfg_{c_i}, \sigma^\sharp)$
3: if $\sigma^{\sharp\prime} = \eta_{c_i}$ then return []
4: $\eta_{c_i} := \sigma^{\sharp\prime}$
5: $report' := Check(\sigma^{\sharp\prime}, A', report)$
6: for all $c_j \in N$ do
7:     if $\phi(\sigma^{\sharp\prime}, pre_{c_i})$ then
8:         report' := report' + $InterCell(\sigma^{\sharp\prime}, c_j, K-1$, report', A', $\eta$)
   return $report'$
```

An optional operation that we omit here, is to perform inter-cell widening. Widening is required for analyses with potential slow convergence such as interval analysis. Adding widening requires an extra condition in the code that checks if the abstract state increases on a given variable. If so, the value for that variable is added as the top element. A narrowing pass can be also performed to improve precision.

*3.2.4 Analysis Criteria and Contracts.* The *Check* function in Algorithm 2 and 3 checks the abstract state after a cell execution and depending on the criteria determine if a violation has occurred. For standard built in analyses (see Section 4) this is hard coded into NBLyzer. However, for the available abstract domains, a user can define *contracts* on lines of code, pre or post conditions on cells or on the global notebook. NBLyzer exposes the set of available abstractions, which can be seen as schema for which users can define queries in a logic-based DSL that can assert expected behaviour.

## 4 INSTANTIATED ANALYSES

In this section we give a brief outline of several instantiations of our analysis framework which we later evaluate in Section 6.

## 4.1 Use Case I: Code Impact Analysis

When a code change occurs users need to know what other code is affected or unaffected by that change. This has a number of usages including automating notebook execution, stale cell state detection, cell cleanup and simplification, among others.

*4.1.1 Abstract Semantics.* We define an abstract domain that maps a variable (including symbols, function names, etc. ) $v$ to a Boolean indicating which variable has changed or not. Practically, the abstract domain is implemented as a set of variables $\bar{v} \subseteq V$. If a variable is in the set it has changed, otherwise it has not. Thus, the lattice is a standard powerset lattice $\wp(V)$ common in data flow analyses [9]. When a variable on the left-hand-side of a statement has changed, we insert the right-hand-side in the set. Below we state the propagation semantics for selected statements. In the implementation, more variations are covered.

(1) Assignment:

$$\lambda\sigma^{\sharp}.[\![\bar{y} = f(\bar{x})]\!] = \left\{ \begin{array}{l} \sigma^{\sharp} \cup \{y\} \text{ iff } f \in \sigma^{\sharp} \vee \\ \exists x \in \bar{x} \text{ s.t. } x \in \sigma^{\sharp} \end{array} \right\}$$

(2) Functions:

$$\lambda\sigma^{\sharp}.[\![f(\bar{x})\{\bar{y}\}]\!] = \left\{ \begin{array}{l} \sigma^{\sharp} \cup \{f\} \text{ iff} \\ \exists x \in \bar{x} \text{ s.t. } x \in \sigma^{\sharp} \vee \\ \exists y \in \bar{y} \text{ s.t. } y \in \sigma^{\sharp} \end{array} \right\}$$

Similarly, joins and meets that arise from control flow are handled by the join operations of the abstract domain, i.e., set union and disjunction.

The $\phi$ operation in this case holds if the intersection of the variable in $\sigma^{\sharp}$ and $pre_{c_j}$ are not null, i.e., there is at least one dependent variable in $c_j$ to propagate to. More formally, we define $\phi$ as follows:

$$\phi(\sigma^{\sharp}_{c_i}, pre_{c_j}) = \{v : v \in \sigma^{\sharp}_{c_i}\} \cap pre_{c_j} \neq \emptyset$$

This analysis has many use cases including automating cell executions for a given change by following the dependencies; stale cell execution where cells that have intermediate impacted cells between them and the source cell, can potentially be stale. Typically, we execute this analysis with a bounded e.g., $K = 3$ for stale cell analysis but in principle can be unbounded. Both options result in similar overheads due to fixpoint subsumption. Other variations include fresh cell analysis that detects cells that cannot cause staleness when changed and an isolated cell analysis that detects cells without dependencies on other cells and thus can be potentially cleaned. These cells are typically found during experimentation phases of development and need to be identified when the notebook program is converted to a production script. This analysis is only performed on $K = 1$ due to its nature.

*4.1.2 Analysis Example.* Consider the example in Figure 1. Here we can see that the execution of cell 1 followed by cell 4 will create staleness. This is because cell 2 is fresh and is the intermediate cell between cell 1 and cell 4 dependencies. Suppose we change the file in cell 1 then the variable $d$ is in our abstract domain. As before we propagate this to cell 2 and hence $x$ is also in our abstract domain. When we further propagate to cell 4 (i.e., $K = 2$) we can report that all the right-hand-side variables are stale if the cell execution sequence 1, 4 is performed.

## 4.2 Use Case II: ML Data Leakage

Data Leakage [12] is a common bug specific to data science. In machine leaning applications a model typically requires normalization of the input data, especially neural networks. Commonly, data is normalized by performing a division of the existing data by its average or maximum. Likewise, data is typically split into training and test subsets. If the normalization is performed using the *overall* data set, then information from the test set will now be influencing the training subset. For this reason, any normalization should be applied individually to the test and training subsets.

While the Data leakage commonly occurs in data science scripts it is even further exacerbated by the execution semantics of notebooks. To this end, we have implemented a light-weight analysis to detect potential data leakages in notebooks. Our abstraction tracks which variable points to which data source and if the variable has been used to train or test a model. When an operation is performed on data that can introduce a leak, e.g., normalization, extrapolation etc. we reset the data source propagation. Otherwise, we propagate the source dependencies of left-hand-side variables to right-hand-side variables. When a variable is an argument to a function that is marked as training or testing a model, the variable is marked as such. We assert that no two variables that are marked as train and test, respectively point to the same data source.

*4.2.1 Abstract Semantics.* We define an abstract domain that maps a variable $v$ to a data leakage abstract domain $\langle L, \sqsubset \rangle$ where $L = \wp(v) \times \wp(\{tr, ts\})$ such that $L$ is partially ordered ($\sqsubset$) point wise by the subset relation $\subset$ with meet $\sqcup$ and join $\sqcap$ are similarly defined using point wise set union $\cup$ and intersection $\cap$, respectively. Thus, an element in the abstract domain is a variable that maps to a set of variables and an indicator if it has been an argument in a train or test function (or both). We differentiate between which tuple element in the product domain is access by $\sigma^{\sharp 1}$ (first tuple element) and $\sigma^{\sharp 2}$ (second tuple element). We define a simplified abstract semantics for three categories of operations below. Note, we do not exhaustively cover all cases below for readability, and only highlight the most important cases.

(1) reset:

$$\lambda\sigma^{\sharp}.[\![\bar{y} = f(\bar{x})]\!] = \left\{ \begin{array}{l} \forall y \in \bar{y}.\sigma^{\sharp}[y \mapsto (\bar{x}, \emptyset)] \\ \text{iff } f \in KB_{\text{reset}} \end{array} \right\}$$

(2) propagate:

$$\lambda\sigma^{\sharp}.[\![\bar{y} = f(\bar{x})]\!] = \left\{ \begin{array}{l} \forall y \in \bar{y}.\sigma^{\sharp}[y \mapsto \sigma^{\sharp}(y) \sqcup \bigsqcup_{x \in \bar{x}} \sigma^{\sharp}(x)] \\ \text{iff } f \notin KB_{\text{reset}}, KB_{\text{test}}, KB_{\text{train}} \end{array} \right\}$$

(3) sinks:

$$\lambda\sigma^{\sharp}.[\![f(\bar{x})]\!] = \left\{ \begin{array}{l} \forall x \in \bar{x}.\sigma^{\sharp}[x \mapsto (\sigma^{\sharp 1}(x), \sigma^{\sharp 2}(x) \sqcup \{tr\})] \\ \text{iff } f \in KB_{\text{train}} \\ \forall x \in \bar{x}.\sigma^{\sharp}[x \mapsto (\sigma^{\sharp 1}(x), \sigma^{\sharp 2}(x) \sqcup \{ts\})] \\ \text{iff } f \in KB_{\text{test}} \end{array} \right\}$$

The reset operations (1), occur when a function f is marked as a reset function in the knowledge base KB. This is library specific and rely on the data scientists to specify which functions may cause leakage. Here we map each right-hand-side variable $y$ to the variables that are arguments to the reset function while resetting its markings of test or train usage to $\emptyset$.

In the case (2), we simply propagate information by joining all abstract states of right-hand-side variables to the left-hand-side variables existing abstract state.

Finally in the case of (3), we mark each argument with a {tr} element if it is an argument to a train function, and {ts} if it is an argument to a test function. If a variable marked as {tr} points to the same source as a function marked as {ts} we issue a warning.

To enable inter-cell propagation, we define the rule:

$$\phi(\sigma^{\sharp}_{c_i}, pre_{c_j}) = pre_{c_j} \subseteq \{v : (v \mapsto x) \in \sigma^{\sharp}_{c_i} \wedge x \neq \bot\} \wedge pre_{c_j} \neq \emptyset$$

Here we make sure the successor cells pre is not empty and is a subset of the incoming cells abstract state variables that are reachable (not mapped to $\bot = (\emptyset, \emptyset)$). This analysis can be performed on a variety of sizes of $K$, however in practice we rely on our fixpoint subsumption and keep $K$ unbounded.

*4.2.2 Analysis Example.* Consider the example in Figure 1. Recall in example, a potential data leakage is shown. Depending on the execution order of the cells i.e., if *cell 2* is executed before *cell 4* and 5. We now describe how our analysis will detect this violation. Assume a what-if analysis is triggered for the event of executing *cell 1*. In other words, we ask *what can happen in future executions if cell 1 is executed?* We first compute an abstract state for *cell 1* which is $\sigma^{\sharp}_{c_1} = d \mapsto (\{data.csv\}, \emptyset)$. Now using abstract state and preconditions of other cells we asses the value of $\phi(\sigma^{\sharp}_{c_1}, pre_{c_j})$ for all cells $c_j$ in the notebook. We find $\phi$ holds for *cell 2*. Next, we compute the abstract state for *cell 2* with the abstract state of *cell 1* as the initial state, obtaining $\sigma^{\sharp}_{c_2} = d \mapsto (\{data.csv\}, \emptyset), x \mapsto (\{d\}, \emptyset)$ as we apply rule (2) as *fit_transform* $\in KB_{reset}$. We evaluate $\phi(\sigma^{\sharp}_{c_2}, pre_{c_j})$ for all cells $c_j$ in the notebook and find that *cell 4* holds. Here all split variables map to $d$ applying rule (1). Again we find that we can only propagate to *cell 5*. Here we have a function in *fit* $\in KB_{train}$ so we have that *x_train* $\mapsto (d, \{tr\})$ and *y_train* $\mapsto (d, \{tr\})$. Next, we have a function *predict* $\in KB_{test}$ and so we have *x_test* $\mapsto (d, \{ts\})$. Since we have 2 or more variables that point to $d$ and have $\{tr\}$ and $\{ts\}$ we flag *cell 5* asserting that the following conditions is violated: *no arguments of train and test functions can point to the same data.* With this analysis condition, NBLyzer warns the user that the execution sequence of cells executions $\langle 1, 2, 4, 5 \rangle$ will result in a data leakage in *cell 5*.

## 5 INTEGRATION AND APPLICATIONS

We have implemented our technique as a notebook server and Microsoft visual code extension. Our implementation currently targets a subset of the python language. It parses the code into an AST from which it constructs a CFG and U-D chains. These low-level code representations are used to perform the analyses implemented in our framework. The user can manually trigger the what-if analysis and pre-select which built-in analyses are turned on for what event. We warn the user of potential violations through use of cell highlighting and messages. The user interface varies with the clients used.

The standard use case is to use NBLyzer as a development time what-if advisor that detects potential bugs before they occur. However NBLyzer can be used for notebook cleaning, where erroneous, idle and isolated cells are flagged for removal; notebook reproducibility where safe execution paths that lead to acceptable results are extracted from the notebook; auditing where security violations for e.g., GDPR compliance [2]; education where the tool can help data scientists write quality code.

## 6 EVALUATION

In this section, we evaluate NBLyzer on a set of real world notebook benchmarks and on the instantiated analyses in Section 4. The evaluation aims to **(1) validate the adequacy of the NBLyzer's performance for our notebook use cases** and to **(2) investigate performance bottlenecks and configuration tuning required to maximize in the performance of NBLyzer**. As a universal service level agreement (SLA) model for user experiences, i.e., the acceptable delays the analyses may exhibit in the notebook environment we refer to the RAIL model [4].

### 6.1 Experimental Setup

All experiments were performed in an Intel(R) Xeon W-2265 CPU @ 3.50 GHz with 64 GB RAM running a 64 bit Windows 10 operating system. Python 3.8.8 was used to execute NBLyzer. We evaluate the execution-time of our static analyses running within NBLyzer on the full set of Kaggle notebooks.

*6.1.1 Static Analyses.* We perform the static analyses instantiated in our framework below. For each analysis type we perform an analysis over all notebooks, where each cell is a source.

- Code Impact Analysis (CIA): the following variations of the analysis discussed in Section 4.1:
  - Isolated Cell Analysis (IsC)
  - Fresh Cell Analysis (FrC)
  - Stale Cell Analysis (StC)
- Data Leakage Analysis (DlK): the analysis discussed in Section 4.2

*6.1.2 Benchmark Characteristics.* We use a benchmark suite consisting for 2211 executable real world notebooks from the Kaggle competition[3] that has previously been used to evaluate data science static analyzers [11]. The benchmark characteristics are summarized in Table 1. We emphasise that this is a fair reflection of typical notebook code.

We see on average, the notebooks in the benchmark suite have 24 cells, where each cell on average has 9 lines of code. In addition, on average branching instructions appear in 33% of cells. Each notebook has on average 3 functions and 0.1 classes defined. We note that these characteristics of low amount of branching, functions and classes is typically advantageous for static analysis precision. We found that every second notebook had a cell that could not be parsed and analyzed due to a syntax errors in it. Overall, this affected 4% of cells in the benchmarks. 2.1 of variables were unbound, from an average of 8.2 variables per cell.

| Characteristic | Mean | SD | Max | Min |
|---|---|---|---|---|
| Cells (per-notebook) | 23.58 | 20.21 | 182 | 1 |
| Lines of code (per-cell) | 9.12 | 13.55 | 257 | 1 |
| Branching instructions (per-cell) | 0.43 | 2.49 | 76 | 0 |
| Functions (per-notebook) | 3.33 | 7.11 | 72 | 0 |
| Classes (per-notebook) | 0.14 | 0.64 | 11 | 0 |
| Non-parsing cells (per-notebook) | 0.5 | 0.98 | 20 | 0 |
| Variables (per-cell) | 8.2 | 2.3 | 552 | 0 |
| Unbound variables (per-cell) | 2.1 | 1.06 | 12 | 0 |

**Table 1: Kaggle Notebook Benchmark Characteristics**

## 6.2 Code Impact Analysis

We evaluate the performance of the code impact analyses for notebook usage. Recall the CIA analyses reason about change propagation in notebook cells. Also recall that many of these analyses by definition have a **fixed** $K$. For the included evaluations, we also evaluate stale cell analysis for various values of $K$ including $K = \infty$, since it can be run with such a parameter value. For each evaluation of CIA analysis, we perform a random change in an source cell and compute the analysis result. We do this for all cells in a notebook, and for all notebooks in the benchmark suite. We omit notebook cells that do not parse.

*6.2.1 Isolated Cells.* In Figure 7 the average analysis executions per-notebook are shown. Overall, the results how that the average isolation analysis on a notebook takes 2.499 milliseconds. The average analysis time, including the maximum outliers, are **well under the threshold for humans to notice a delay** and does not degrade the user experience. We were able to detect that 14% of cells were in fact isolated and candidates for notebook cleaning or simplification. **This highlights the need for automated cleaning/simplification tooling for notebooks** and the ability of NBLyzer to detect such cells. Our manual observation of the results could not detect any false positives.

*6.2.2 Fresh Cell Analysis.* In Figure 8 the average fresh cell analysis executions are shown. The results show that the average fresh cell analysis on a notebook takes 2.98 milliseconds. Similarity, the analysis time for average and maximum outliers is **well under the threshold for users to notice a delay** and does not degrade the user experience. The analysis found that 74% of cells are fresh and no false positives were observed by our manual inspection.

*6.2.3 Stale Cell Analysis.* In Figure 9 the average and maximum stale analysis executions are shown. We show maximum results because we ran the experiments for $K = 3$ and thus a propagation occurs. The results show that the average stale cell analysis on a notebook takes 2.49 milliseconds. The average maximum analysis per notebook take 22.1 milliseconds, with a global maximum of 472.99 milliseconds. The analysis time for average and maximum cases are **well under the threshold for users to notice a delay** and does not degrade the user experience. While the global maximum analysis time is above the unnoticeable threshold, **it is still well under the threshold of any degradation of the user experience**. The analysis found that 24% of cells can cause staleness from a random change, highlighting the **significant possibility of such bugs occurring** and utility of this analysis. Our manual inspection found no false positives. We conjecture this is due to the simplicity of data science code. Note, we do not expect this to be the case for general python code as our analysis does not model dynamic semantics.

## 6.3 Data Leakage Analysis

We evaluate the performance and utility of the data leakage analysis. This analysis is run on $K = \infty$, however we investigate its performance on various fixed $K$ values. This analysis is also diverse in its use cases. On one hand it can be used during development time to warn users of potential bugs and on the other hand it can be used in a batch mode for semantic reproducibility of notebooks [16]. We evaluate if the performance of this analysis is compatible with these use cases.

In Figure 4 the average and maximum data leakage analysis for $K = \infty$ executions are shown. The results how that the average data leakage analysis on a notebook takes 41.45 milliseconds. The average maximum analysis per notebook take 880.9 milliseconds, with a global maximum of 233 seconds. **The analysis time for average case is well under the threshold for users to notice any delay** and does not degrade the user experience. **The average maximum recorded analysis time is above the immediate fell threshold, but below the threshold for the task feeling out of flow** (1000ms). The global maximum does cause a considerable delay and user degradation. Below we investigate the cause and remedies for such cases but note they are not common and only 4% of all analyses execute for more than 1000ms and only 1% for more than 5000ms.

*6.3.1 Varying K Bounds.* To demonstrate the affect of reducing $K$ in Figures 5a and 5b we show the effect of vary the $K$ from $\infty$ to bounded values of $K = 8, 4, 2$ and 1. We note that the speedup of the analysis with smaller $K$ values **is not significant enough on average to result in major performance improvements** overall for either analysis. A major reason for this as shown in Figure 5c is that our fixpoint subsumption optimization increases for large values of $K$ resulting in modest average maximum depths as shown in Figure 5e. This is further corroborated by the Figures 5d and 5f.

*6.3.2 Propagation Rate.* Another explanation for the achieved performance is the rate at which propagation occurs to other cells. Given a worst case scenario this propagation rate could be large and result in an execution tree that is very wide and deep. In Figure 6 we plot the average and maximum propagation rates for each notebook (where each cell was a source cell). Here we find that $\phi$ holds on average 9% of the time and the maximum propagation rate for each notebook is on average 13% of the time. This figure coincides with our experience **that a typical notebook has several alternate executions but not to the extent that all cells depend on each other**.

*6.3.3 Bottleneck Sources.* Next we investigate the 4% of notebooks that take more than 1000ms to execute to determine where the bottleneck is occurring and what can be done to bring them under 1000ms. For the 103 notebooks with a maximum analysis execution of larger than 1000ms, we reduce $K = 4$. Here we were able to bring 33% (34 notebooks) of the notebook executions to under the 1000ms. **Thus, we are able to compute 98.7% of notebooks in under 1000ms**. We note, that this reduction exclusively occurred for notebooks with maximum execution times $< 10$ seconds. Of the 4 cases $> 100s$ we found that they in fact had **no significant speedups by reducing the $K$ value**. We have investigated these

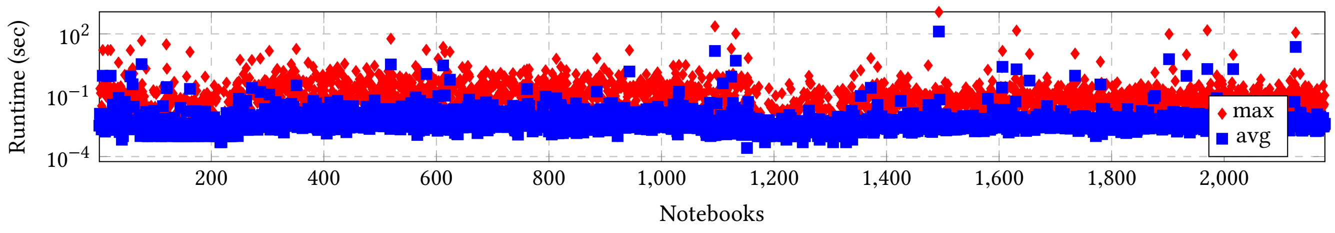


**Figure 4: Data Leakage Analysis Avg. and Max. Analysis Times**

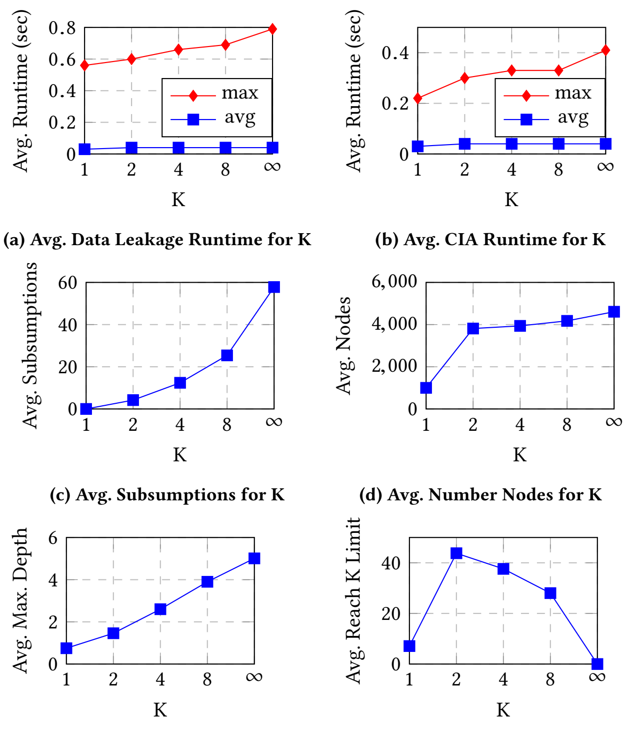


**Figure 5: Avg. Performance for Benchmarks for K Values**

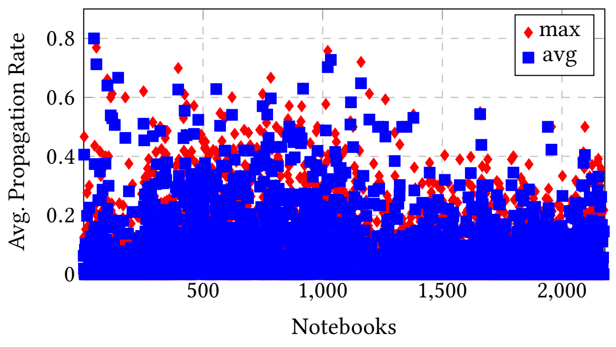


**Figure 6: Data Leakage Analysis Avg. and Max. Propagation Rates**

notebook in question and narrowed down the poor performance to a single cells with very large number and depth of branching and large number of lines of code. For example, one of the notebooks had a cell with 257 LOC and 71% of these were branching statements often deeply nested. We argue that such code is not characteristic of regular notebooks and would cause a challenge to most static analyzers for the time frames we target. To mitigate such cases we would need to improve our rather standard intra-cell analysis fixpoint iteration techniques and employ techniques such as [8] which is left for future work.

## 7 RELATED WORK

Compared to static analysis tools for data science scripts [15], NBLyzer targets notebooks and incorporates their semantics in the analysis. We do this by deciding on-the-fly which cell should be analysed next depending on our cell propagation dependency graph. The use of static provenance is related to our technique in the sense that provenance information is propagated forward and can be modeled as an abstract domain [11]. Unlike NBLyzer this work targets scripts and is limited to loop free programs. The lineage technique in [10] targets notebooks. Using this static lineage information computed by data flow analysis and runtime timestamps the technique is able to perform stale state detections. This technique relies on both runtime information and compile time (liveness data-flow analysis). NBLyzer can perform such analyses statically and does not require information at cell execution. Moreover, this technique is limited to a single analysis where NBLyzer is a general static analysis framework and can incorporate various abstract domains. The technique in [16] attempts to reconstruct executions in notebooks by finding dependencies using syntactic means on the AST. NBLyzer builds dependencies wrt. the abstract domain and performs a semantic analysis. Regarding our ML data leakage analysis, we have not found any static analysis method for detecting data leaks in data science code.

## 8 CONCLUSION

In this paper we have described NBLyzer, a static analysis framework that considers the execution semantics of notebook environments. We have instantiated several analyses in our framework, with applications including notebook debugging, notebook verification, notebook cleaning, and notebook reproducibility. As far as we aware, we are the first to suggest a general abstract interpretation-based static analysis framework specific for notebook semantics.

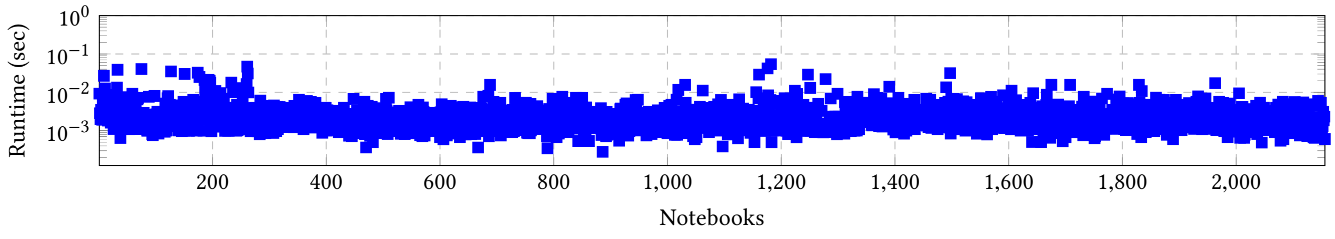


**Figure 7: Isolated Cell Analysis Avg. Times**

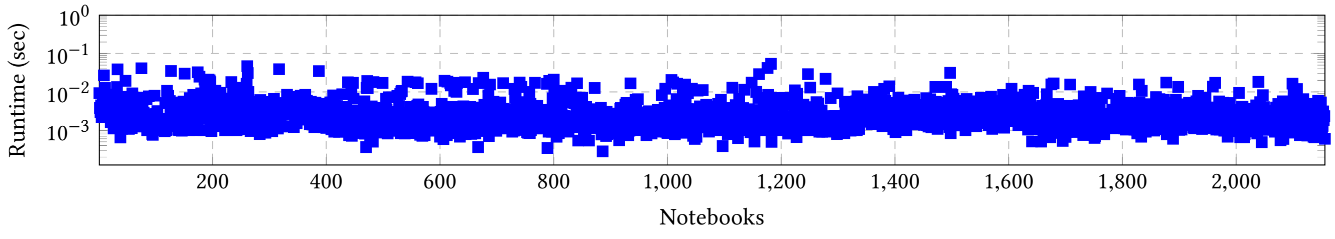


**Figure 8: Fresh Cell Analysis Avg. Analysis Times**

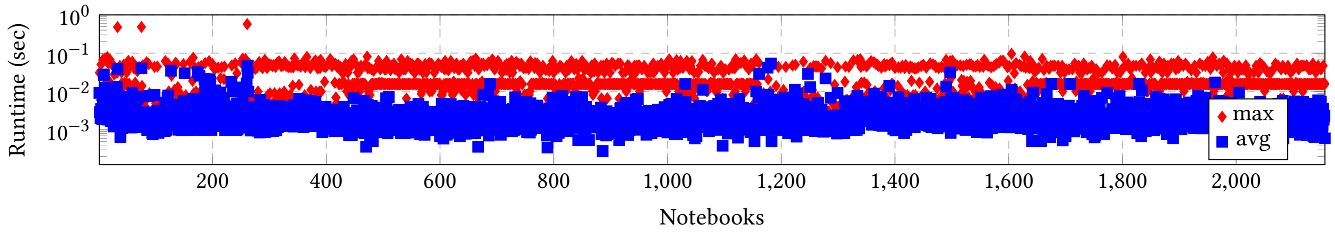


**Figure 9: Stale Cell Analysis Avg. and Max Analysis Times**

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