Program Analysis for Adaptive Data Analysis

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Data analyses are usually designed to identify some property of the population from which the data are drawn, generalizing beyond the specific data sample. For this reason, data analyses are often designed in a way that guarantees that they produce a low generalization error. That is, they are designed so that the result of a data analysis run on a sample data does not differ too much from the result one would achieve by running the analysis over the entire population.

An adaptive data analysis can be seen as a process composed by multiple queries interrogating some data, where the choice of which query to run next may rely on the results of previous queries. The generalization error of each individual query/analysis can be controlled by using an array of well-established statistical techniques. However, when queries are arbitrarily composed, the different errors can propagate through the chain of different queries and bring to high generalization error. To address this issue, data analysts are designing several techniques that not only guarantee bounds on the generalization errors of single queries, but that also guarantee bounds on the generalization error of the composed analyses. The choice of which of these techniques to use, often depends on the chain of queries that an adaptive data analysis can generate.

In this work, we consider adaptive data analyses implemented as while-like programs and we design a program analysis which can help with identifying which technique to use to control their generalization error. More specifically, we formalize the intuitive notion of *adaptivity* as a quantitative property of programs. We do this because the adaptivity level of a data analysis is a key measure to choose the right technique. Based on this definition, we design a program analysis for soundly approximating this quantity. The program analysis generates a representation of the data analysis as a weighted dependency graph, where the weight is an upper bound on the number of times each variable can be reached, and uses a path search strategy to guarantee an upper bound on the adaptivity. We implement our program analysis and show that it can help to analyze the adaptivity of several concrete data analyses with different adaptivity structures.

Additional Key Words and Phrases: Adaptive data analysis, program analysis, dependency graph

1 INTRODUCTION

Consider a dataset X consisting of n independent samples from some unknown population P . How can we ensure that the conclusions drawn from X generalize to the population P ? Despite decades of research in statistics and machine learning on methods for ensuring generalization, there is an increased recognition that many scientific findings generalize poorly (e.g. [\[Gelman and Loken](#page-26-0) [2014;](#page-26-0) [Ioannidis](#page-26-1) [2005\]](#page-26-1)). While there are many reasons a conclusion might fail to generalize, one that is receiving increasing attention is *adaptivity*, which occurs when the choice of method for analyzing the dataset depends on previous interactions with the same dataset [\[Gelman and Loken](#page-26-0) [2014\]](#page-26-0).

Adaptivity can arise from many common practices, such as exploratory data analysis, using the same data set for feature selection and regression, and the re-use of datasets across research projects. Unfortunately, adaptivity invalidates traditional methods for ensuring generalization and statistical validity, which assume that the method is selected independently of the data. The misinterpretation of adaptively selected results has even been blamed for a "statistical crisis" in empirical science [\[Gelman and Loken](#page-26-0) [2014\]](#page-26-0).

A line of work initiated by [Dwork et al.](#page-25-0) [\[2015c\]](#page-25-0), [Hardt and Ullman](#page-26-2) [\[2014\]](#page-26-2) posed the question: Can we design general-purpose methods that ensure generalization in the presence of adaptivity, together with guarantees on their accuracy? The idea that has emerged in these works is to use randomization to help ensure generalization. Specifically, these works have proposed to mediate the access of an adaptive data analysis to the data by means of queries from some pre-determined

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Fig. 1. Overview of our Adaptive Data Analysis model. We have a population that we are interested in studying, and a dataset containing individual samples from this population. The adaptive data analysis we are interested in running has access to the dataset through queries of some pre-determined family (e.g., statistical or linear queries) mediated by a mechanism. This mechanism uses randomization to reduce the generalization error of the queries issued to the data.

family (we will consider here a specific family of queries often called "statistical" or "linear" queries) that are sent to a mechanism which uses some randomized process to guarantee that the result of the query does not depend too much on the specific sampled dataset. This guarantees that the result of the queries generalizes well. This approach is described in Figure [1.](#page-1-0) This line of work has identified many new algorithmic techniques for ensuring generalization in adaptive data analysis, leading to algorithms with greater statistical power than all previous approaches. Common methods proposed by these works include, the addition of noise to the result of a query, data splitting, etc. Moreover, these works have also identified problematic strategies for adaptive analysis, showing limitations on the statistical power one can hope to achieve. Subsequent works have then further extended the methods and techniques in this approach and further extended the theoretical underpinning of this approach, e.g. [\[Bassily et al.](#page-25-1) [2016;](#page-25-1) [Dwork et al.](#page-25-2) [2015a](#page-25-2)[,b;](#page-25-3) [Feldman and Steinke](#page-26-3) [2017;](#page-26-3) [Jung et al.](#page-26-4) [2020;](#page-26-4) [Rogers et al.](#page-26-5) [2020;](#page-26-5) [Steinke and Zakynthinou](#page-27-0) [2020;](#page-27-0) [Ullman et al.](#page-27-1) [2018\]](#page-27-1).

A key development in this line of work is that the best method for ensuring generalization in an adaptive data analysis depends to a large extent on the number of rounds of adaptivity, the depth of the chain of queries. As an informal example, the program $x \leftarrow q_1(D); y \leftarrow q_2(D,x); z \leftarrow q_3(D,y)$ has three rounds of adaptivity, since q_2 depends on D not only directly because it is one of its input but also via the result of q_1 , which is also run on D, and similarly, q_3 depends on D directly but also via the result of q_2 , which in turn depends on the result of q_1 . The works we discussed above showed that, not only does the analysis of the generalization error depend on the number of rounds, but knowing the number of rounds actually allows one to choose methods that lead to the smallest possible generalization error - we will discuss this further in Section [2.](#page-3-0)

For example, these works showed that when an adaptive data analysis uses a large number of rounds of adaptivity then a low generalization error can be achieved by mechanism of adding to the result of each query Gaussian noise scaled to the number of rounds. When instead an adaptive data analysis uses a small number of rounds of adaptivity then a low generalization error can be achieved by using more specialized methods, such as data splitting mechanism or the reusable holdout technique from [Dwork et al.](#page-25-0) [\[2015c\]](#page-25-0). To better understand this idea, we show in Figure [2](#page-2-0) two experiments showcasing these situations. More precisely, in Figure [2\(](#page-2-0)a) we show the results of a specific analysis^{[1](#page-1-1)} with two rounds of adaptivity. This analysis can be seen as a classifier which first runs 500 non-adaptive queries on the first 500 attributes of the data, looking for correlations between the attributes and a label, and then runs one last query which depends on all these correlations. Without any mechanism the generalization error is pretty large, and the lower generalization error is achieved when the data-splitting method is used. In Figure $2(b)$ $2(b)$, we show the results of a specific analysis^{[2](#page-1-2)} with four hundreds rounds of adaptivity. This analysis can be seen as a classifier which

⁹⁶ ¹We will use formally a program implementing this analysis (Figure [3\)](#page-5-0) as a running example in the rest of the paper.

⁹⁷ ²We will present this analysis formally in Section [6.](#page-19-0)

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Fig. 2. The generalization errors of two adaptive data analysis examples, under different choices of mechanisms. (a) Data analysis with adaptivity 2, (b) Data analysis with adaptivity 400.

114 115 116 at each step runs an adaptive query based on the result of the previous ones. Again, without any mechanism the generalization error is pretty large, and the lower generalization error is achieved when the Gaussian noise is used.

117 118 119 120 121 This scenario motivates us to explore the design of program analysis techniques that can be used to estimate the number of *rounds of adaptivity* that a program implementing a data analysis can perform. These techniques could be used to help a data analyst in the choice of the mechanism to use, and they could be ultimately be integrated into a tool for adaptive data analysis such as the Guess and Check framework by [Rogers et al.](#page-26-5) [\[2020\]](#page-26-5).

122 123 124 125 126 127 128 129 130 131 132 The first problem we face is how to define formally a model for adaptive data analysis which is general enough to support the methods we discussed above and would permit to formulate the notion of adaptivity these methods use. We take the approach of designing a programming framework for submitting queries to some mechanism giving access to the data mediated by one of the techniques we mentioned before, e.g., adding Gaussian noise, randomly selecting a subset of the data, using the reusable holdout technique, etc. In this approach, a program models an analyst asking a sequence of queries to the mechanism. The mechanism runs the queries on the data applying one of the methods discussed above and returns the result to the program. The program can then use this result to decide which query to run next. Overall, we are interested in controlling the generalization of the results of the queries which are returned by the mechanism, by means of the adaptivity.

133 134 135 136 137 138 139 140 141 142 143 144 145 146 The second problem we face is how to define the adaptivity of a given program. Intuitively, a query Q may depend on another query P , if there are two values that P can return which affect in different ways the execution of Q. For example, as shown in [\[Dwork et al.](#page-25-3) [2015b\]](#page-25-3), and as we did in our example in Figure [2\(](#page-2-0)a), one can design a machine learning algorithm for constructing a classifier which first computes each feature's correlations with the label via a sequence of queries, and then constructs the classifier based on the correlation values. If one feature's correlation changes, the classifier depending on features is also affected. This notion of dependency builds on the execution trace as a causal history. In particular, we are interested in the history or provenance of a query up until this is executed, we are not then concerned about how the result is used — except for tracking whether the result of the query may further cause some other query. This is because we focus on the generalization error of queries and not their post-processing. To formalize this intuition as a quantitative program property, we use a trace semantics recording the execution history of programs on some given input — and we create a dependency graph, where the dependency between different variables (query is also assigned to variable) is explicit and track which variable 148 149 150 151 is associated with a query request. We then enrich this graph with weights describing the maximal number of times each variable is evaluated in a program evaluation starting with an initial state. The adaptivity is then defined as the length of the walk visiting most query-related variables on this graph.

152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 The third problem we face is how to estimate the adaptivity of a given program. The adaptive data analysis model we consider and our definition of adaptivity suggest that for this task we can use a program analysis that is based on some form of dependency analysis. This analysis needs to take into consideration: 1) the fact that, in general, a query Q is not a monolithic block but rather it may depend, through the use of variables and values, on other parts of the program. Hence, it needs to consider some form of data flow analysis. 2) the fact that, in general, the decision on whether to run a query or not may depend on some other value. Hence, it needs to consider some form of control flow analysis. 3) the fact that. in general, we are not only interested in whether there is a dependency or not, but in the length of the chain of dependencies. Hence, it needs to consider some quantitative information about the program dependencies. To address these considerations and be able to estimate a sound upper bound on the adaptivity of a program, we develop a program analysis algorithm, named AdaptFun, which combines data flow and control flow analysis with reachability bound analysis [\[Gulwani and Zuleger](#page-26-6) [2010\]](#page-26-6). This new program analysis gives tighter bounds on the adaptivity of a program than the ones one would achieve by directly using the data and control flow analyses or the ones that one would achieve by directly using reachability bound analysis techniques alone.

168 169 170 To Summarize, our work aims at the design of a static analysis for programs implementing adaptive analysis that can estimate their rounds of adaptivity. Specifically, our contributions are as follows:

- (1) A programming framework for adaptive data analyses where the program represents an analyst that can query a generalization-preserving mechanism mediating the access to some data.
- (2) A formal definition of the notion of adaptivity under the analyst-mechanism model. This definition is built on a variable-based dependency graph that is constructed using sets of program execution traces.
- (3) A static program analysis algorithm AdaptFun combining data flow, control flow and reachability bound analysis in order to provide tight bounds on the adaptivity of a program.
- (4) A soundness proof of the program analysis showing that the adaptivity estimated by AdaptFun bounds the true adaptivity of the program.
- (5) An implementation of AdaptFun and an experimental evaluation the bounds this implementation provides on several examples.

2 OVERVIEW

Some results in Adaptive Data Analysis. In Adaptive Data Analysis an analyst is interested in studying some distribution P over some domain X . Following previous works [\[Bassily et al.](#page-25-1) [2016;](#page-25-1) [Dwork et al.](#page-25-0) [2015c;](#page-25-0) [Hardt and Ullman](#page-26-2) [2014\]](#page-26-2), we focus on the setting where the analyst is interested in answers to statistical queries (also known as linear queries) over the distribution. A statistical query is usually defined by some function query : $X \rightarrow [-1,1]$ (often other codomains such as [0, 1] or $[-R, +R]$, for some R, are considered). The analyst wants to learn the *population mean*, which (abusing notation) is defined as $\text{query}(P) = \mathop{\mathbb{E}}_{X \sim P} [\text{query}(X)].$

However, the distribution P can only be accessed via a set of samples X_1, \ldots, X_n drawn from . We assume that the samples are drawn independently and identically distributed (i.i.d.). These

197 198 samples are held by a mechanism $M(X_1, \ldots, X_n)$ who receives the query query and computes an answer $a \approx$ query(P).

199 200 201 The naïve way to approximate the population mean is to use the *empirical mean*, which (abusing notation) is defined as $query(X_1, ..., X_n) = \frac{1}{n} \sum_{i=1}^n query(X_i)$. However, the mechanism M can then adopt some methods for improving the generalization error.

202 203 204 205 206 207 In this work we consider analysts that ask a sequence of k queries query₁,..., query_k. If the queries are all chosen in advance, independently of the answers of each one of them, then we say they are non-adaptive. If the choice of each query query, depend on the prefix query₁, a_1, \ldots , query_{j-1}, a_{j-1} then they are fully adaptive. An important intermediate notion is r-round adaptive, where the sequence can be partitioned into r batches of non-adaptive queries. Note that non-interactive queries are 1-round and fully adaptive queries are k rounds.

We now review what is known about the problem of answering r -round adaptive queries.

THEOREM 2.1. For any distribution P , and any k non-adaptive statistical queries, the empirical *mean satisfies* max_{j=1,...,k} |a_j – query_j(P)| = $O\left(\sqrt{\frac{\log k}{n}}\right)$ $\frac{1}{n}$), and for any $r\geq 2$ and any r-round adaptive statistical queries, it satisfies max_{j=1,...,k} |a_j – query_j(P)| = $O\left(\sqrt{\frac{k}{n}}\right)$ Ι

In fact, these bounds are tight (up to constant factors) which means that even allowing one extra round of adaptivity leads to an exponential increase in the generalization error of the empirical mean, from $\log k$ to k.

[Dwork et al.](#page-25-0) [\[2015c\]](#page-25-0) and [Bassily et al.](#page-25-1) [\[2016\]](#page-25-1) showed that by using an alternative mechanism M which uses randomization in order to limit the dependency of a single query on the specific data instance, one can actually achieve much stronger generalization error as a function of the number of queries, specifically.

THEOREM 2.2 ([BASSILY ET AL. [2016;](#page-25-1) DWORK ET AL. [2015c\]](#page-25-0)). For any k , there exists a mechanism such that for any distribution P, and any $r \geq 2$ any r-round adaptive statistical queries, it satisfies

$$
\max_{j=1,\dots,k} |a_j - \text{query}_j(P)| = O\left(\frac{\sqrt[4]{k}}{\sqrt{n}}\right)
$$

Notice that Theorem [2.2](#page-4-0) has different quantification in that the optimal choice of mechanism depends on the number of queries. Thus, we need to know the number of queries a priori to choose the best mechanism.

[Dwork et al.](#page-25-0) [\[2015c\]](#page-25-0) also gave more refined bounds in terms of the number of rounds of adaptivity.

THEOREM 2.3 ([DWORK ET AL. [2015c\]](#page-25-0)). For any r and k, there exists a mechanism such that for any distribution P, and any $r \geq 2$ any r-round adaptive statistical queries, it satisfies

$$
\max_{j=1,\dots,k} |a_j - \text{query}_j(P)| = O\left(\frac{r\sqrt{\log k}}{\sqrt{n}}\right)
$$

This suggests that if one knows a good a priori upper bound on the number of rounds of adaptivity, one can get a much better guarantee of generalization error, but only by using an appropriate choice of the mechanism. The examples in Figure [2](#page-2-0) are experimental results on realistic two rounds and multiple rounds data analysis algorithms, illustrating these theorems.

A formal model for adaptivity. Motivated by the results discussed above, we will present a static analysis aimed at giving good a priori upper bounds on the number of rounds of adaptivity of a program. Before introducing the static analysis, we motivate the definition of adaptivity we will 1:6 Anon.

255 256 257 258 259 260 261 Fig. 3. (a) The program towRounds(k), an example with two rounds of adaptivity (b) The corresponding execution-based dependency graph (c) The corresponding program-based dependency graph from AdaptFun. use through a simple example illustrated in Figure [3\(](#page-5-0)a), which implements a simple "two rounds strategy" in our query while language (presented in Section [3\)](#page-7-0) and where the commands are labelled with the unique line numbers. We also show a execution-based dependency graph we use to define the adaptivity in Figure [3\(](#page-5-0)b) and the program-based dependency graph we estimate using our static analysis framework AdaptFun in Figure [3\(](#page-5-0)c).

262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 As shown in Figure [3\(](#page-5-0)a), the analyst asks in total $k+1$ queries to the mechanism in two phases. In the first phase, the analyst asks *k* queries and stores the answers that are provided by the mechanism. In the second phase, the analyst constructs a new query based on the results of the previous k queries and sends this query to the mechanism. More specifically, we assume that, in this example, the domain X contains at least k numeric attributes, which we index just by natural numbers. The queries inside the while loop correspond to the first phase and compute an approximation of the product of the empirical mean of the first k attributes. The query outside the loop corresponds to the second phase and computes an approximation of the empirical mean where each record is weighted by the sum of the empirical mean of the first k attributes. Since statistical queries computes the empirical mean of a function on rows, we use χ to abstract a possible row in the database and queries are of the form query(ψ), where ψ is a special expression (see syntax in Section [3\)](#page-7-0) representing a function : $X \to U$ on rows. We use U to denote the codomain of queries and it could be $[-1, 1]$, $[0, 1]$ or $[-R, +R]$, for some R we consider. This function characterizes the linear query we are interested in running. As an example, $x \leftarrow \text{query}(\chi[i] \cdot \chi[k])$ computes an approximation, according to the used mechanism, of the empirical mean of the product of the i^{th} attribute and k^{th} attribute, identified by $\chi[j] \cdot \chi[k]$. Notice that we don't materialize the mechanism but we assume that it is implicitly run when we execute the query.

270 280 281 282 283 284 285 286 287 288 289 290 291 292 293 This example is intuitively 2-rounds adaptive since we have two clearly distinguished phases, and the queries that we ask in the first phase do not depend on each other (the query $query(y[j] \cdot \chi[k])$ at line 3 only relies on the counter *j* and input k), while the last query (at line 6) depends on the results of all the previous queries. However, capturing this concept formally is surprisingly difficult. The difficulty comes from the fact that a query can depend on the result of another query in multiple ways, by means of data dependency or control flow dependency. In order to find the right definition for our goal, we take inspiration from the known results on the data analysis model we discussed above. This theory tells us that what we want to measure is the generalization error on the result of a query, and not an arbitrary manipulation of the query. Indeed, arbitrary manipulations can change the generalization error. As an example, suppose that v is the result we get from running a query, if we multiply this result by some constant, we are also changing the incurred error. Moreover, this theory tells us that we can always consider a non-adaptive set of queries as to being adaptive, and more importantly, that we can transform an adaptive query into a non-adaptive one, incurring an exponential blow up of the number of queries. For example, we could ask many queries upfront and depending on the results of some of them, we could return the results of others.

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302 303 304 305 306 307 308 309 To address these challenges, we first build a directed graph representing the possible dependencies between queries of a program and then we define the adaptivity of the program using this graph. We call this graph: execution-based dependency graph. The vertices in the graph represent the variables that are assigned in some command of the program. The edges represent dependency relations between vertices. The dependency relations are computed by looking at the execution traces of a program (see Section [4\)](#page-9-0). Additionally, we add weights to every vertex. The weight of a vertex is a function that given a starting state returns a natural number representing the number of times the vertex is visited when the program is executed starting from this state.

310 311 312 313 314 315 316 317 318 319 As an example, let us consider the graph in Figure [3\(](#page-5-0)b). This graph is built by considering all the possible execution traces of the program in Figure [3\(](#page-5-0)a). Each vertex in this graph has a superscript representing its weight, and a subscript 1 or 0 telling if the vertex corresponds to a query or not. We will call this subscript a query annotation. For example the vertex l^6 : $\frac{w_1}{l}$, has weight w_1 , a constant function which returns 1 for every starting state, since this query at line 6 is at most executed once regardless of the initial trace. The query annotation of this vertex is 1, which indicates that [l ← query($\chi[k]*a$]⁶ is a query request. Another vertex, $x^3 : \frac{w_k}{l}$, appears in the while loop. It has as weight a function w_k that for every initial state returns the value that k has in this state, since this is also the number the while loop will be iterated. The node j^4 : $\frac{w_k}{0}$ has as a subscript 0 representing a non-query assignment.

320 321 322 323 324 325 326 327 Since the edges between two vertices represent the fact that one program variable may depend on the other, we can define the program adaptivity with respect to a initial trace by means of a walk traversing the graph, visiting each vertex no more than its weight with respect to the initial trace, and visiting as many query nodes as possible. So, looking again at our example, we can see that in the walk along the dotted arrows, $l^6 \rightarrow a^5 \rightarrow x^3$, there are 2 vertices with query annotation 1 and that this number is maximal, i.e. we cannot find another walk having more than 2 vertices with query annotation 1, under the assumption that $k \geq 1$. So the adaptivity of the program in Figure [3\(](#page-5-0)a) is 2, as expected.

320 330 331 332 333 334 335 336 337 Static analysis for adaptivity. Our static analysis provides an upper bound on the adaptivity for this example as follows. AdaptFun constructs a program-based dependency graph, for our example we show this graph in Figure [3\(](#page-5-0)c). The edges of this graph are built by considering both control flow and data flow between assigned variables (the algorithm is presented in Section [5.3.3\)](#page-15-0). The weight of every vertex is estimated by using a reachability-bound estimation algorithm (presented in Section [5.3.2\)](#page-14-0), which can be symbolic and provide a sound upper bound on the weight of the corresponding vertex in the execution-based dependency graph. For instance, the weight k of the vertex x^3 in Figure [3\(](#page-5-0)c) is a sound upper bound on the weight w_k of vertex x^3 in Figure 3(b), with the same starting trace. The soundness of this step is proved in Theorem [5.1.](#page-14-1)

338 339 340 341 342 AdaptFun search a walk on this graph which overapproximate the adaptivity of the program (this is done by an algorithm AdaptSearch presented in Section [5.4\)](#page-15-1). For instance, in Figure [3\(](#page-5-0)c), AdaptSearch first finds a path $l^6: \frac{1}{1} \to a^5: \frac{k}{1} \to x^3: \frac{k}{1}$, and then approximate a walk with this path. Every vertex on this walk is visited once, and the number of vertices with query annotation 1 traversed in this path is 2, which is the upper bound we expect. It is worth to note here that even 344 345 though the node x^3 has weight depending on k, it is only visited once, similarly for l^6 , hence the overall upper bound on the adaptivity is 2, as we expect.

347 3 LABELED QUERY WHILE LANGUAGE

348 349 350 351 In this section, we formally introduce the language we will focus on for writing data analyses. This is a standard while language with some primitives for calling queries. After defining the syntax of the language and showing an example, we will define its trace-based operational semantics. This is the main technical ingredient we will use to define the program's adaptivity.

353 3.1 Syntax

We use $VAR, VAL, QVAL, C, DB$ and QD to stand for the set of variables, values, query values, commands, databases and the codomain of queries, respectively.

365 366 367 368 369 370 371 An expression is either a standard arithmetic expression or a boolean expression, or a list of expressions. Our language supports primitives for queries, where a specific query is specified by a query expression ψ . A query expression contains the necessary information for a query request, for example, $\gamma[a]$ represents the values at a certain index a in a row γ of the database. Query expressions combine access to the database with other expressions, for example, χ [3] + 5 represents a query which asks the value from the column 3 of each database raw χ , adds 5 to each of these values, and then computes the average of these values.

372 373 374 375 376 377 378 A labeled command c is just a command with a label — we assume that labels are unique, so that they can help to identify uniquely every subexpression. We have skip, assignment $x \leftarrow e$, the composition of two commands $c; c$, an if statement if (b, c, c) , a while statement while b do c . The main novelty of the syntax is the query request command $x \leftarrow q(\psi)$. For instance, if a data analyst wants to ask a simple linear query which returns the first element of the row, they can simply use the command $x \leftarrow q(\chi[1])$ in their data analysis program. We use $\mathcal{L}V$ to represent the universe of all the labeled variables.

3.2 Trace-based Operational Semantics

381 382 383 384 385 386 An event tracks useful information about each step of the evaluation, as a quadruple. Its first element is either an assigned variable (from an assignment command) or a boolean expression (from the guard of if or while command), follows by the label associated to this event, the value evaluated either from the expression assigned to the variable, or the boolean expression in the guard. The last element stores the query information, which a query value whose default is \bullet . We declare event projection operator π_i , which projects the *i*th element from an event.

Event ϵ ::= $(x, l, v, \bullet) | (x, l, v, \alpha)$ Assignment Event (k, l, v, \bullet) Testing Event

389 390 391 A trace $\tau \in \mathcal{T}$ is a list of events, collecting the events generated along the program execution. \mathcal{T} represents the set of traces. There are some useful operators: the trace concatenation operator $\cdot_+ : \mathcal{T} \to \mathcal{T} \to \mathcal{T}$, combines two traces. The belongs to operator $\in: \mathcal{E} \to \mathcal{T} \to \{true, false\}$

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Command × Trace → Command × Trace	$(c, \tau) \rightarrow (c', \tau')$					
$\langle \tau, e \rangle \Downarrow_e v$	$\epsilon = (x, l, v, \bullet)$	$\tau, \psi \Downarrow_q \alpha$	$\text{query}(\alpha) = v$	$\epsilon = (x, l, v, \alpha)$		
$\langle [x \leftarrow e]^l, \tau \rangle \rightarrow \langle [\text{skip}]^l, \tau : : \epsilon \rangle$	assn	$\tau, \psi \Downarrow_q \alpha$	$\text{query}(\alpha) = v$	$\epsilon = (x, l, v, \alpha)$	$\text{query}(\tau) = (x, l, v, \alpha)$	
$\tau, b \rightarrow_b \text{ true}$	$\epsilon = (b, l, \text{ true}, \bullet)$	$\tau, b \rightarrow_b \text{ false}$	$\epsilon = (b, l, \text{ false}, \bullet)$	$\text{while } [b]^l \text{ do } c, \tau \rangle \rightarrow \langle c; \text{ while } [b]^l \text{ do } c), \tau : : \epsilon \rangle$	$\text{while } [b]^l, \text{ do } c, \tau \rangle \rightarrow \langle [\text{skip}]^l, \tau : : \epsilon \rangle$	$\text{while } [b]^l, \text{ do } c, \tau \rangle \rightarrow \langle [\text{skip}]^l, \tau : \epsilon \rangle$
$\langle c_1, \tau \rangle \rightarrow \langle [\text{skip}]^l, \tau' \rangle$	$\langle [\text{skip}]^l, \langle c_2, \tau' \rangle \rightarrow \langle [\text{skip}]^l, \tau'' \rangle$	seq	$\tau, b \rightarrow_b \text{ true}$	$\epsilon = (b, l, \text{ true}, \bullet)$		
$\langle c_1, \tau \rangle \rightarrow \langle [\text{skip}]^l, \tau' \rangle$	$\langle [\text{skip}]^l, \langle c_2, \tau'$					

Fig. 5. Trace-based Operational Semantics for Language.

and its opposite ∉ express whether or not an event belongs to a trace. Another operator $\iota : \mathcal{T} \to$ $VAR \rightarrow \{N\} \cup \{\perp\}$, takes a trace and a variable as input and returns the label of the latest assignment event which assigns value to that variable. A trace can be regarded as the program history, which records queries asked by the analyst during the execution of the program. We collect the trace with a trace-based operational semantics based on transitions of the form $\langle c, \tau \rangle \rightarrow \langle c', \tau' \rangle$. It states that a configuration $\langle c, \tau \rangle$, which consists of a command c to be evaluated and a starting trace τ , evaluates to another configuration with the trace updated along with the evaluation of the command c to the normal form of the command skip.

The function $\theta : \mathcal{T} \to \mathcal{V} \mathcal{A} \mathcal{R} \to \mathcal{V} \mathcal{A} \mathcal{L} \cup \{\perp\}$, which maps a trace and a variable to the latest value assigned to this variable on the trace is defined as follows.

$$
\theta(\tau::(x, l, v, \bullet))x \triangleq v \quad \theta(\tau::(y, l, v, \bullet))x \triangleq \theta(\tau)x, y \neq x \quad \theta(\tau::(b, l, v, \bullet))x \triangleq \theta(\tau)x
$$

$$
\theta(\tau::(x, l, v, \alpha))x \triangleq v \quad \theta(\tau::(y, l, v, \alpha))x \triangleq \theta(\tau)x, y \neq x \quad \theta([\cdot])x \triangleq \bot
$$

We give a selection of rules of the trace-based operational semantics in Figure [5.](#page-8-0)

The rule assn evaluates a standard assignment $x \leftarrow e$, the expression e is first evaluated by our expression evaluation $\langle \tau, e \rangle \parallel_e v$, presented below. And the result v of evaluating e is used to construct a new event $\epsilon = (x, l, v, \bullet)$ and attach to the previous trace.

$$
\frac{\langle \tau, a \rangle \rightarrow_a v}{\langle \tau, a \rangle \downarrow_e v} \qquad \frac{\langle \tau, b \rangle \rightarrow_b v}{\langle \tau, b \rangle \downarrow_e v} \qquad \frac{\langle \tau, e_1 \rangle \downarrow_e v_1 \cdots \langle \tau, e_n \rangle \downarrow_e v_n}{\langle \tau, [e_1, \cdots, e_n] \rangle \downarrow_e [v_1, \cdots, v_n]} \qquad \frac{\langle \tau, a \rangle \downarrow_e v}{\langle \tau, v \rangle \downarrow_e v}
$$

425 426 The expression evaluation rules also rely on the evaluation of arithmetic expressions $\langle \tau, a \rangle \rightarrow_a v$ and boolean expressions $\langle \tau, b \rangle \rightarrow_b v$. The full rules can be found in the appendix.

Distinguished from the standard assignment evaluation, the rule query evaluates a query requesting command $[x \leftarrow query(\psi)]^l$ in two steps. The query expression ψ is first evaluated into a query value α by following the rules below. Then, by sending this query request query(α) to a hidden mechanism, this query is evaluated to a result value returned from it, $v = \frac{query(\alpha)}{log(\alpha)}$. Also, the generated event stores both the query value α here, and the result value of the query request.

$$
\frac{\langle \tau, a \rangle \rightarrow_a n}{\langle \tau, a \rangle \downarrow_q n} \qquad \frac{\langle \tau, \psi_1 \rangle \downarrow_q \alpha_1 \quad \langle \tau, \psi_2 \rangle \downarrow_q \alpha_2}{\langle \tau, \psi_1 \oplus_a \psi_2 \rangle \downarrow_q \alpha_1 \oplus_a \alpha_2} \qquad \frac{\langle \tau, a \rangle \rightarrow_a n}{\langle \tau, \chi[a] \rangle \downarrow_q \chi[n]} \qquad \frac{\langle \tau, a \rangle \rightarrow_a n}{\langle \tau, \alpha \rangle \downarrow_q \alpha}
$$

436 437 438 The rules for if and while both have two versions, when the boolean expressions in the guards are evaluated to true and false, respectively. In these rules, the evaluation of the guard generates a testing event and the trace is updated as well by appending this event.

439 440 If we observe the operational semantics rules, we can find that no rule will shrink the trace. It is proved in the appendix.

441

442 4 TRACE-BASED DEPENDENCY AND ADAPATIVITY

In this section, we present our definition of adaptivity on basis of an execution-based dependency graph. The construction of this graph requires us to think about the dependency relation between two queries using what we have at hand - the trace generated in Section [3.](#page-7-0)

4.1 Design choice of Dependency

In the data analysis model our programming framework supports, we define that a query is adaptively chosen when it is affected by answers of previous queries. The next thing is to decide how do we define whether one query is "affected" by previous answers, with the limited information we have? As a reminder, when the analyst asks a query, the only known information will be the answers to previous queries and the current execution trace of the program.

There are two possible situations that a query will be "affected", either when the query expression directly uses the results of previous queries (data dependency), or when the control flow of the program with respect to a query (whether to ask this query or not) depends on the results of previous queries (control flow dependency).

Since the the results of previous queries can be stored or used in variables which aren't associated to the query request, it is necessary to track the dependency between queries, through all the program's variables, and then we can distinguish variables which are assigned with query requests. We give a definition of when one variable may -depend on a previous variable with two candidates.

- (1) One variable may depend on a previous variable if and only if a change of the value assigned to the previous variable may also change the value assigned to the variable.
- (2) One variable may depend on a previous variable if and only if a change of the value assigned to the previous variable may also change the appearance of the assignment command to this variable during execution.

467 468 469 470 471 472 473 The first definition is defined as the witness of a variation on the value assigned to the same variable through two executions, according to the change of the value assigned to another variable in pretrace. In particular for query requests, the variation we observe is on the query value instead of on the query requesting results. In the simple program $c_1 = x \leftarrow$ query($\chi[2]$); $y \leftarrow$ query($\chi[3] + x$). From our perspective, query(χ [1]) is different from query(χ [2])). Informally, we think query(χ [3] + χ) may depend on the query query(γ [2])), because equipped function of the former γ [3] + x may depend on the data stored in x assigned with the result of query(χ [2])), according to this definition.

474 475 476 477 478 479 Nevertheless, the first definition fails to catch control dependency because it just monitors the changes to a query, but misses the appearance of the query when the answers of its previous queries change. For instance, it fails to handle $c_2 = x \leftarrow \text{query}(\chi[1])$; if $(x > 2, y \leftarrow \text{query}(\chi[2])$, skip), but the second definition can. However, it only considers the control dependency and misses the data dependency. This reminds us to define a may -dependency relation between labeled variables by combining the two definitions to capture the two situations.

4.2 Dependency

To define the may dependency relation on two labeled variables, we rely on the limited information at hand - the trace generated by the operational semantics. In this end, we first define the may dependency between events, and use it as a foundation of the variable may-dependency relation.

DEFINITION 1 (EVENTS DIFFERENT UP TO VALUE (Diff)). Two events $\epsilon_1, \epsilon_2 \in \mathcal{E}$ are Different up to Value, denoted as $Diff(\epsilon_1, \epsilon_2)$ if and only if:

$$
\pi_1(\epsilon_1) = \pi_1(\epsilon_2) \land \pi_2(\epsilon_1) = \pi_2(\epsilon_2)
$$
\n
$$
\land \big((\pi_3(\epsilon_1) \neq \pi_3(\epsilon_2) \land \pi_4(\epsilon_1) = \pi_4(\epsilon_2) = \bullet) \lor (\pi_4(\epsilon_1) \neq \bullet \land \pi_4(\epsilon_2) \neq \bullet \land \pi_4(\epsilon_1) \neq q \pi_4(\epsilon_2)) \big)
$$

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491 492 493 494 495 496 497 498 We compare two events by defining Diff(ϵ_1, ϵ_2). We use $\psi_1 = q \psi_2$ and $\psi_1 \neq q \psi_2$ to notate query expression equivalence and in-equivalence, distinct from standard equality. A program c's labeled variables is a subset of the labeled variables $\mathcal{L}V$, denoted by $\mathbb{L}\mathbb{V}(c) \in \mathcal{P}(\mathcal{V} \mathcal{R}\mathcal{R} \times \mathcal{L}) \subseteq \mathcal{L}V$. We also define the set of query variables for a program c , $\mathbb{Q} \mathbb{V} : C \to \mathcal{P}(\mathcal{L} \mathcal{V})$. A program c's query variables is a subset of its labeled variables, $\mathbb{Q}\mathbb{V}(c) \subseteq \mathbb{L}\mathbb{V}(c)$. We have the operator $\mathbb{TL} : \mathcal{T} \to \mathcal{L}$, which gives the set of labels in every event belonging to the trace. Then we introduce a counting operator cnt : $\mathcal{T} \to \mathbb{N} \to \mathbb{N}$, which counts the occurrence of of a labeled variable in the trace, whose behavior is defined as follows,

$$
\mathsf{cnt}(\tau::(l, l, l, l)) \triangleq \mathsf{cnt}(\tau, l) + 1 \quad \mathsf{cnt}(\tau::(l, l', l, l)) \triangleq \mathsf{cnt}(\tau, l), l' \neq l \quad \mathsf{cnt}([l, l) \triangleq 0
$$

The full definitions of these above operators can be found in the appendix.

 $\exists \tau_0, \tau_1, \tau' \in \mathcal{T}, \epsilon_1' \in \mathcal{E}^{\text{asn}}, c_1, c_2 \in C$. Diff $(\epsilon_1, \epsilon_1') \wedge$

DEFINITION 2 (EVENT MAY-DEPENDENCY)..

An event ϵ_2 is in the event may-dependency relation with an assignment event $\epsilon_1 \in \mathcal{E}^{\text{asn}}$ in a program c with a hidden database D and a trace $\tau \in \mathcal{T}$ denoted as $DEF_{\mathcal{E}}(\epsilon_1, \epsilon_2, [\epsilon_1]_{++} \tau_{++}[\epsilon_2], c, D)$, iff

504 505 506

$$
\frac{50t}{507}
$$

$$
\frac{508}{505}
$$

 $(\exists \epsilon_2' \in \mathcal{E} \cdot)$ \vec{r} $\langle c, \tau_0 \rangle \rightarrow^* \langle c_1, \tau_1 + [\epsilon_1] \rangle \rightarrow^* \langle c_2, \tau_1 + [\epsilon_1] + \tau_+ [\epsilon_2] \rangle$ $\wedge \langle c_1, \tau_{1}([\epsilon_1']) \rangle \rightarrow^* \langle c_2, \tau_{1}([\epsilon_1'] + \tau'_{1}([\epsilon_2']) \rangle$ \wedge Diff(ϵ_2, ϵ'_2) \wedge cnt($\tau, \pi_2(\epsilon_2)$) = cnt($\tau', \pi_2(\epsilon'_2)$) $\Big\}$ $\forall \exists \tau_3, \tau_3' \in \mathcal{T}, \epsilon_b \in \mathcal{E}^{\text{test}}$. $\overline{}$ « $\langle c, \tau_0\rangle\rightarrow^* \langle c_1,\tau_{1^{++}}[\epsilon_1]\rangle\rightarrow^* \langle c_2,\tau_{1^{++}}[\epsilon_1]_{^{++}}\tau_{^{++}}[\epsilon_b]_{^{++}}\tau_3\rangle$ $\wedge \quad \langle c_1, \tau_{1}([\epsilon_1']) \rangle \rightarrow^* \langle c_2, \tau_{1}([\epsilon_1'] + \tau' + [(\neg \epsilon_b)] + \tau_3' \rangle$ \bigwedge $\mathbb{TL}_{\tau_3} \cap \mathbb{TL}_{\tau_3'} = \emptyset \wedge \text{cnt}(\tau', \pi_2(\epsilon_b)) = \text{cnt}(\tau, \pi_2(\epsilon_b)) \wedge \epsilon_2 \in \tau_3 \wedge \epsilon_2 \notin \tau_3'$ ª ®)

514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 Our event *may-dependency* relation of two events $\epsilon_1 \in \mathcal{E}^{\text{asn}}$ and $\epsilon_2 \in \mathcal{E}$, for a program c and hidden database D is w.r.t to a trace $[\epsilon_1]_{\mu+\tau+\lceil\epsilon_2\rceil}$. The $\epsilon_1 \in \mathcal{E}^{\text{asn}}$ is an assignment event because only a change on an assignment event will affect the execution trace, according to our operational semantics. In order to observe the changes of ϵ_2 under the modification of ϵ_1 , this trace $[\epsilon_1]_{+\tau}$ ++ $[\epsilon_2]$ starts with ϵ_1 and ends with ϵ_2 . The *may-dependency* relation considers both the value dependency and value control dependency as discussed in Section [4.1.](#page-9-1) The relation can be divided into two parts naturally in Definition [2](#page-10-0) (line 2 − 4, 5 − 8 respectively, starting from line 1). The idea of the event ϵ_1 may depend on ϵ_2 can be briefly described: we have one execution of the program as reference (See line 2 and 6, for the two kinds of dependency). When the value assigned to the first variable in ϵ_1 is modified, the reference trace $\tau_1 + [\epsilon_1]$ is modified correspondingly to $\tau_1 + [\epsilon'_1]$. We use Diff(ϵ_1, ϵ'_1) at line 1 to express this modification, which guarantees that ϵ_1 and ϵ'_1 only differ in their assigned values and are equal on variable name and label. We perform a second run of the program by continuing the execution of the same program from the same execution point, but with the modified trace τ_{1} + $[\epsilon'_1]$ (See line 3, 7). The expected may dependency will be caught by observing two different possible changes (See line 4, 8 respectively) when comparing the second execution with the reference one (similar definitions as in [\[Cousot](#page-25-4) [2019\]](#page-25-4)).

530 531 532 533 534 535 536 537 538 In the first part (line 2–4 of Definition [2\)](#page-10-0), we witness the appearance of ϵ'_2 in the second execution, and a variation between ϵ_2 and ϵ'_2 on their values. We have special requirement Diff(ϵ_2, ϵ'_2), which guarantees that they have the same variable name and label but only differ in their evaluated values. In particularly for queries, if ϵ_2 and ϵ'_2 are generated from query requesting, then <code>Diff(ϵ_2,ϵ'_2)</code> guarantees that they differ in their query values rather than the query requesting results. Additionally, in order to handle multiple occurrences of the same event through iterations of the while loop, where ϵ_2 and ϵ'_2 could be in different while loops, we restrict the same occurrence of ϵ_2 's label in τ from the first execution with the occurrence of ϵ_2 's label in τ ' from the second execution, through cnt $(\tau, \pi_2(\epsilon_2))$ = cnt $(\tau', \pi_2(\epsilon'_2))$ at line 4.

.

540 541 542 543 544 545 546 547 548 In the second part (line 5–8 of Definition [2\)](#page-10-0), we witness the disappearance of ϵ_2 through observing the change of a testing event ϵ_b . To witness the disappearance, the command that generates ϵ_2 must not be executed in the second execution. The only way to control whether a command will be executed, is through the change of a guard's evaluation result in an if or while command, which generates a testing event ϵ_b in the first place. So we observe when ϵ_b changes into $\neg \epsilon_b$ in the second execution firstly, whether it follows with the disappearance of ϵ_2 in the second trace. We restrict the occurrence of ϵ_b 's label in the two traces being the same through $\text{cnt}(\tau', \pi_2(\epsilon_b)) = \text{cnt}(\tau, \pi_2(\epsilon_b))$ to handle the while loop. Again, for queries, we observe the disappearance based on the query value equivalence.

549 550 Considering all events generated during a program's executions under an initial trace, as long as there is one pair of events satisfying the event may-dependency relation in Definition [2,](#page-10-0) we say the two related variables satisfy the variable may-dependency relation, in Definition [3.](#page-11-0)

DEFINITION 3 (VARIABLE MAY-DEPENDENCY)..

A variable $x_2^{l_2} \in \mathbb{LV}(\mathfrak{c})$ is in the variable may-dependency relation with another variable $x_1^{l_1} \in \mathbb{LV}(\mathfrak{c})$ in a program c, denoted as $\text{DEP}_{var}(x_1^{l_1}, x_2^{l_2}, c)$, if and only if.

$$
\exists \epsilon_1, \epsilon_2 \in \mathcal{E}^{\text{asn}}, \tau \in \mathcal{T}, D \in \mathcal{DB} \ . \ \pi_1(\epsilon_1)^{\pi_2(\epsilon_1)} = x_1^{l_1} \wedge \pi_1(\epsilon_2)^{\pi_2(\epsilon_2)} = x_2^{l_2} \wedge \text{DEP}_e(\epsilon_1, \epsilon_2, \tau, c, D)
$$

4.3 Execution Based Dependency Graph

Based on the variable may-dependency relation, we define the execution-based dependency graph.

DEFINITION 4 (EXECUTION BASED DEPENDENCY GRAPH). Given a program c, its execution-based dependency graph $G_{trace}(c) = (V_{trace}(c), E_{trace}(c), W_{trace}(c), Q_{trace}(c))$ is defined as follows,

$$
\begin{array}{rcl}\n\text{Vertices} & \mathsf{V}_{\text{trace}}(c) & := & \left\{ x^l \in \mathcal{L} \mathcal{V} \, \Big| \, x^l \in \mathbb{L} \mathbb{V}(c) \right\} \\
\text{Directed Edges} & \mathsf{E}_{\text{trace}}(c) & := & \left\{ (x^l, y^j) \, \Big| \, x^i, y^j \in \mathbb{L} \mathbb{V}(c) \land \text{DEP}_{\text{var}}(x^i, y^j, c) \right\} \\
\text{Weights} & \mathbb{W}_{\text{trace}}(c) & := & \left\{ (x^l, w) \, \Big| \, w : \mathcal{T} \to \mathbb{N} \land x^l \in \mathbb{L} \mathbb{V}(c) \right. \\
\text{Matrix} & \mathbb{V}_{\text{trace}}(c) & := & \left\{ (x^l, w) \, \Big| \, w : \mathcal{T} \to \mathbb{N} \land x^l \in \mathbb{L} \mathbb{V}(c) \right. \\
\text{Query Annotation} & \mathbb{Q}_{\text{trace}}(c) & := & \left\{ (x^l, n) \, \Big| \, x^l \in \mathbb{L} \mathbb{V}(c) \land n = 1 \Leftrightarrow x^l \in \mathbb{Q} \mathbb{V}(c) \land n = 0 \Leftrightarrow x^l \notin \mathbb{Q} \mathbb{V}(c) \right\}\n\end{array}
$$

569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 There are four components of the execution-based dependency graph. The vertices $V_{trace}(c)$ is the set of program c 's labeled variables $LV(c)$, which are statically collected. The query annotation is a set of pairs $Q_{\text{trace}}(c) \in \mathcal{P}(\mathcal{L}V \times \{0,1\})$ mapping each $x^l \in V_{\text{trace}}(c)$ to 0 or 1, indicating whether this labeled variable is in program c's query variable set $\mathbb{Q}\mathbb{V}(c)$. The weights is a set of pairs, $(x^l, w) \in LV \times (T \to \mathbb{N})$, with a labeled variable as first component and its weight w the second component. Weight w for x^l is a function $w : \mathcal{T} \to \mathbb{N}$ mapping from a starting trace to a natural number. When program executes under this starting trace τ , $\langle c, \tau \rangle \rightarrow^* \langle \text{skip}, \tau_{++} \tau' \rangle$, it generates an execution trace τ' . This natural number is the evaluation times of the labeled command corresponding to the vertex, computed by the counter operator $w(\tau) = \text{cnt}(\tau', l)$. We can see in the execution-based dependency graph of twoRounds in Figure [3\(](#page-5-0)b), the weight of vertices in the while loop is $\theta(\tau)$, which depends on the value of the user input k specified in the starting trace τ . The directed edges $E_{\text{trace}}(c)$ is also a set of pairs with two labeled variables $(x^i, y^j) \in \mathcal{L}(\mathcal{V} \times \mathcal{L}(\mathcal{V}),$ from x^{i} pointing to y^{j} in the graph. The edges are constructed directly from our variable may-dependency relation. For any two vertices x^i and y^j in $V_{\text{trace}}(c)$, if they satisfy the variable may-dependency relation DEP_{var} (x^{i}, y^{j}, c) , there is a direct edge between the two vertices in our execution-based dependency graph for program c .

585 586 587 In most data analysis programs c we are interested, there are usually some user input variables, such as k in twoRounds. We denote $\mathcal{T}_0(c)$ as the set of initial traces in which all the input variables in c are initialized, it is also reflected in $W_{trace}(c)$.

Fig. 6. The overview of AdaptFun

4.4 Trace-based Adaptivity

Given a program c's execution-based dependency graph $G_{trace}(c)$, we define adaptivity with respect to an initial trace $\tau_0 \in \mathcal{T}_0(c)$ by the finite walk in the graph, which has the most query requests along the walk. We show the definition of a finite walk as follows.

DEFINITION 5 (FINITE WALK (K)).

Given the execution-based dependency graph $G_{trace}(c) = (V_{trace}(c), E_{trace}(c), W_{trace}(c), Q_{trace}(c))$ of a program c, a finite walk k in $G_{trace}(c)$ is a function $k : \mathcal{T} \to \mathcal{E}$ sequence of edges. For a initial trace $\tau_0 \in \mathcal{T}_0(c)$, $k(\tau_0)$ is a sequence of edges $(e_1 \ldots e_{n-1})$ for which there is a sequence of vertices (v_1, \ldots, v_n) such that:

• $e_i = (v_i, v_{i+1}) \in E_{\text{trace}}(c)$ for every $1 \leq i < n$.

• every $v_i \in V_{\text{trace}}(c)$ and $(v_i, w_i) \in W_{\text{trace}}(c)$, v_i appears in (v_1, \ldots, v_n) at most $w(\tau_0)$ times.

The length of $k(\tau_0)$ is the number of vertices in its vertices sequence, i.e., $len(k) (\tau_0) = n$.

We use $W\mathcal{K}(\mathsf{G}_{\text{trace}}(c))$ to denote the set containing all finite walks k in $\mathsf{G}_{\text{trace}}(c)$; and $k_{v_1\rightarrow v_2} \in$ $\mathcal{W}\mathcal{K}(\mathsf{G}_{\textsf{trace}}(c))$ with $v_1, v_2 \in \mathsf{V}_{\textsf{trace}}(c)$ denotes the walk from vertex v_1 to v_2 .

We are interested in queries, so we need to recover the variables corresponding to queries from the walk. We define the query length of a walk, instead of counting all the vertices in k 's vertices sequence, we just count the number of vertices which correspond to query variables in this sequence.

Definition 6 (Query Length of the Finite Walk(1en^q)). .

Given the execution-based dependency graph $G_{trace}(c) = (V_{trace}(c), E_{trace}(c), W_{trace}(c), Q_{trace}(c))$ of a program c, and a finite walk $k \in W\mathcal{K}(\mathsf{G}_{\text{trace}}(c))$. The query length of k is a function $\textsf{len}^{\mathsf{q}}(k)$: $\mathcal{T} \to \mathbb{N}$, such that with an initial trace $\tau_0 \in \mathcal{T}_0(c)$, len $\mathfrak{q}(k)(\tau_0)$ is the number of vertices which correspond to query variables in the vertices sequence of the walk $k(\tau_0)$ (v_1, \ldots, v_n) as follows,

 $\text{len}^q(k)(\tau_0) = |(v \mid v \in (v_1, \ldots, v_n) \land Q(v) = 1)|.$

The definition of adaptivity is then presented in Def [7](#page-12-0) below.

DEFINITION 7 (ADAPTIVITY OF A PROGRAM)..

Given a program c, its adaptivity $A(c)$ is function $A(c) : \mathcal{T} \to \mathbb{N}$ such that for an initial trace $\tau_0 \in \mathcal{T}_0(c),$

$$
A(c)(\tau_0) = \max\left\{\text{len}^{\mathsf{q}}(k)(\tau_0) \mid k \in \mathcal{W}\mathcal{K}(\mathsf{G}_{\text{trace}}(c))\right\}
$$

5 THE STATIC ANALYSIS ALGORITHM ON PROGRAMS

In this section, we present our static program analysis for computing an upper bound on the adaptivity of an arbitrary program c , as we define in last section.

633 5.1 A guide to the static program analysis framework

634 635 636 Our program analysis framework AdaptFun can be divided as two steps: 1) to construct a weighted depdenency graph based on c . 2) to find a path in this graph, which is used to estimate an upper bound on the adaptivity of c.

638 639 640 641 5.1.1 Graph Estimation. According to adaptivity defined over program's execution-based dependency graph (in Definition [4\)](#page-11-1), we first build a similar graph to over-approximate that graph. The construction considers the vertices, edges, and the weight of every vertex, as well as some annotations which mark queries. The overall picture of this step is organized as follows.

- (1) Vertices are the assigned variables with unique labels, extracted directly from the program, see Section [5.2.](#page-13-0)
- 644 645 (2) Query annotations are also decided directly from the program, when there is a query request, the associated variable will be marked as 1, otherwise, 0. See Section [5.2.](#page-13-0)
	- (3) Every vertex has a weight, which tells the maximal times this vertex can be visited in a possible execution. This weight is estimated by a reachability bound analysis on each vertex. See Section [5.3.2.](#page-14-0)
		- (4) Edges between vertices consider both control flow and data flow, See Section [5.3.3.](#page-15-0)
		- (5) Finally, with all the ingredients ready, we construct the final approximated program-based dependency graph in Section [5.4.](#page-15-1)

Overall, this program-based graph has a similar topology as the execution-based dependency graph. It has the same vertices and query annotation, but approximated edges and weights. We call this generated approximation graph, program-based dependency graph.

658 659 5.1.2 Adaptivity Computation. Likewise the adaptivity is defined as a finite walk in the execution based dependency graph, our static estimation on this adaptivity also relies on finding a walk in the program-based dependency graph. We discuss some challenges in finding the 'appropriate' walk in the graph, and how our algorithm responds to these challenges as in Section [5.4.](#page-15-1)

5.2 Vertices Estimation and Query Annotation Estimation

The vertices in the program-based dependency graph are identical to the execution-based dependency graph, which are assigned variables in the program annotated with unique labels, $V_{\text{prog}}(c) \triangleq V_{\text{trace}}(c)$.

In the same way, the query annotation in program-based dependency graph is identical to the execution-based dependency graph. We define $Q_{prog}(c) \triangleq Q_{trace}(c)$.

5.3 Weight and Edge Estimation

The weight of every vertex in the execution-based graph relies on program's execution traces. In order to over-approximate the weight statically but still tightly, we present a symbolic reachability bound analysis for estimation of the weight of each vertex(label) in Section [5.3.2,](#page-14-0) in spirit of some reachablility bound techniques.

Since the edges of the execution-based graph of a program relies on the dependency relation, which handles both control flow and data flow, as an over-approximation of this graph, the edges of our program-based dependency graph also cover these two kind of flows. We develop a feasible data flow relation to catch them, in Section [5.3.3.](#page-15-0)

The edge and weight estimation are both performed on basis of an abstract control flow graph of the program, we first show how to generate this abstract execution control flow graph before the introduction of the edge and weight estimation.

681 682 683 684 685 5.3.1 Abstract Execution Control Flow graph. We define an abstract control flow graph for program c, whose vertices are the unique labels from c 's labeled commands with a special label ex for the exit of the program. Each edge (l_1, dc, l_2) of our abstract control flow graph is annotated with a difference constraint, which is used to describe the execution of l_1 . The edge itself talks about the transition between l_1 to l_2 . Still for the same twoRounds(k) example as overview, its generated

642 643

696 697 Fig. 7. (a) The same towRounds(k) program as Figure [3](#page-5-0) (b) The abstract control flow graph for towRounds(k) (c) The abstract control flow graph with the reachability bound for towRounds(k).

698 699 700 701 702 703 704 705 706 707 708 709 710 abstract control flow graph is shown in Figure [7\(](#page-14-2)b). For example, the edge $(0, a \le 0, 1)$ on the top, tells us the command $[a \leftarrow 0]^0$ is executed with next continuation location 1, where the command $[j \leftarrow k]^1$ will be executed next. The constraint $a \le 0$ is a difference constraint, generated by abstracting from the assignment command $a \leftarrow 0$, representing that value of *a* is less than or equals to 0 after location 0 before executing command at line 1. The difference constraint is an inequality relation. The left-hand side of the inequality talks about variables before the execution and the right-hand side ascribes those after the execution. The difference constraint $a < a + x$ on the edge $(5, a < a+x, 2)$ describes the execution of the command $[a \leftarrow a+x]^5$. The cycle $2 \rightarrow 4 \rightarrow 5 \rightarrow 2$ in Figure [7\(](#page-14-2)b). Please also look at the edge from 3 to 4, which talks about the query. The $x < Q_m$ describes the execution of a query request (the command at line 3), the query results stored in x is bounded by Q_m . Q_m is the maximal value for query requesting result from the database DB. ⊤ means there is no assignment executed, for example, we have the difference constraint ⊤ on the edge 2 to 6, means at line 2, there is no assignment (it is a testing guard $j > 0$.)

711 712 713 714 715 716 717 718 719 720 721 722 5.3.2 Weight Estimation. In order to estimate weight for every vertex in the program-based dependency graph, we perform the symbolic reachability bound analysis on the abstract control flow graph and add weight as shown in Figure [7\(](#page-14-2)c). We use $absW(c)$ for the computed weights, a set of pairs (l, w) where w is the weight for label *l* from the abstract control flow graph of c. w is an arithmetic expression over N and input variables, denoted by \mathcal{A}_{in} . This analysis is inspired from the program complexity analysis method in [\[Sinn et al.](#page-27-2) [2017a\]](#page-27-2). The detail of our symbolic reachability bound analysis which uses the difference constraint of the abstract control flow graph can be found in the appendix. Then we compute the weight for each vertex in $V_{\text{bros}}(c)$, as a set of pairs $(x^l, w) \in \mathcal{L} \times \overline{\mathcal{A}}_{in}$ mapping each $x^l \in V_{\text{prog}}(c)$ to an arithmetic expression over N and input variables. Because the vertices in the two graph share the same unique label, the line number of the same command, we define $W_{\text{brog}}(c)$ as follows,

$$
W_{\text{prog}}(c) \triangleq \{ (x^l, w) \mid x^l \in V_{\text{prog}}(c) \land (l, w) \in \text{absW}(c) \}.
$$

We prove that this arithmetic expression for $x^l \in V_{\text{prog}}(c)$ is a sound upper bound of the maximum visiting times of x^l over all execution traces of c, with the full proof in the appendix.

THEOREM 5.1 (SOUNDNESS OF THE REACHABILITY BOUNDS ESTIMATION). Given a program c with its estimated weight $W_{\text{prog}}(c)$ we have:

$$
\forall (x^l, w) \in W_{\text{prog}}, \tau_0 \in \mathcal{T}_0(c), \tau \in \mathcal{T}, v \in \mathbb{N}. \langle c, \tau_0 \rangle \rightarrow^* \langle \text{skip}, \tau_{0^{++}} \tau \rangle \land \langle \tau_0, w \rangle \Downarrow_e v \implies \text{cnt}(\tau, l) \leq v
$$

Example. As in Figure [3\(](#page-5-0)c), the weight for a^5 is k. which is a sound estimated weight. For any initial $\tau_0 \in \mathcal{T}_0(c)$, we know $\langle \tau_0, k \rangle \Downarrow_e \theta(\tau_0) k$ and the weight w_k for vertex a^5 from Figrue [3\(](#page-5-0)b) $w_k(\tau_0) = \theta(\tau_0)k$. In the same way, the weights for all the other vertices are sound.

1:16 Anon. **Anon.** Anon. **Anon.** Anon. **Anon.** Anon. **Anon.** Anon. **Anon.** Anon. **Anon.**

736 737 738 5.3.3 Edge Estimation. We show how to estimate the directed edges for the program-based dependency graph. We develop a variant of data flow analysis, called Feasible Data-Flow Generation, which produces a sound approximation of the edges in the execution based dependency graph.

Feasible Data-Flow Generation. We generate edges by using both control and data flow in the following flowsTo relation, which uses the results of reaching definition analysis, as $RD(l, c)$ for every label l in a program c . FV computes the set of free variables in an expression.

DEFINITION 8 (FEASIBLE DATA-FLOW). *Given a program* c *and two labeled variables* x^{i} , y^{j} *in this* program, flowsTo (x^{i}, y^{j}, c) is

We prove that this *Feasible Data-Flow* relation is a sound approximation of the *variable may-*Dependency relation over labeled variables for every program, in the appendix.

Edge Estimation. Then we define the estimated directed edges between vertices in $V_{\text{prog}}(c)$, as a set of pairs $E_{\text{prog}}(c) \in \mathcal{P}(\mathcal{L}V \times \mathcal{L}V)$ indicating a directed edge from the first vertex to the second one in each pair as follows,

$$
\mathsf{E}_{\text{prog}}(c) \triangleq \{ (y^j, x^i) \mid y^j, x^i \in \mathsf{V}_{\text{prog}}(c) \land \exists n, z_1^{r_1}, \dots, z_n^{r_n} \in \mathbb{L}\mathbb{V}(c) .
$$

\n
$$
n \geq 0 \land \text{flowsTo}(x^i, z_1^{r_1}, c) \land \dots \land \text{flowsTo}(z_n^{r_n}, y^j, c) \}
$$

We prove that this estimated directed edge set $E_{\text{prog}}(c)$ is a sound approximation of the edge set in 's execution-based dependency graph in the appendix.

Example. Look at Figure [3\(](#page-5-0)c), and take the edge (l^6, a^5) for example. By flowsTo(l^6, a^5, c), we can see *a* is used directly in the query expression $\chi[k] * a$, in the assignment command [l ← query($\chi[k]*a$]^{l}, i.e., $a \in FV(\chi[k]*a)$. Also, from the reaching definition analysis, we know $a^5 \in RD(6, \text{twoRounds}(k))$. Then we have flowsTo(l^6, a^5, c) and construct the edge (l^6, a^5). And the same way for constructing the rest edges. Also, the edge (x^3, j^5) in the same graph represents the control flow, caught by our flowsTo relation.

5.4 Adaptivity Upper Bound Computation

We notate our dependency graph as follows:

$$
G_{\text{prog}}(c) = (V_{\text{prog}}(c), E_{\text{prog}}(c), W_{\text{prog}}(c), Q_{\text{prog}}(c))
$$

775 776 777 778 779 780 781 782 783 with $V_{\text{prog}}(c)$, $E_{\text{prog}}(c)$, $W_{\text{prog}}(c)$ and $Q_{\text{prog}}(c)$ as computed in each steps above. Its formal definition can be found in the appendix. We compute the adaptivity upper bound for a program c by the maximum query length over all finite walks in the program-based data dependency graph $G_{\text{prog}}(c)$, defined formally in Definition [9.](#page-16-0) We use $\mathcal{W}\mathcal{K}(\mathsf{G}_{\text{prog}}(c))$ to represent the walks over the programbased dependency graph for c. Different from the walks on $G_{trace}(c)$, $k \in \mathcal{WK}(G_{\text{broy}}(c))$ doesn't rely on the initial trace. The occurrence time of every v_i in k's vertices sequence is bound by an arithmetic expression w_i where $(v_i, w_i) \in W_{\text{prog}}(c)$ is v_i 's estimated weight. Then we have len^q(k) \in \mathcal{A}_{in} as well. The full definition for $W\mathcal{K}(\mathsf{G}_{\text{prog}}(c))$ and len^q over $W\mathcal{K}(\mathsf{G}_{\text{prog}}(c))$ is in the appendix.

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Fig. 8. (a) The simple while loop example (b) The program-based dependency graph generated from AdaptFun. DEFINITION 9 (PROGRAM-BASED ADAPTIVITY).

Given a program c and its program-based graph $G_{\text{brog}}(c)$ the program-based adaptivity for c is defined as

$$
A_{\text{prog}}(c) \triangleq \max\left\{ \text{len}^{\text{q}}(k) \mid k \in \mathcal{W}\mathcal{K}(\mathsf{G}_{\text{prog}}(c)) \right\}.
$$

Based on our soundness of the program-based adaptivity, our program-based adaptivity is a sound upper bound of its adaptivity in Definition [7.](#page-12-0)

THEOREM 5.2 (SOUNDNESS OF $A_{\text{prog}}(c)$). For every program c, its program-based adaptivity is a sound upper bound of its adaptivity.

$$
\forall \tau_0 \in \mathcal{T}_0(c) \ . \ \langle A_{\text{prog}}(c), \tau_0 \rangle \Downarrow_e n \implies n \geq A(c)(\tau_0)
$$

To estimate a sound and precise upper bound on adaptivity, we develop an adaptivity estimation algorithm called AdaptSearch (in the appendix Alg. I), which uses both the deep first search and breath first search strategy to find the walk. We also show that the estimated adaptivity from our AdaptSearch is sound with respect to the program-based adaptivity.

THEOREM 5.3 (SOUNDNESS OF AdaptSearch). For every program c.

AdaptSearch($G_{\text{prog}}(c)$) $\geq A_{\text{prog}}(c)$.

The full proofs and details of all the soundness can be found in the appendix.

811 812 813 The key novelty of AdaptSearch is its walk finding part, we first discuss two challenges when we try to find the walks in the program-based dependency graph, and show that how we solve them using our algorithms.

814 815 816 817 818 81^c 820 Non-Termination Challenge: One naive walk finding method is to simply traverse on this program-based dependency graph by decreasing the weight of every node by one after every visit. However, this simple traversing strategy leads to a non-termination dilemma for most programs we are interested in because the weight can be a symbolic expression. Look at the simple example in Figure [8,](#page-16-1) where k is the input variable from domain N. If we traverse on the program-based dependency graph, and decrease the weight of x^3 (the weight k is symbolic) by one after every visit, we will never terminate because we only know $k \in \mathbb{N}$.

821 822 823 824 825 826 To solve this non-termination challenge, we switch to another walk finding approach: we first find a longest path in the program-based dependency graph and then approximate the walk with the path. Through a simple deep first search algorithm, we find the longest weighted path as the dotted arrow in Figure [8,](#page-16-1) $x^3 : \frac{1}{1} \to x^1 : \frac{1}{1}$. Then, by summing up the weights on this path where the vertices have query annotation 1, deep first search algorithm gives the adaptivity bound $1 + k$. This is a tight bound for this program's adaptivity. This approach is the fundamental of AdaptSearch.

827 828 829 830 831 832 Approximation Challenge: We adopt a deep first strategy to search for the longest weighted path, and then use the path to approximate the adaptivity. We find that this gives us overapproximation to a large extend. This over-approximation could result in an ∞ adaptivity upper bound on the program with actual adaptivity 2. Look at twoRounds in overview, we find the longest weighted path is $x^3 : \frac{k}{1} \to a^5 : \frac{k}{0} \to l^6 : \frac{1}{0}$ in Figure [3\(](#page-5-0)c) with weighted query length 1 + k. If we use this path to approximate a finite walk, and weight of each vertex as its visiting times, we

834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 have the estimated walk $x^3 \to \cdots \to x^3 \to a^5 \to \cdots \to a^5 \to l^6$, in which x^3 appears k times. Obviously, its weighted query length, $1 + k$, over approximates the adaptivity of this example to a large extend, which is supposed to be 2. The reason of the over-approximation comes from the missing consideration of the restriction on vertex's visiting times in a walk. Moreover, the restriction plays different roles in cases whether there is cycle in the graph. This leads us to consider cycle in the program-based dependency graph in AdaptSearch, and we develop an auxiliary algorithm to estimate the adaptivity for cycles in the graph, $AdaptSearch_{src} (G)$ as in Alg. [1.](#page-17-0) AdaptSearch_{scc} takes an strong connected graph, which is an strong connected component (SCC) of $G_{\text{prog}}(c)$ and approximates the path to a precise walk to compute the adaptivity of this subgraph. In general, AdaptSearch will now first find all the SCCs of $G_{\text{prog}}(c)$ by using the Kosaraju's algorithm[\[Sharir](#page-27-3) [1981\]](#page-27-3). Then AdaptSearch simplifies the input graph by replacing every strong connected components with, a vertex whose weight is the adaptivity of the SCC, calculated by AdaptSearch_{scc} (G). Then AdaptSearch performs the standard breath first search strategy to find the longest weighted path on this simplified graph and returns the estimation on adaptivity as we shown before. The full details of AdaptSearch is in the appendix Alg. 2.

873 874 875 876 877 878 879 880 881 Adaptivity Computation Algorithm on SCC Graph (AdaptSearch_{scc} (G)). This algorithm in Alg. [1](#page-17-0) takes a subgraph of the program-based dependency graph(SCC), and the output is the adaptivity of the input. For an SCC containing only one vertex, it returns the query annotation of this vertex as adaptivity. For SCC containing at least one edge, There are three steps: 1. find out all the paths in the input 2. calculate the adaptivity of every path using our designed adaptivity counting method. 3. return the maximal adaptivity among all the paths. Because our input graph is SCC, when we start traversing from a vertex, we will finally go back to this vertex. The paths we find in step 1 are all those with the same starting and ending vertex. The most interesting part is step 2. For the SCC containing at least one edge, we compute the adaptivity for each path on the fly of searching

Fig. 9. (a) The nested while loop example, (b) The program-based dependency graph generated from AdaptFun.

for the paths in the recursion algorithm dfs. It is designed based on a deep first search strategy from line: 6-16. In order to guarantee the visiting times of each vertex by its weight and compute the adaptivity accurately, we use a special parameter flowcapacity to track the minimum weight along the path during the searching procedure, and a parameter querynum to track the total number of vertices with query annotation 1 along the path.

flowcapacity is a list of arithmeitc expression \mathcal{A}_{in} recording the minimum weight when the path reaches that vertex, which is initialized by ∞ .

querynum is a list of integer initialized by query annotation $Q(v)$ for every vertex.

902 903 904 905 906 907 908 The updating operations during the traverse (line: 8) and at the end of the traverse (line: 11) are interesting, specifically flowcapacity $[v] \times$ querynum $[v]$ computes the query length for this path. it guarantees the visiting times of each vertex on the path reaching a vertex v is no more than the maximum visiting times it can be on a qualified walk, through flowcapacity[v], and in the same time compute the query length instead of weighted length accurately through querynum[v]. In this way, we resolve the Approximation Challenge without losing the soundness, formally in the appendix.

909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 Now, we show an example illustrating how our two updating operations for adaptivity for each path can guarantee both the accuracy and the soundness. Look at a Nested While Loop example program in Figure [9.](#page-18-0) We first search for a path: $y^6 \rightarrow y^6$, and compute the adaptivity for this path as k . Notice here, another special operation we have in the second branch is Non-updating of querynum and flowcapacity. This guarantees both the accuracy and the soundness. Specifically, if this vertex is visited, it indicates that a cycle is monitored and the traversing on this cycle is finished by going back to this vertex. When we continuously search for walks heading out of this vertex, the minimum weight on this cycle does not affect the walks going out of this vertex that will not pass this cycle. However, if we keep recording the minimum weight, then we restrict the visiting times of vertices on a walk by using the minimum weight of vertices not on this walk. Then, it is obviously that this leads to unsoundness. If we update the flowcapacity [y^6] as k after visiting y^6 the second time on this walk, and continuously visit x^9 , then the flowcapacity[k] is updated as $min(k, k^2)$. So the visiting times of x^9 is restricted by k on the walk $y^6 \rightarrow y^6 \rightarrow x^9$. This restriction excludes the finite walk $y^6 \to y^6 \to x^9 \to x^9$ where y^6 and x^9 visited by k^2 times in the computation. However, the finite walk $y^6 \to y^6 \to x^9 \to x^9$ where y^6 is visited k times and x^9 is visited k^2 times, is a qualified walk, and exactly the longest walk we aim to find. So, by Non-updating the flowcapacity after visiting y again, we guarantee that the visiting times of vertices on every searched walk will not be restricted by weights not on this walk. In the last line of this dfs algorithm, line: 16, it returns the adaptivity heading out from its input vertex. By applying this deep first search strategy on every vertex on this SCC, we compute the adaptivity of this SCC by taking the maximum value over every vertex. The soundness is formally guaranteed in the appendix.

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942 Fig. 10. (a) The simplified multiple rounds example (b) The program-based dependency graph from AdaptFun

943 6 EXAMPLES AND IMPLEMENTATIONS

We present four examples, illustrating AdaptFun. Then we show our implementation of AdaptFun and its experimental results on 18 examples including these four examples.

6.1 Examples

Example 6.1 (Multiple Rounds Algorithm). We look at an advanced adaptive data analysis algo-rithm - multiple rounds algorithm, as in Figure [10\(](#page-19-1)a). It takes the user input k which decides the number of iterations. It starts from an initialized empty tracking list I , goes k rounds and at every round, tracking list *I* is updated by a query result of query(χ [*I*]). After *r* rounds, the algorithm returns the columns of the hidden database D not specified in the tracking list I . We use functions updnscore(p , a), updcscore(p , a), update(I , ns , cs) to simplify the complex update computations of $Nscore$, Cscore and the tracking list I , which will not affect our analysis.

The interesting part here is the query asked in each iteration is not independent any more. The query in one iteration *i* now depends on the tracking list *I* from its previous iteration $j - 1$, which is updated by the query result in the same iteration $j - 1$. The connection between queries from different iterations, which means these queries are adaptively chosen according to our Theorem [2.3.](#page-4-1)

The program-based dependency graph is presented in Figure [10\(](#page-19-1)b). Its execution-based dependency graph has the same graph, except different weight so we do not show it again. We can simply replaces k with a function w_k which takes a trace and returns the value of k in this trace. The weight 1 is replaced as a constant function w_1 taking whatever trace and returns 1 for the execution-based dependency graph. For consistence, we use w_k and w_1 for all the examples in this section. As the adaptivity definition in our formal adaptivity model in Definition [7,](#page-12-0) there is a finite walk along the dashed arrows, $a^6 \rightarrow I^9 \rightarrow ns^7 \rightarrow \cdots \rightarrow ns^7$, where every vertex is visited $w_k(\tau_0)$ times for an initial trace $\tau_0 \in \mathcal{T}_0(c)$. There is one vertex a^6 visited $w_k(\tau_0)$ times with query annotation 1, So we have the adaptivity with τ_0 for this program as $w_k(\tau_0)$.

Next, we show AdaptFun providing the tight upper bound for this example. If first finds a path $a^6: \frac{k}{1} \to I^9: \frac{k}{0} \to ns^7: \frac{k}{0}$ with three weighted vertices, and then AdaptSearch approximate this path to a walk, in which a^6 , I^9 , ns^7 is visited k times. So the estimated adaptivity is k. We know for any initial trace τ_0 where $\langle \tau_0, k \rangle \Downarrow_e v$ and $w_k(\tau_0) = v$. So k from AdaptFun is a tight bound.

Example 6.2 (Linear Regression Algorithm with Gradient Decent Optimization). The linear regression algorithm with gradient decent Optimization works well in our AdaptFun as well. Analysis Result: $A_{\text{prog}}(linearRegressionGD(k, rate)) = k$

This linear regression algorithm aims to model a linear relationship between a dependent variable y , and an independent variable x , $y = a \times x + c$, specifically approximating the model parameter a and c. In order to have a good approximation on the model parameter a and c , it sends query to a training

990 991 992 993 994 Fig. 11. (a) The linear regression algorithm (b) The program-based dependency graph from AdaptFun data set adaptively in every iteration. This training data set contains two columns (can extend to higher dimensional data sets), first column is used as the observed value for the independent variable x, second column is used as the observed label value for the dependent variable ψ . This algorithm is written in our Query While language in Figure [11\(](#page-20-0)a) as linearRegressionGD(k, rate).

995 996 997 998 999 1000 1001 1002 1003 1004 1005 1006 1007 1008 1009 This linear regression algorithm starts from initializing the linear model parameters and the counter variable, and then goes into the training iterations. In each iteration, it computes the differential value w.r.t. parameter a and c respectively, through requesting two queries, query(-2 ∗ $(\chi[1] - (\chi[0] \times a + c)) \times (\chi[0])$ and query(-2 * ($\chi[1] - (\chi[0] \times a + c)$)) at line 4 and 5. Then, it uses these two differential values stored in variable da and dc to update the linear model parameters a and c . Its the program-based dependency graph is shown in Figure [11\(](#page-20-0)b). Its execution-based dependency graph share the same graph, only needs to change the weight, k into w_k and 1 for w_1 as we do in the previous example. In the execution-based dependency graph, there are multiple walks having the same longest query length. For example, the walk $c^7 \rightarrow dc^6 : \rightarrow c^7 \rightarrow \cdots \rightarrow dc^6$ along the dotted arrows, where each vertex is visited $w_k(\tau_0)$ times for an initial trace τ_0 . There is actually other walks having the same query length k, the walk $a^7 \to da^6 \to a^7 \to \cdots \to da^6$ along the dotted arrows, where each vertex is visited $w_k(\tau_0)$ times. But it doesn't affect the adaptivity for this program, which is still the maximal query length $w_k(\tau_0)$ with respect to initial trace τ_0 . Also, AdaptFun, estimates the adaptivity k for this example. Similarly as the multiple round example, we can show it is a tight bound.

Example 6.3 (Over-approximation Algorithm). The AdaptFun comes across an over-approximation on the estimation due to its path-insensitive nature. It occurs when the control flow can be decided in a particular way in front of conditional branches, while the static analysis fails to witness.

We show the over-approximation, in Figure [12\(](#page-21-0)a), we call it a multiple rounds odd iteration algorithm. In this algorithm, at line 5 of every iteration, a query query($\chi[x]$) based on previous query results stored in x is asked by the analyst like in the multiple rounds strategy. The difference is that only the query answers from the even iterations ($i = 0, 2, \dots$) are used in the query in line 7, query($\chi[\ln(u)]$). Because the execution trace only updates x using the query answers in even iterations, so the answers from odd iterations do not affect the queries in even iterations. From the execution-based dependency graph in Figure [12\(](#page-21-0)b), we can see that the weight for the vertex u^5 is $w_k/2$ a function which takes any initial trace τ_0 , return the value of $k/2$ evaluated in τ_0 . However, AdaptFun fails to realize that odd iteration will always execute the then branch and even iteration means else branch, so it considers both branches for every iteration. In this sense, the weight estimated for y^5 and p^6 are both k as in Figure [12\(](#page-21-0)c). As a result, AdaptFun estimates the longest walk from Figure [12\(](#page-21-0)c), $y^5 \to x^7 \to y^5 \to \cdots \to x^7$ with each vertex visited k times, as the dotted arrows. And the adaptivity computed is $1 + 2 * k$, instead of $1 + k$.

Example 6.4 (Over-Defined Adaptivtiy Example). The program's adaptivity in our formal model, in Definition [7](#page-12-0) also comes across an over-approximation on the program's intuitive adaptivity rounds.

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1047 1048

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(b)

1050 1051 1052 It is resulted from difference between its weight calculation and the variable may-dependency definition. It occurs when the weight is computed over the traces different from the traces used in witness the *variable may-dependency* relation.

1053 1054 1055 1056 1057 1058 1059 1060 1061 1062 1063 1064 1065 1066 1067 1068 As the program in Figure [13\(](#page-21-1)a), which is a variant of the multiple rounds strategy, named multipleRoundSingle(k) with input k . In this algorithm, at line 7 of every iteration, a query query($\gamma[y] + p$) based on previous query results stored in p and y is asked by the analyst like in the multiple rounds strategy. The difference is that only the query answers from the one single iterations ($j = k - 2$) are used in this query query($\chi[y] + p$). Because the execution trace updates p using the constant 0 for all the iterations where $(j \neq k-2)$ at line 10 after the query request at line 7. In this way, all the query answers stored in p will not be accessed in next query request at line 7 in the iterations where ($j \neq k - 2$). Only query answer at one single iteration where ($j = k - 2$) will be used in next query request query(χ [y] + p) at line 7. So the adaptivity for this example is 2. However, our adaptivity model fails to realize that there is only dependency relation between p^7 and p^7 in one single iteration, not the others. As shown in the execution-based dependency graph in Figure [13\(](#page-21-1)b), there is an edge from p^7 to itself representing the existence of *Variable* May-Dependency from p^7 on itself, and the visiting times of labeled variable p^7 is $w_k(\tau_0)$ with a initial trace τ_0 . As a result, the walk with the longest query length is $p^7 \to \cdots \to p^7 \to y^4 \to z^1$ with the vertex p^7 visited $w_k(\tau_0)$, as the dotted arrows. The adaptivity based on this walk is $2+w(\tau_0)$, instead of 2. Though the AdaptFun is able to give us $2 + k$, as an accurate bound w.r.t this definition.

1070 6.2 Implementation Results

(a)

1071 1072 1073 1074 1075 1076 1077 We implemented AdaptFun as a tool which takes a labeled command as input and outputs an upper bound on the program adaptivity and on the number of query requests. This implementation consists of an abstract control flow graph generation, weight estimation (as presented in Section [5.3.2\)](#page-14-0), edge estimation (as presented in Section [5.3.3\)](#page-15-0) in Ocaml, and the adaptivity computation algorithm shown in Section [5.4](#page-15-1) in Python. The OCaml program takes the labeled command as input and outputs the program-based dependency graph, feeds into the python program and the python program provides the adaptivity upper bound and the query number as the final output.

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1079 1080 1081 1082 1083 1084 1085 1086 We evaluated this implementation on 17 example programs with the evaluation results shown in Table [1.](#page-22-0) In this table, the first column is the name of each program. For each program c, the second column is its intuitive adaptivity rounds, the third column is the $A(c)$ we defined through our formal semantic model in Section [4.](#page-9-0) In the third column, we use k represent the weight function w_k (in program's execution-based dependency graph) which return value of variable k from an initial trace τ_0 , same for natural numbers. The last column is the output of the AdaptFun implementation, which consists of two expressions. The first one is the upper bound for adaptivity and the second one is the upper bound for the total number of query requests in the program.

1087 1088 1089 1090 1091 1092 1093 1094 1095 1096 1097 1098 1099 1100 The first 3 programs we evaluated are twoRoundsComplete (k) , multipleRoundsComplete (k) , and the linearRegressionGD(k, rate) which we discussed in overview and Section [6.](#page-19-0) For these examples, $A(c)$ give the accurate adaptivity definition, simultaneously the AdaptFun outputs the tight bounds for both of the adaptivity and query requesting number as expected. But for the the forth program multipleRoundOdd(k), AdaptFun outputs an over-approximated upper bound $1 + 2 * k$ for the $A(c)$, which is consistent with our expectation as discussed in Example [6.3.](#page-20-1) The fifth program is the evaluation results for the example in Example [6.4,](#page-20-2) where AdaptFun outputs the tight bound for $A(c)$ but $A(c)$ is a loose definition of the program's actual adaptivity rounds. The programs in the table from $seq()$ to nestedWhileMultiPathMultiVarRecAcross (k) are designed for testing the programs under different possible situitions. These programs contain control dependency, data value dependency, the nested while, dependency through multiple variables, dependency across nested loops, and so on. Overall for these examples, our system gives both the accurate adaptivity definition and adaptivity upper bound simultaneously through the dynamic analysis and static analysis. The full programs can be found in the appendix, and the implementation in Github.

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Table 1. Experimental results of AdaptFun implementation

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7 RELATED WORK

1120 1121 1122 In terms of techniques, our work relies on ideas from both static analysis and dynamic analysis. We discuss closely related work in both areas.

1123 1124 1125 1126 1127 Static program analysis. Our algorithm in Section [5](#page-12-1) is influenced by many areas of static program analysis such as effect systems, control-flow analysis, and data-flow analysis [\[Ryder and Paull](#page-27-4) [1988\]](#page-27-4). The idea of statically estimating a sound upper bound for the adaptivity from the semantics is indirectly inspired from prior work on cost analysis via effect systems [Cicek et al. [2017a;](#page-25-5) 1128 1129 1130 1131 1132 1133 1134 1135 1136 1137 1138 1139 1140 1141 1142 1143 1144 1145 1146 [Qu et al.](#page-26-7) [2019;](#page-26-7) [Radicek et al.](#page-26-8) [2018\]](#page-26-8). The idea of defining adaptivity using data flow is inspired by the work of graded Hoare logic [\[Gaboardi et al.](#page-26-9) [2021\]](#page-26-9), which reasons about data flows as a resource. One of the most important ingredients of our work is the estimation of the program-based dependency graph. There are many ways to construct a dependency graph statically. Some of the most related work focuses on the testing of graphical user interfaces (GUIs), using an event graph. For example, [Memon](#page-26-10) [\[2007\]](#page-26-10) proposes an event-flow model using an algorithm to construct an event-flow graph, representing all the possible event interactions. This event-flow graph has a vertex for every GUI event such as click-to-paste and an edge between pairs of events that can be performed immediately one after the other. Our program-based dependency graph uses the edge to track the may-dependence of one variable with respect to another variable. The main difference is in the way the graph is constructed. AdaptFun relies on the structure of the target program, while the event-flow model only considers the event type. Another work [\[Arlt et al.](#page-25-6) [2012\]](#page-25-6) constructs a weighted event-dependency graph, capturing data dependencies between events by analyzing bytecode. Every weighted edge indicates a dependency between two events, meaning one event possibly reads data written by the other event, with the weight showing the intensity of the dependency (the quantity of data involved). Our approach of generating the program-based dependency graph shares the idea of tracking data dependency via static analysis on the source code. However, because of the different domains, we care about assigned variables, and we use the weight in a different way to find a finite walk in the graph.

1147 1148 1149 1150 1151 1152 1153 1154 1155 1156 1157 1158 Moreover, the state-of-art data-flow analysis techniques do not consider the quantitative information on how many times each variable is dependent on the other. Our weight estimation is inspired by works in program complexity analysis and worst case execution time analysis areas, focusing on analyzing the cost of the entire program. The techniques are based on type system [\[Çiçek et al.](#page-25-7) [2017b;](#page-25-7) [Rajani et al.](#page-26-11) [2021\]](#page-26-11), Hoare logic [\[Carbonneaux et al.](#page-25-8) [2015\]](#page-25-8), abstract interpretation [\[Gustafsson](#page-26-12) [et al.](#page-26-12) [2005;](#page-26-12) [Humenberger et al.](#page-26-13) [2018\]](#page-26-13), invariant generation through cost equations or ranking functions [\[Albert et al.](#page-25-9) [2008;](#page-25-9) [Alias et al.](#page-25-10) [2010;](#page-25-10) [Brockschmidt et al.](#page-25-11) [2016;](#page-25-11) [Flores-Montoya and Hähnle](#page-26-14) [2014\]](#page-26-14) or a combination of program abstraction and invariant inferring [\[Gulwani et al.](#page-26-15) [2009;](#page-26-15) [Gulwani](#page-26-6) [and Zuleger](#page-26-6) [2010;](#page-26-6) [Sinn et al.](#page-27-5) [2017b\]](#page-27-5). In general, these techniques give the approximated upper bound of the program's total running time or resource cost. However, they failed to consider the case where the cost – the adaptivity– could decrease when there isn't a dependency relation between variables.

1160 1161 1162 1163 1164 1165 1166 1167 1168 1169 1170 1171 1172 1173 1174 1175 Dynamic program analysis. Our framework constructs a execution-based dependency graph based on the execution traces of a program. We define semantic dependence on this graph by considering (intraprocedural) data and control dependency [\[Bilardi and Pingali](#page-25-12) [1996;](#page-25-12) [Cytron et al.](#page-25-13) [1991;](#page-25-13) [Pollock and Soffa](#page-26-16) [1989\]](#page-26-16). One related work [\[Austin and Sohi](#page-25-14) [1992\]](#page-25-14) presents a methodology to construct a dynamic dependency graph (DDG) based on the dynamic execution of a program in an imperative language, where edges represent dependency between instructions. Data dependency, control dependency, storage dependency, and resource dependency between instructions are all considered. Our execution-based dependency graph only needs data dependency and control dependency between variable assignment results. DDGs have been used in many other domains. [Nagar and Jagannathan](#page-26-17) [\[2018\]](#page-26-17) use DDGs to find serializability violations. [Hammer et al.](#page-26-18) [\[2006a\]](#page-26-18) use similar program dependency graphs [\[Ferrante et al.](#page-26-19) [1987\]](#page-26-19) for dynamic program slicing. [\[Hammer](#page-26-20) [et al.](#page-26-20) [2006b\]](#page-26-20) propose ways of constructing different kinds of program slices, by choose different program dependency. They actually use a combination of static and dynamic dependency graphs but in a manner that is different from how we use the two. Their slicing uses both static and dynamic dependency graphs, while we use the dynamic dependency graph as the basis of a definition, which is then soundly approximated by an analysis based on the static dependency graph.

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1177 1178 1179 1180 1181 1182 Our execution-based data dependency relation definition over variables is inspired by the method in [\[Cousot](#page-25-4) [2019\]](#page-25-4), where the dependency relation is also identified by looking into the differences on two execution traces. However, Cousot excludes timing channels [\[Sabelfeld and Myers](#page-27-6) [2003\]](#page-27-6) and empty observation, which are also not considered as a form of dependency in traditional dependency analysis [\[Denning and Denning](#page-25-15) [1977\]](#page-25-15). Our definition includes timing channels and empty observation by observing both the disappearance and value variation.

1184 1185 1186 1187 1188 1189 1190 1191 1192 1193 Generalization in Adaptive Data Analysis. Starting from the works by [Dwork et al.](#page-25-0) [\[2015c\]](#page-25-0) and [Hardt and Ullman](#page-26-2) [\[2014\]](#page-26-2), several works have designed methods that ensure generalization for adaptive data analyses. Some examples are: [\[Bassily et al.](#page-25-1) [2016;](#page-25-1) [Dwork et al.](#page-25-2) [2015a](#page-25-2)[,b;](#page-25-3) [Feldman](#page-26-3) [and Steinke](#page-26-3) [2017;](#page-26-3) [Jung et al.](#page-26-4) [2020;](#page-26-4) [Rogers et al.](#page-26-5) [2020;](#page-26-5) [Steinke and Zakynthinou](#page-27-0) [2020;](#page-27-0) [Ullman et al.](#page-27-1) [2018\]](#page-27-1). Several of these works drew inspiration from the idea of using methods designed to ensure differential privacy, a notion of formal data privacy, in order to guarantee generalization for adaptive data analyses. By limiting the influence that an individual can have on the result of a data analysis, even in adaptive settings, differential privacy can also be used to limit the influence that a specific data sample can have on the statistical validity of a data analysis. This connection is actually in two directions, as discussed for example by [Yeom et al.](#page-27-7) [\[2018\]](#page-27-7).

1194 1195 1196 1197 1198 1199 1200 1201 1202 1203 1204 1205 1206 1207 1208 1209 1210 Considering this connection between generalization and privacy, it is not surprising that some of the works on programming language techniques for privacy-preserving data analysis are related to our work. Adaptive Fuzz [\[Winograd-Cort et al.](#page-27-8) [2017\]](#page-27-8) is a programming framework for differential privacy that is designed around the concept of adaptivity. This framework is based on a typed functional language that distinguish between several forms of adaptive and non-adaptive composition theorem with the goal of achieving better upper bounds on the privacy cost. Adaptive Fuzz uses a type system and some partial evaluation to guarantee that the programs respect differential privacy. However, it does not include any technique to bound the number of rounds of adaptivity. [Lobo-Vesga et al.](#page-26-21) [\[2021\]](#page-26-21) propose a language for differential privacy where one can reason about the accuracy of programs in terms of confidence intervals on the error that the use of differential privacy can generate. These are akin to bounds on the generalization error. This language is based on a static analysis which however cannot handle adaptivity. The way we formalize the access to the data mediated by a mechanism is a reminiscence of how the interaction with an oracle is modeled in the verification of security properties. As an example, the recent works by [Barbosa](#page-25-16) [et al.](#page-25-16) [\[2021\]](#page-25-16) and [Aguirre et al.](#page-25-17) [\[2021\]](#page-25-17) use different techniques to track the number of accesses to an oracle. However, reasoning about the number of accesses is easier than estimating the adaptivity of these calls, as we do instead here.

8 CONCLUSION AND FUTURE WORKS

1214 1215 1216 1217 1218 1219 We presented AdaptFun, a program analysis useful to provide an upper bound on the adaptivity of a data analysis under a specific data analysis model, as well as the total number of queries asked. This estimation can help data analysts to control the generalization errors of their analyses by choosing different algorithmic techniques based on the adaptivity. Besides, a key contribution of our works is the formalization of the notion of adaptivity for adaptive data analysis. Also, our implementation shows the potential application of our work into real world.

1220 1221 1222 1223 1224 In the future, we plan to address the over-approximation of AdaptFun. Our algorithm may over-estimate the adaptivity of a program, as shown in Section [6,](#page-19-0) due to its path-insensitive nature. We plan to explore the possibility of making AdaptFun path-sensitive. We also see the over-approximation when we estimate weight in Section [5.3.2](#page-14-0) in some complicated examples with nested while loops, the corresponding improvement is also in our plan.

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