# 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 2014; Ioannidis 2005]). 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 2014].

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 2014].

A line of work initiated by Dwork et al. [2015c], Hardt and Ullman [2014] 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. 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. 2016; Dwork et al. 2015a,b; Feldman and Steinke 2017; Jung et al. 2020; Rogers et al. 2020; Steinke and Zakynthinou 2020; Ullman et al. 2018].

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.

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. [2015c]. To better understand this idea, we show in Figure 2 two experiments showcasing these situations. More precisely, in Figure 2(a) we show the results of a specific analysis<sup>1</sup> 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), we show the results of a specific analysis<sup>2</sup> with four hundreds rounds of adaptivity. This analysis can be seen as a classifier which

<sup>96</sup> <sup>1</sup>We will use formally a program implementing this analysis (Figure 3) as a running example in the rest of the paper.

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<sup>&</sup>lt;sup>2</sup>We will present this analysis formally in Section 6.

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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.

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.

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. [2020].

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

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

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.

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

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:

- 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. 2016; Dwork et al. 2015c; Hardt and Ullman 2014], 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 query(*P*) =  $\underset{X \sim P}{\mathbb{E}}$  [query(*X*)].

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

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

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.

In this work we consider analysts that ask a sequence of k queries  $query_1, \ldots, query_k$ . 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  $query_j$  depend on the prefix  $query_1, a_1, \ldots, query_{j-1}, a_{j-1}$ 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  $\max_{j=1,...,k} |a_j - \operatorname{query}_j(P)| = O\left(\sqrt{\frac{\log k}{n}}\right)$ , and for any  $r \ge 2$  and any r-round adaptive statistical queries, it satisfies  $\max_{j=1,...,k} |a_j - \operatorname{query}_j(P)| = O\left(\sqrt{\frac{k}{n}}\right)$ 

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. [2015c] and Bassily et al. [2016] 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; DWORK ET AL. 2015c]). For any k, there exists a mechanism such that for any distribution P, and any  $r \ge 2$  any r-round adaptive statistical queries, it satisfies

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

Notice that Theorem 2.2 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. [2015c] also gave more refined bounds in terms of the number of rounds of adaptivity.

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

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

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 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

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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(a), which implements a simple "two rounds strategy" in our query while language (presented in Section 3) 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(b) and the program-based dependency graph we estimate using our static analysis framework AdaptFun in Figure 3(c).

As shown in Figure 3(a), the analyst asks in total k + 1 queries to the mechanism in two phases. In 262 the first phase, the analyst asks k queries and stores the answers that are provided by the mechanism. 263 In the second phase, the analyst constructs a new query based on the results of the previous k264 queries and sends this query to the mechanism. More specifically, we assume that, in this example, 265 the domain X contains at least k numeric attributes, which we index just by natural numbers. The 266 queries inside the while loop correspond to the first phase and compute an approximation of the 267 product of the empirical mean of the first k attributes. The query outside the loop corresponds 268 to the second phase and computes an approximation of the empirical mean where each record 269 is weighted by the sum of the empirical mean of the first k attributes. Since statistical queries 270 computes the empirical mean of a function on rows, we use  $\chi$  to abstract a possible row in the 271 database and queries are of the form query( $\psi$ ), where  $\psi$  is a special expression (see syntax in 272 Section 3) representing a function :  $X \to U$  on rows. We use U to denote the codomain of queries 273 and it could be [-1, 1], [0, 1] or [-R, +R], for some R we consider. This function characterizes the 274 linear query we are interested in running. As an example,  $x \leftarrow query(\chi[j] \cdot \chi[k])$  computes an 275 approximation, according to the used mechanism, of the empirical mean of the product of the  $j^{th}$ 276 attribute and  $k^{th}$  attribute, identified by  $\chi[j] \cdot \chi[k]$ . Notice that we don't materialize the mechanism 277 but we assume that it is implicitly run when we execute the query. 278

This example is intuitively 2-rounds adaptive since we have two clearly distinguished phases, and 279 the queries that we ask in the first phase do not depend on each other (the query  $query(\chi[i] \cdot \chi[k])$ ) 280 at line 3 only relies on the counter i and input k), while the last query (at line 6) depends on the 281 results of all the previous queries. However, capturing this concept formally is surprisingly difficult. 282 The difficulty comes from the fact that a query can depend on the result of another query in multiple 283 ways, by means of data dependency or control flow dependency. In order to find the right definition 284 for our goal, we take inspiration from the known results on the data analysis model we discussed 285 above. This theory tells us that what we want to measure is the generalization error on the result of 286 a query, and not an arbitrary manipulation of the query. Indeed, arbitrary manipulations can change 287 the generalization error. As an example, suppose that v is the result we get from running a query, if 288 we multiply this result by some constant, we are also changing the incurred error. Moreover, this 289 theory tells us that we can always consider a non-adaptive set of queries as to being adaptive, and 290 more importantly, that we can transform an adaptive query into a non-adaptive one, incurring an 291 exponential blow up of the number of queries. For example, we could ask many queries upfront 292 and depending on the results of some of them, we could return the results of others. 293

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

310 As an example, let us consider the graph in Figure 3(b). This graph is built by considering all the 311 possible execution traces of the program in Figure 3(a). Each vertex in this graph has a superscript 312 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  $l^6 : \frac{w_1}{1}$ , has weight  $w_1$ , a constant 313 314 function which returns 1 for every starting state, since this query at line 6 is at most executed 315 once regardless of the initial trace. The query annotation of this vertex is 1, which indicates that  $[l \leftarrow query(\chi[k] * a)]^6$  is a query request. Another vertex,  $x^3 : \frac{w_k}{1}$ , appears in the while loop. It 316 317 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  $j^4 : {}^{w_k}_0$  has as a subscript 0 318 319 representing a non-query assignment.

320 Since the edges between two vertices represent the fact that one program variable may depend 321 on the other, we can define the program adaptivity with respect to a initial trace by means of a 322 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 323 that in the walk along the dotted arrows,  $l^6 \rightarrow a^5 \rightarrow x^3$ , there are 2 vertices with query annotation 324 1 and that this number is maximal, i.e. we cannot find another walk having more than 2 vertices 325 326 with query annotation 1, under the assumption that  $k \ge 1$ . So the adaptivity of the program in 327 Figure 3(a) is 2, as expected. 328

Static analysis for adaptivity. Our static analysis provides an upper bound on the adaptivity for 329 this example as follows. AdaptFun constructs a program-based dependency graph, for our example 330 we show this graph in Figure 3(c). The edges of this graph are built by considering both control 331 flow and data flow between assigned variables (the algorithm is presented in Section 5.3.3). The 332 weight of every vertex is estimated by using a reachability-bound estimation algorithm (presented 333 in Section 5.3.2), which can be symbolic and provide a sound upper bound on the weight of the 334 corresponding vertex in the execution-based dependency graph. For instance, the weight k of the 335 vertex  $x^3$  in Figure 3(c) is a sound upper bound on the weight  $w_k$  of vertex  $x^3$  in Figure 3(b), with 336 the same starting trace. The soundness of this step is proved in Theorem 5.1. 337

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). For instance, in Figure 3(c), AdaptSearch first finds a path  $l^6 : {}_1^1 \rightarrow a^5 : {}_1^k \rightarrow x^3 : {}_1^k$ , 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

though the node  $x^3$  has weight depending on k, it is only visited once, similarly for  $l^6$ , hence the 344 overall upper bound on the adaptivity is 2, as we expect. 345

#### LABELED QUERY WHILE LANGUAGE 3 347

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

#### 3.1 Syntax 353

354	Arithmetic Expression	а	::=	$n \mid x \mid a \oplus_a a \mid \log a \mid \operatorname{sign} a \mid \max(a, a) \mid \min(a, a)$
355	Boolean Expression	b	::=	true   false   $\neg b \mid b \oplus_b b \mid a \sim a$
356	Expression	е	::=	$v \mid a \mid b \mid [e, \ldots, e]$
357	Value	v	::=	$n \mid \texttt{true} \mid \texttt{false} \mid [] \mid [v, \dots, v]$
358	Query Expression	ψ	::=	$\alpha \mid a \mid \psi \oplus_a \psi \mid \chi[a]$
359	Query Value	α	::=	$n \mid \chi[n] \mid \alpha \oplus_a \alpha \mid n \oplus_a \chi[n] \mid \chi[n] \oplus_a n$
360	Label	l	∈	$\mathbb{N} \cup \{in, ex\}$
361	Labeled Command	С	::=	$[x \leftarrow e]^l \mid [x \leftarrow query(\psi)]^l \mid while [b]^l do c$
362				$ c;c $ if( $[b]^l,c,c)$   [skip] <sup>l</sup>

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

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

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

#### 3.2 **Trace-based Operational Semantics**

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

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

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

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

and its opposite  $\notin$  express whether or not an event belongs to a trace. Another operator  $\iota : \mathcal{T} \to \mathcal{VAR} \to \{\mathbb{N}\} \cup \{\bot\}$ , 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  $\langle c, \tau \rangle \to \langle c', \tau' \rangle$ . It states that a configuration  $\langle c, \tau \rangle$ , which consists of a command *c* to be evaluated and a starting trace  $\tau$ , 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  $\theta$  :  $\mathcal{T} \to \mathcal{VAR} \to \mathcal{VAL} \cup \{\bot\}$ , which maps a trace and a variable to the latest value assigned to this variable on the trace is defined as follows.

$$\begin{array}{l} \theta(\tau::(x,l,v,\bullet))x \triangleq v \quad \theta(\tau::(y,l,v,\bullet))x \triangleq \theta(\tau)x, y \neq x \quad \theta(\tau::(b,l,v,\bullet))x \triangleq \theta(\tau)x \\ \theta(\tau::(x,l,v,\alpha))x \triangleq v \quad \theta(\tau::(y,l,v,\alpha))x \triangleq \theta(\tau)x, y \neq x \quad \theta([])x \triangleq \bot \end{array}$$

We give a selection of rules of the trace-based operational semantics in Figure 5.

The rule **assn** evaluates a standard assignment  $x \leftarrow e$ , the expression *e* is first evaluated by our expression evaluation  $\langle \tau, e \rangle \downarrow_e v$ , 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.

$$\frac{\langle \tau, a \rangle \to_a v}{\langle \tau, a \rangle \Downarrow_e v} \qquad \frac{\langle \tau, b \rangle \to_b v}{\langle \tau, b \rangle \Downarrow_e v} \qquad \frac{\langle \tau, e_1 \rangle \Downarrow_e v_1 \cdots \langle \tau, e_n \rangle \Downarrow_e v_n}{\langle \tau, [e_1, \cdots, e_n] \rangle \Downarrow_e [v_1, \cdots, v_n]} \qquad \overline{\langle \tau, v \rangle \Downarrow_e v}$$

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  $\psi$  is first evaluated into a query value  $\alpha$  by following the rules below. Then, by sending this query request  $query(\alpha)$  to a hidden mechanism, this query is evaluated to a result value returned from it,  $v = query(\alpha)$ . Also, the generated event stores both the query value  $\alpha$  here, and the result value of the query request.

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

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.

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

## 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.

### 447 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.

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,  $query(\chi[1])$  is different from  $query(\chi[2])$ . Informally, we think  $query(\chi[3] + x)$ may depend on the query  $query(\chi[2])$ , because equipped function of the former  $\chi[3] + x$  may depend on the data stored in x assigned with the result of  $query(\chi[2])$ , according to this definition.

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  $c_2 = x \leftarrow query(\chi[1])$ ;  $if(x > 2, y \leftarrow query(\chi[2]), skip)$ , 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:

$$\pi_1(\epsilon_1) = \pi_1(\epsilon_2) \land \pi_2(\epsilon_1) = \pi_2(\epsilon_2) \land ((\pi_3(\epsilon_1) \neq \pi_3(\epsilon_2) \land \pi_4(\epsilon_1) = \pi_4(\epsilon_2) = \bullet) \lor (\pi_4(\epsilon_1) \neq \bullet \land \pi_4(\epsilon_2) \neq \bullet \land \pi_4(\epsilon_1) \neq_q \pi_4(\epsilon_2)))$$

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We compare two events by defining  $\text{Diff}(\epsilon_1, \epsilon_2)$ . We use  $\psi_1 =_q \psi_2$  and  $\psi_1 \neq_q \psi_2$  to notate query 491 expression equivalence and in-equivalence, distinct from standard equality. A program c's labeled 492 variables is a subset of the labeled variables  $\mathcal{LV}$ , denoted by  $\mathbb{LV}(c) \in \mathcal{P}(\mathcal{VAR} \times \mathcal{L}) \subseteq \mathcal{LV}$ . We 493 also define the set of query variables for a program  $c, \mathbb{QV} : C \to \mathcal{P}(\mathcal{LV})$ . A program *c*'s query 494 variables is a subset of its labeled variables,  $\mathbb{QV}(c) \subseteq \mathbb{LV}(c)$ . We have the operator  $\mathbb{TL}: \mathcal{T} \to \mathcal{L}$ , 495 which gives the set of labels in every event belonging to the trace. Then we introduce a counting 496 operator cnt :  $\mathcal{T} \to \mathbb{N} \to \mathbb{N}$ , which counts the occurrence of of a labeled variable in the trace, 497 whose behavior is defined as follows, 498

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

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

Definition 2 (Event May-Dependency). .

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

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$$\exists \tau_{0}, \tau_{1}, \tau' \in \mathcal{T}, \epsilon_{1}' \in \mathcal{E}^{\operatorname{asn}}, c_{1}, c_{2} \in \mathcal{C} . \operatorname{Diff}(\epsilon_{1}, \epsilon_{1}') \wedge \\ (\exists \epsilon_{2}' \in \mathcal{E} . \begin{pmatrix} \langle c, \tau_{0} \rangle \rightarrow^{*} \langle c_{1}, \tau_{1} + [\epsilon_{1}] \rangle \rightarrow^{*} \langle c_{2}, \tau_{1} + [\epsilon_{1}] + \tau_{+}[\epsilon_{2}] \rangle \\ \wedge \langle c_{1}, \tau_{1} + [\epsilon_{1}'] \rangle \rightarrow^{*} \langle c_{2}, \tau_{1} + [\epsilon_{1}'] + \tau' + [\epsilon_{2}'] \rangle \\ \wedge \operatorname{Diff}(\epsilon_{2}, \epsilon_{2}') \wedge \operatorname{cnt}(\tau, \pi_{2}(\epsilon_{2})) = \operatorname{cnt}(\tau', \pi_{2}(\epsilon_{2}')) \end{pmatrix} \\ \vee \exists \tau_{3}, \tau_{3}' \in \mathcal{T}, \epsilon_{b} \in \mathcal{E}^{\operatorname{test}} . \\ \begin{pmatrix} \langle c, \tau_{0} \rangle \rightarrow^{*} \langle c_{1}, \tau_{1} + [\epsilon_{1}] \rangle \rightarrow^{*} \langle c_{2}, \tau_{1} + [\epsilon_{1}] + \tau + [\epsilon_{b}] + \tau_{3} \rangle \\ \wedge \langle c_{1}, \tau_{1} + [\epsilon_{1}'] \rangle \rightarrow^{*} \langle c_{2}, \tau_{1} + [\epsilon_{1}'] + \tau' + [(\neg \epsilon_{b})] + \tau_{3}' \rangle \\ \wedge \mathbb{TL}_{\tau_{3}} \cap \mathbb{TL}_{\tau_{3}'} = \emptyset \wedge \operatorname{cnt}(\tau', \pi_{2}(\epsilon_{b})) = \operatorname{cnt}(\tau, \pi_{2}(\epsilon_{b})) \wedge \epsilon_{2} \in \tau_{3} \wedge \epsilon_{2} \notin \tau_{3}' \end{pmatrix} )$$

Our event *may-dependency* relation of two events  $\epsilon_1 \in \mathcal{E}^{asn}$  and  $\epsilon_2 \in \mathcal{E}$ , for a program *c* and 514 hidden database D is w.r.t to a trace  $[\epsilon_1]_{++\tau_{++}}[\epsilon_2]$ . The  $\epsilon_1 \in \mathcal{E}^{asn}$  is an assignment event because 515 only a change on an assignment event will affect the execution trace, according to our operational 516 semantics. In order to observe the changes of  $\epsilon_2$  under the modification of  $\epsilon_1$ , this trace  $[\epsilon_1]_{+\tau_{+}}[\epsilon_2]$ 517 starts with  $\epsilon_1$  and ends with  $\epsilon_2$ . The may-dependency relation considers both the value dependency 518 519 and value control dependency as discussed in Section 4.1. The relation can be divided into two parts naturally in Definition 2 (line 2 - 4, 5 - 8 respectively, starting from line 1). The idea of the 520 event  $\epsilon_1$  may depend on  $\epsilon_2$  can be briefly described: we have one execution of the program as 521 reference (See line 2 and 6, for the two kinds of dependency). When the value assigned to the first 522 variable in  $\epsilon_1$  is modified, the reference trace  $\tau_{1++}[\epsilon_1]$  is modified correspondingly to  $\tau_{1++}[\epsilon'_1]$ . We 523 use Diff $(\epsilon_1, \epsilon'_1)$  at line 1 to express this modification, which guarantees that  $\epsilon_1$  and  $\epsilon'_2$  only differ 524 in their assigned values and are equal on variable name and label. We perform a second run of the 525 program by continuing the execution of the same program from the same execution point, but 526 with the modified trace  $\tau_{1^{++}}[\epsilon'_1]$  (See line 3, 7). The expected may dependency will be caught by 527 observing two different possible changes (See line 4, 8 respectively) when comparing the second 528 execution with the reference one (similar definitions as in [Cousot 2019]). 529

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

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In the second part (line 5–8 of Definition 2), we witness the disappearance of  $\epsilon_2$  through observing 540 the change of a testing event  $\epsilon_b$ . To witness the disappearance, the command that generates  $\epsilon_2$ 541 542 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 543 generates a testing event  $\epsilon_b$  in the first place. So we observe when  $\epsilon_b$  changes into  $\neg \epsilon_b$  in the second 544 execution firstly, whether it follows with the disappearance of  $\epsilon_2$  in the second trace. We restrict the 545 occurrence of  $\epsilon_b$ 's label in the two traces being the same through  $\operatorname{cnt}(\tau', \pi_2(\epsilon_b)) = \operatorname{cnt}(\tau, \pi_2(\epsilon_b))$ 546 547 to handle the while loop. Again, for queries, we observe the disappearance based on the query value equivalence. 548

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, we say the two related variables satisfy the *variable may-dependency* relation, in Definition 3.

DEFINITION 3 (VARIABLE MAY-DEPENDENCY). .

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

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

#### 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,

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

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  $W_{trace}(c)$ .

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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  $k : \mathcal{T} \rightarrow$  sequence of edges. For a initial trace  $\tau_0 \in \mathcal{T}_0(c), k(\tau_0)$  is a sequence of edges  $(e_1 \dots e_{n-1})$  for which there is a sequence of vertices  $(v_1, \dots, v_n)$  such that:

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

• every  $v_i \in V_{trace}(c)$  and  $(v_i, w_i) \in W_{trace}(c)$ ,  $v_i$  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  $\mathcal{WK}(G_{trace}(c))$  to denote the set containing all finite walks k in  $G_{trace}(c)$ ; and  $k_{v_1 \rightarrow v_2} \in \mathcal{WK}(G_{trace}(c))$  with  $v_1, v_2 \in V_{trace}(c)$  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  ${\rm Walk}({\tt len}^q))$  .

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  $k \in W\mathcal{K}(G_{trace}(c))$ . The query length of k is a function  $len^{q}(k) : \mathcal{T} \to \mathbb{N}$ , such that with an initial trace  $\tau_0 \in \mathcal{T}_0(c)$ ,  $len^{q}(k)(\tau_0)$  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,

 $len^{q}(k)(\tau_{0}) = |(v | v \in (v_{1}, \dots, v_{n}) \land Q(v) = 1)|.$ 

The definition of adaptivity is then presented in Def 7 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  $\tau_0 \in \mathcal{T}_0(c)$ ,

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

## 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.

## 5.1 A guide to the static program analysis framework

Our program analysis framework AdaptFun can be divided as two steps: 1) to construct a weighted dependency 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.

5.1.1 Graph Estimation. According to adaptivity defined over program's execution-based de pendency graph (in Definition 4), 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.
- (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.
  - (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.
    - (4) Edges between vertices consider both control flow and data flow, See Section 5.3.3.
    - (5) Finally, with all the ingredients ready, we construct the final approximated program-based dependency graph in Section 5.4.

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*.

*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.

## 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,  $V_{prog}(c) \triangleq V_{trace}(c)$ .

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, in spirit of some reachability 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.

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.

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

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Fig. 7. (a) The same towRounds(k) program as Figure 3 (b) The abstract control flow graph for towRounds(k) (c) The abstract control flow graph with the reachability bound for towRounds(k).

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

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

$$\mathsf{W}_{\mathsf{prog}}(c) \triangleq \{ (x^l, w) \mid x^l \in \mathsf{V}_{\mathsf{prog}}(c) \land (l, w) \in \mathsf{absW}(c) \}$$

We prove that this arithmetic expression for  $x^l \in V_{prog}(c)$  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  $W_{prog}(c)$  we have:

$$\forall (x^{l}, w) \in \mathsf{W}_{\mathsf{prog}}, \tau_{0} \in \mathcal{T}_{0}(c), \tau \in \mathcal{T}, v \in \mathbb{N} . \langle c, \tau_{0} \rangle \rightarrow^{*} \langle \mathsf{skip}, \tau_{0} \leftrightarrow \tau \rangle \land \langle \tau_{0}, w \rangle \Downarrow_{e} v \implies \mathsf{cnt}(\tau, l) \leq v$$

*Example.* As in Figure 3(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 Figure 3(b)  $w_k(\tau_0) = \theta(\tau_0)k$ . In the same way, the weights for all the other vertices are sound.

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Edge Estimation. We show how to estimate the directed edges for the program-based de-736 5.3.3 pendency graph. We develop a variant of data flow analysis, called Feasible Data-Flow Generation, 737 738 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

745	$flowsTo(x^i, y^j, [x \leftarrow e]^l)$	$\triangleq (x^i, y^j) \in \{(y^i, x^l)   y \in FV(e) \land y^i \in RD(l, [x \leftarrow e]^l)\}$
746	$flowsTo(x^i, y^j, [x \leftarrow query(\psi)]^l)$	$\triangleq (x^{i}, y^{j}) \in \{(y^{i}, x^{l})   y \in FV(\psi) \land y^{i} \in RD(l, [x \leftarrow query(\psi)]^{l})\}$
747	$flowsTo(x^i, y^j, [skip]^l)$	$= \emptyset$
748	$flowsTo(x^i, y^j, if([b]^l, c_1, c_2))$	$\triangleq$ flowsTo $(x^i, y^j, c_1) \lor$ flowsTo $(x^i, y^j, c_2)$
749		$\forall (x^i, y^j) \in \{(x^i, y^j)   x \in FV(b) \land x^i \in RD(l, if([b]^l, c_1, c_2)) \land y^j \in \mathbb{LV}(c_1)$
		$\forall (x^i, y^j) \in \{(x^i, y^j)   x \in FV(b) \land x^i \in RD(l, if([b]^l, c_1, c_2)) \land y^j \in \mathbb{LV}(c_2) $
750	flowsTo $(x^i, y^j, while [b]^l do c_w)$	$\triangleq$ flowsTo $(x^i, y^j, c_w) \lor$
751		$(x^i, y^j) \in \{(x^i, y^j)   x \in FV(b) \land x^i \in RD(l, \text{ while } [b]^l \text{ do } c_w) \land y^j \in \mathbb{LV}(c_w)$
752	flowsTo $(x^i,y^j,c_1;c_2)$	$\triangleq$ flowsTo $(x^i, y^j, c_1) \lor$ flowsTo $(x^i, y^j, c_2)$

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  $\mathsf{E}_{\mathsf{prog}}(c) \in \mathcal{P}(\mathcal{LV} \times \mathcal{LV})$  indicating a directed edge from the first vertex to the second one in each pair as follows,

$$\mathsf{E}_{\mathsf{prog}}(c) \triangleq \{ (y^j, x^i) \mid y^j, x^i \in \mathsf{V}_{\mathsf{prog}}(c) \land \exists n, z_1^{r_1}, \dots, z_n^{r_n} \in \mathbb{LV}(c) . \\ n \ge 0 \land \mathsf{flowsTo}(x^i, z_1^{r_1}, c) \land \dots \land \mathsf{flowsTo}(z_n^{r_n}, y^j, c) \}$$

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

*Example.* Look at Figure 3(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  $[l \leftarrow query(\chi[k] * a)]^l$ , i.e.,  $a \in FV(\chi[k] * a)$ . Also, from the reaching definition analysis, we know  $a^5 \in \mathsf{RD}(6, \mathsf{twoRounds}(\mathsf{k}))$ . 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 771

772 We notate our dependency graph as follows:

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

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

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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  $G_{prog}(c)$  the program-based adaptivity for c is defined as

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

Based on our soundness of the program-based adaptivity, our program-based adaptivity is a sound upper bound of its adaptivity in Definition 7.

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

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

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

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

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.

**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, where k is the input variable from domain  $\mathbb{N}$ . 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  $k \in \mathbb{N}$ .

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,  $x^3 : {k \atop 1} \to x^1 : {1 \atop 1}$ . 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.

**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  $\infty$  adaptivity upper bound on the program with actual adaptivity 2. Look at twoRounds in overview, we find the longest weighted path is  $x^3 : {}_1^k \rightarrow a^5 : {}_0^k \rightarrow l^6 : {}_0^1$  in Figure 3(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

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

Alg	$\mathbf{gorithm~1}$ Adaptivity Computation Algorithm on SCC Graph AdaptSearch <sub>scc</sub> (G):
Re	<b>quire:</b> <i>G</i> = (V, E, W, Q) #{An Strong Connected program based dependency Graph}
1:	init $r_{scc}$ : <i>a</i> , arithmetic expression, initialized 0, the Adaptivity of this SCC
	visited : {0, 1} List, #{length  V , initialize with 0 for every vertex}
	$r: a$ , arithmetic expression List, #{length $ V $ , initialize with $Q(v)$ for every vertex }
	flowcapacity: <i>a</i> List, #{length $ V $ , initialize with $\infty$ for every vertex}
	querynum: INT List, #{length $ V $ , initialize with $Q(v)$ for every vertex. }
2:	<b>if</b> $ V  = 1$ and $ E  = 0$ : <b>return</b> $Q(v)$
3:	<pre>def dfs(G, c, visited):</pre>
4:	<b>for</b> every vertex <i>v</i> connected by a directed edge from <i>c</i> :
5:	if visited[v] = false:
6:	flowcapacity[v] = min(W(v), flowcapacity[c]);
7:	<pre>querynum[v] = querynum[c] + Q(v);</pre>
8:	$r[v] = max(r[v], flowcapacity[v] \times querynum[v]);$
9:	visited[v] = 1; dfs(G, v, visited);
10:	<b>else</b> : #{There is a cycle finished, update the adaptivity}
11:	$r[v] = \max(r[v], r[c] + \min(W(v), flowcapacity[c]) * (querynum[c] + Q(v)));$
12:	return r[c]
13:	<pre>for every vertex v in V: initialize the visited, r, flowcapacity, querynum;</pre>
14:	$r_{scc} = max(r_{scc}, dfs(G, v, visited));$
15:	return r <sub>scc</sub>

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

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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 arithmetic expression  $\mathcal{A}_{in}$  recording the minimum weight when the path reaches that vertex, which is initialized by  $\infty$ .

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

The updating operations during the traverse (line: 8) and at the end of the traverse (line: 11) are interesting, specifically flowcapacity[v] × 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.

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

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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 algorithm - multiple rounds algorithm, as in Figure 10(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( $\chi[I]$ ). 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 j 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.

The program-based dependency graph is presented in Figure 10(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, 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  $\tau_0$  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  $a^6 : {}^k_1 \to I^9 : {}^k_0 \to ns^7 : {}^k_0$  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  $\tau_0$  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:  $A_{prog}(linearRegressionGD(k, rate)) = k$ 

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

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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 y. This algorithm is written in our Query While language in Figure 11(a) as linearRegressionGD(k, rate).

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

1013 We show the over-approximation, in Figure 12(a), we call it a multiple rounds odd iteration 1014 algorithm. In this algorithm, at line 5 of every iteration, a query query  $(\chi[x])$  based on previous 1015 query results stored in x is asked by the analyst like in the multiple rounds strategy. The difference 1016 is that only the query answers from the even iterations ( $i = 0, 2, \dots$ ) are used in the query in line 1017 7, query( $\chi[\ln(y)]$ ). Because the execution trace only updates x using the query answers in even 1018 iterations, so the answers from odd iterations do not affect the queries in even iterations. From the 1019 execution-based dependency graph in Figure 12(b), we can see that the weight for the vertex  $y^5$  is 1020  $w_k/2$ . a function which takes any initial trace  $\tau_0$ , return the value of k/2 evaluated in  $\tau_0$ . However, 1021 AdaptFun fails to realize that odd iteration will always execute the then branch and even iteration 1022 means else branch, so it considers both branches for every iteration. In this sense, the weight 1023 estimated for  $y^5$  and  $p^6$  are both k as in Figure 12(c). As a result, AdaptFun estimates the longest 1024 walk from Figure 12(c),  $y^5 \rightarrow x^7 \rightarrow y^5 \rightarrow \cdots \rightarrow x^7$  with each vertex visited k times, as the dotted 1025 arrows. And the adaptivity computed is 1 + 2 \* k, instead of 1 + k. 1026

*Example 6.4 (Over-Defined Adaptivity Example).* The program's adaptivity in our formal model, in Definition 7 also comes across an over-approximation on the program's intuitive adaptivity rounds.

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Fig. 13. (a) The multi rounds single example (b) The execution-based dependency graph.

(b)

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

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

#### **Implementation Results** 6.2 1070

(a)

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

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We evaluated this implementation on 17 example programs with the evaluation results shown in 1079 Table 1. In this table, the first column is the name of each program. For each program *c*, the second 1080 column is its intuitive adaptivity rounds, the third column is the A(c) we defined through our 1081 formal semantic model in Section 4. In the third column, we use k represent the weight function  $w_k$ 1082 (in program's execution-based dependency graph) which return value of variable k from an initial 1083 trace  $\tau_0$ , same for natural numbers. The last column is the output of the AdaptFun implementation, 1084 which consists of two expressions. The first one is the upper bound for adaptivity and the second 1085 1086 one is the upper bound for the total number of query requests in the program.

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

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Table 1. Experimental results of AdaptFun implementation

1102				
1103	Program c	adaptivity rounds	A(c)	AdaptFun
1105	<pre>twoRoundsComplete(k)</pre>	2	2	2, k
1104	<pre>multipleRoundsComplete(k)</pre>	k	k	k, k
1105	linearRegressionGD(k,rate)	k	k	k, 2 * k
1106	multipleRoundsOdd(k)	1 + k	1 + k	1 + 2 * k, 1 + 2 * k
1107	<pre>multipleRoundsSingle(k)</pre>	2	2 <b>+</b> <i>k</i>	2 + k, $2 + k$
1109	seq()	4	4	4, 4
1100	<pre>seqMultiVar()</pre>	4	4	4, 4
1109	ifValueDependency	3	3	3, 3
1110	ifControlDependency()	3	3	3, 3
1111	whileRec(k)	1 + k	1 + k	1 + k
1112	<pre>whileMultipleVar(k)</pre>	1 + 2 * k	1 + 2 * k	1 + 2 * k, 2 + 3 * k
1112	<pre>whileValueControlDependency(k)</pre>	1 + 2 * k	1 + 2 * k	1 + 2 * k, 2 + 2 * k
1115	<pre>whileMultiplePathValueControlDependency(k)</pre>	2 + k	2 + k	2 + k, 1 + 2 * k
1114	<pre>nestWhileValueDependency(k)</pre>	$2 + k^2$	$2 + k^2$	$2 + k^2$ , $1 + k + k^2$
1115	<pre>nestedWhileRecAcross(k)</pre>	1 + 2 * k	1 + 2 * k	$1 + 2 * k, 1 + k + k^2$
1116	<pre>nestedWhileMultiVarRecAcross(k)</pre>	$1 + k + k^2$	$1 + k + k^2$	$1 + k + k^2$ , $2 + k + k^2$
1117	${\tt nestedWhileMultiPathMultiVarRecAcross(k)}$	$1 + k + k^2$	$1 + k + k^2$	$1 + k + k^2$ , $2 + k + k^2$

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### 7 RELATED WORK

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

Static program analysis. Our algorithm in Section 5 is influenced by many areas of static program analysis such as effect systems, control-flow analysis, and data-flow analysis [Ryder and Paull 1988]. 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 [Çiçek et al. 2017a;

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

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

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

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Our execution-based data dependency relation definition over variables is inspired by the method in [Cousot 2019], where the dependency relation is also identified by looking into the differences on two execution traces. However, Cousot excludes timing channels [Sabelfeld and Myers 2003] and empty observation, which are also not considered as a form of dependency in traditional dependency analysis [Denning and Denning 1977]. Our definition includes timing channels and empty observation by observing both the disappearance and value variation.

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Generalization in Adaptive Data Analysis. Starting from the works by Dwork et al. [2015c] and 1184 Hardt and Ullman [2014], several works have designed methods that ensure generalization for 1185 adaptive data analyses. Some examples are: [Bassily et al. 2016; Dwork et al. 2015a,b; Feldman 1186 and Steinke 2017; Jung et al. 2020; Rogers et al. 2020; Steinke and Zakynthinou 2020; Ullman et al. 1187 2018]. Several of these works drew inspiration from the idea of using methods designed to ensure 1188 1189 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, 1190 even in adaptive settings, differential privacy can also be used to limit the influence that a specific 1191 data sample can have on the statistical validity of a data analysis. This connection is actually in 1192 two directions, as discussed for example by Yeom et al. [2018]. 1193

1194 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 1195 our work. Adaptive Fuzz [Winograd-Cort et al. 2017] is a programming framework for differential 1196 privacy that is designed around the concept of adaptivity. This framework is based on a typed 1197 functional language that distinguish between several forms of adaptive and non-adaptive composi-1198 1199 tion 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 1200 privacy. However, it does not include any technique to bound the number of rounds of adaptivity. 1201 Lobo-Vesga et al. [2021] propose a language for differential privacy where one can reason about 1202 1203 the accuracy of programs in terms of confidence intervals on the error that the use of differential 1204 privacy can generate. These are akin to bounds on the generalization error. This language is based 1205 on a static analysis which however cannot handle adaptivity. The way we formalize the access 1206 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 1207 et al. [2021] and Aguirre et al. [2021] use different techniques to track the number of accesses to an 1208 1209 oracle. However, reasoning about the number of accesses is easier than estimating the adaptivity of 1210 these calls, as we do instead here. 1211

### 8 CONCLUSION AND FUTURE WORKS

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.

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, 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 in some complicated examples with nested while loops, the corresponding improvement is also in our plan.

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