

LOCALIZING FAULTS IN NUMERICAL SOFTWARE USING A VALUE-BASED CAUSAL MODEL

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List of Abbreviations

- OMIM: Online mendelian inheritance in man
- GWAS: Genome-wide association study
- UMLS: Unified medical language system
- CBIR: Content-based image retrieval
- SIFT: Scale invariant feature transformation
- HOG: Histograms of oriented gradients
- SVM: support vector machine
- HPRD: Human protein reference database
- PPI: Protein-protein interaction
- HDN: Human disease network
- CRC: Colorectal cancer
- PD: Parkinson's disease
- DMN: Disease manifestation network
- IMPC: International mouse phenotyping consortium
- FDA: Food and drug administration

Localizing Faults in Numerical Software Using a Value-Based Causal Model
LOCALIZING FAULTS IN NUMERICAL SOFTWARE USING A VALUE-BASED
CAUSAL MODEL

Abstract

by

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Causal statistical fault localization (CSFL) thechnique has been approved to be effective in localizing software faults with test profiles and outcome. But when applying CSFL on numerical software fault localization, t most research on SFL, execution dynamics have been characterized either purely by code-coverage profiles, indicating which statements, branches, or paths were covered by each execution (e.g., [1]), or by indicators of the outcomes of predicates (e.g., [2]) ? both existing branch predicates and predicates inserted specifically to enhance SFL (e.g., ones that compare the values of numeric variables to zero). Although the outcomes of such predicates reflect the values of program variables to some extent, they often do so inadequately for SFL, e.g., because predicates or conditions were omitted mistakenly, because they are hidden in library code, or because few predicates are actually required in the program. Even predicates inserted in a program to enhance SFL are likely to characterize the values of numeric variables inadequately, unless application-specific information is available that indicates which predicates should be inserted. These facts make coverage and predicate-based SFL techniques poorly suited to localizing faults in numerical programs and subprograms having relatively few conditional branches.

We first investigates the performance of Baah et al?s causal regression model

for fault localization when an important precondition for causal inference, called positivity, is violated. Two kinds of positivity violations are considered: structural and random ones. We prove that random, but not structural nonpositivity may harm the performance of Baah et al?'s causal estimator. To address the problem of random nonpositivity, we propose a modification to the way suspiciousness scores are assigned. Empirical results are presented that indicate it improves the performance of Baah et al?'s technique. We also present a probabilistic characterization of Baah et al?'s estimator, which provides a more efficient way to compute it.

Then we proposed NUMFL. NUMFL is a value-based causal inference model for localizing faults in numerical software. NUMFL combines causal and statistical analyses to characterize the causal effects of individual numerical expressions on output errors. Given value-profiles for an expression's variables, NUMFL uses generalized propensity scores (GPSs) or covariate balancing propensity scores (CBPSs) to reduce confounding bias caused by evaluation of other, faulty expressions. It estimates the average failure-causing effect of an expression using quadratic regression models fit within GPS or CBPS subclasses. We report on an empirical evaluation of NUMFL involving components from four Java numerical libraries, in which it was compared to five alternative statistical fault localization metrics. The results indicate that NUMFL is the most effective technique overall. We also found that NUMFL works fairly well with data from failing runs alone.

Chapter 1

The Importance of Being Positive in Causal Statistical Fault Localization

1.1 Introduction

Coverage-based statistical fault localization (SFL) techniques apply statistical or machine learning techniques to code-coverage profiles (or “spectra”) and PASS/-FAIL labels for a set of observed program executions, in order to identify possible locations of the fault(s) that caused some of the executions to fail. These techniques equate the “suspiciousness” of a program element with a statistical measure of the association between coverage of that element and the occurrence of program failures. For example Baah et al showed [7] that the Tarantula metric [17], the Ochiai metric [6], and the F1-measure [7] each embed an estimator of the conditional probability of program failure given that a statement is covered, which we denote by $P(F|s)$.

It should be noted, first of all, that these and other suspiciousness metrics do *not* directly estimate the probability that is *faulty*, because doing so would require data about observed faults, not just data about *failures*. One might hope instead

that such suspiciousness metrics yield good estimates of the *average causal effect* [18] of executing a given program element on the occurrence of failures, which we shall call the *average failure-causing effect* (AFCE). Average causal effect estimates are used to study causality in a variety of fields, such as epidemiology, econometrics, and social science. However, as Baah et al pointed out [7], SFL suspiciousness metrics often produce biased estimates of a program element’s AFCE, due to the effects of other program elements. For example, Figure 1.1 shows a small function that contains a bug in statement s_3 , which should be $y = x + 2$. Appropriately, $P(F|s_3) = 1$. However, because the faulty statement s_3 is always executed before either of the correct statements s_5 or s_8 is executed, $P(F|s_5) = P(F|s_8) = 1$, which suggests misleadingly that s_5 and s_8 are faulty.

Statements	Sample Code
	double foo(int a ,int b) {
s_1	int x = 0, int y = 0;
s_2	if (a > 0) {
s_3	y = x + 1; // fault
s_4	if (b > 0) {
s_5	output(y + 1);
	}
	else {
s_8	output(y + 2);
	}
	else {
s_{11}	output(y + 3);
	}
	}

Figure 1.1: Motivating Example

This problem, which is an instance of *confounding bias* (or just *confounding*) [18], is due to the fact that execution of the control dependence region [9] containing statements s_3 and s_4 is a *common cause* of program failure and of execution of state-

ment s_5 or s_8 . More generally, confounding of the effect of a “treatment” variable T on an outcome variable Y is bias due to the presence of a common cause C of T and Y . Confounding bias cannot be eliminated, in general, without considering the causal relationships between the variables under study. These relationships are typically represented in a *causal* DAG [18], which is a directed acyclic graph in which there is an edge $A \rightarrow B$ just in case variable A is a direct cause of variable B . For example, Figure 1.2 is a very simple causal graph showing the causal relationships between a treatment T , an outcome Y , and a confounder C . For SFL, Baah et al [1, 6] proposed using a causal DAG derived from the *program dependence graph* (PDG) [12], in which the nodes represent binary coverage indicator variables.

Confounding can be reduced or eliminated by adjusting or controlling for a suitable set of variables during statistical analysis. A well-known result of Pearl, the *Back-Door Adjustment Theorem* [18], states that a set of covariates X in a causal DAG G is sufficient for confounding adjustment if it “blocks” all “backdoor paths” between the treatment T and the outcome Y . A *backdoor path* between T and Y is a path with an arrow $T \leftarrow$ entering T . A path is *blocked* by \mathbf{X} if the path (1) contains a configuration of the form $\rightarrow Z \rightarrow$ or $\leftarrow Z \rightarrow$ such that $Z \in \mathbf{X}$ or (2) contains a “collider” $\rightarrow Z \leftarrow$ such that neither Z nor any of its descendants is in \mathbf{X} . For example, in Figure 1.2 the path $T \leftarrow C \rightarrow Y$ is a backdoor path, which is blocked by C .

To adjust (partially) for confounding bias in *causal SFL* (CSFL), Baah et al proposed estimating the AFCE of a particular statement s by using a linear regression model of the form

$$Y = \beta_0 + \beta_1 T_s + \beta_2 C_s + \sigma, \quad (1.1)$$

where σ is the treatment (coverage) indicator for s (1: covered, 0: not covered); C_s is a coverage indicator for the *forward control dependence predecessor* of s [9], which we denote by $\text{pred}(s)$; Y is a failure indicator (1: fails; 0: passes); β_0 , β_1 , and β_2

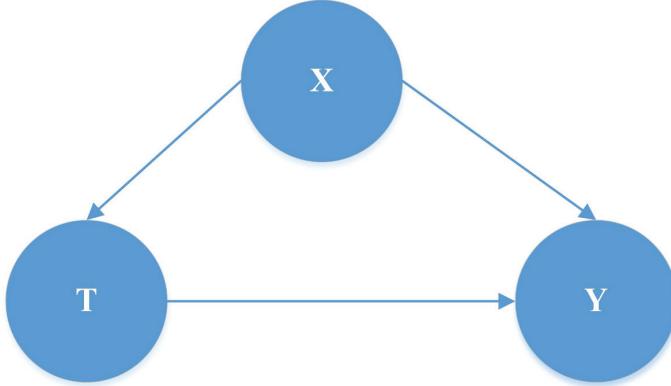


Figure 1.2: Causal Diagram of treatment, outcome and confounder

are coefficients, and σ is a random error term. (Model (1) is not applicable to s if $pred(s)$ does not exist.) Note that the units being “treated” are program executions. The covariate C_s is used for confounding adjustment in this model because, in the forward control dependence subgraph of the PDG of a structured program, $pred(s)$ blocks all backdoor paths between T_s and Y . (It does not generally block backdoor paths involving data dependences, however.) The AFCE estimate for s is given by the estimated value $\hat{\beta}_1$ of the coefficient β_1 of T_s in model (1). This estimate is used as the suspiciousness score of s . Note that an instance of model (1) is fitted for each statement. We shall refer to model (1) as Baah et al’s CSFL *regression model*. (Note that Baah et al also proposed another approach to CSFL based on matching instead of regression [8], and it does address data dependences.)

Interestingly, model (1) performed well when evaluated [7] even though the coverage data it requires often violates an important precondition for valid causal inference, called the “positivity” condition. In the remainder of this paper, we shall examine why this is so and suggest improvements to Baah et al’s technique based on our conclusions.

1.2 The Problem of Positivity Violations

Positivity [15] is an important condition for valid causal inference but is often overlooked in SFL research.

Definition. The positivity condition holds with respect to a treatment variable T and a set X of covariates for confounding adjustment if the conditional probability $P(T = t|X = x)$ of receiving treatment value t , given the covariate values $X = x$, is greater than zero for all t and for all x such that $P(X = x) > 0$. Suppose that s is a statement with a unique forward control dependence predecessor $\text{pred}(s)$. In terms of Baah et al's CSFL regression model (2.1), positivity requires that, whether $\text{pred}(s)$ is covered ($C_s = 1$) or is not covered ($C_s = 0$), the probability of s being covered ($T_s = 1$) and the probability of s not being covered ($T_s = 0$) are both positive. If either probability is zero then we say that the positivity condition is violated.

There are two distinct ways in which positivity can be violated [9, 10]:

- Structural violations of positivity occur if units with certain values of X cannot possibly be treated (or untreated). For example, when the function in Figure 1.1 is executed, if statements s_3 and s_4 are not covered then neither of statements s_5 and s_8 will be covered. In the presence of structural non-positivity, causal inferences cannot be made about the entire population of units. The inference needs to be restricted to strata with X values for which structural positivity holds.
- Random violations of positivity occur, in the absence of structural violations, due to sampling variability. That is, a sample is drawn containing some units with a value x of X such that for a certain treatment value t , no unit in the sample having $X = x$ also has $T = t$. For example, given a set of tests of the function in Figure 1.1, it may be that none of them covers statement s_8 , even

though it is possible to construct a test that does so.

1.2.1 Research Questions

In the remainder of this paper, we will consider three research questions concerning nonpositivity.

RQ1: Is Baah et al’s causal inference model (2.1) subject to structural violations of positivity? If so, how does this influence the AFCE estimates it yields? In model (2.1), T_s and C_s are both binary variables, so we might conceive of four different (T_s, C_s) pairs: $(T_s = 0, C_s = 0)$, $(T_s = 0, C_s = 1)$, $(T_s = 1, C_s = 0)$ and $(T_s = 1, C_s = 1)$. However, $(T_s = 1, C_s = 0)$ cannot occur with execution data from a structured program, because if an execution does not cover $\text{pred}(s)$, it cannot cover s . Thus $P(T_s = 1 | C_s = 0) = 0$, and so model (2.1) is subject to structural nonpositivity. This means that it is impossible to identify the average causal effect of T_s on Y when C_s is not restricted to be 1. However, the empirical evaluation of model (2.1) reported by Baah et al [7], as well as our own experimentation with the model, suggest that this does not seriously harm its fault localization performance in practice. In Section III.A, we employ linear algebra to determine why this is so.

RQ2: What are the consequences if model (2.1) is used despite random violations of positivity? Ideally, model (2.1) would be applied with execution data such that for each statement , both $(T_s = 1, C_s = 1)$ and $(T_s = 0, C_s = 1)$ occur. This would be the case, for example, with a test set that achieves branch coverage. In practice, however, it is possible that one or both of these pairs does not occur. In this case, either the treated group of executions or the untreated group is empty. If s is not covered, there is no basis at all for estimating its AFCE. This leaves the question of what to do if is covered whenever $\text{pred}(s)$ is covered. We examine this issue in Section III.B.

RQ3: Given that model (2.1) is subject to structural nonpositivity, is the estimate $\hat{\beta}_1$ of the coefficient β_1 a valid causal effect estimate? In Section III.C, we present a probabilistic characterization of $\hat{\beta}_1$ that clarifies this issue.

In Section IV, we also investigate RQ2 and RQ3 empirically.

1.3 Analysis of the Research Questions

1.3.1 Analysis of RQ1

In Section 1.2.1, we saw that Baah et al's CSFL regression model (2.1) is subject to structural violations of positivity. In this section, we analyze model (2.1) to see why this apparently does not harm its fault localization performance. Let \mathbf{y} , \mathbf{t}_s , and \mathbf{c}_s be column vectors of corresponding values of the failure indicator Y and the coverage indicators T_s and C_s , respectively, observed over a set of executions. Let $\mathbf{1}$ be a column vector of 1s of the same length n . Let \mathbf{X} be the matrix $[\mathbf{1}, \mathbf{t}_s, \mathbf{c}_s]$ and let $\boldsymbol{\beta}$ be the column vector $[\beta_0, \beta_1, \beta_2]'$ (we use ' here to indicate vector or matrix transpose). Then the regression model in equation (2.1) can be rewritten as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \quad (1.2)$$

where $\boldsymbol{\epsilon}$ is a column vector of random errors.

Assume that the parameters in model (2.2) are estimated by ordinary least squares. Then the causal effect estimator $\hat{\beta}_1$ is given by [16]

$$\hat{\beta}_1 = \frac{(cov(\mathbf{c}_s, \mathbf{c}_s) \cdot cov(\mathbf{t}_s, \mathbf{y}) - cov(\mathbf{t}_s, \mathbf{c}_s) \cdot cov(\mathbf{c}_s, \mathbf{y}))}{(cov(\mathbf{t}_s, \mathbf{t}_s) \cdot cov(\mathbf{c}_s, \mathbf{c}_s) - cov(\mathbf{t}_s, \mathbf{c}_s) \cdot cov(\mathbf{t}_s, \mathbf{c}_s))} \quad (1.3)$$

where $cov(\mathbf{a}, \mathbf{b})$ denotes the covariance of sample vectors \mathbf{a} and \mathbf{b} . Letting the

length of \mathbf{a} and \mathbf{b} be n , we have

$$cov(\mathbf{a}, \mathbf{b}) = \frac{1}{n-1} \sum_i (a_i - \bar{\mathbf{a}})(b_i - \bar{\mathbf{b}}) \quad (1.4)$$

Here, $\bar{\mathbf{a}}$ and $\bar{\mathbf{b}}$ denote the means of vectors \mathbf{a} and \mathbf{b} , respectively. Applying equation (1.4) to equation (2.3) and rearranging terms, the numerator of the quotient in equation (2.3) is:

$$(\mathbf{c}_s \cdot \mathbf{c}_s)(\mathbf{t}_s \cdot \mathbf{y}) - (\mathbf{c}_s \cdot \mathbf{t}_s)(\mathbf{c}_s \cdot \mathbf{y}) - n\bar{\mathbf{c}}_s^2(\mathbf{t}_s \cdot \mathbf{y}) + n\bar{\mathbf{c}}_s\bar{\mathbf{t}}_s(\mathbf{c}_s \cdot \mathbf{y}) \quad (1.5)$$

and the denominator of the quotient in equation (2.3) is

$$(\mathbf{c}_s \cdot \mathbf{c}_s)(\mathbf{t}_s \cdot \mathbf{t}_s) - (\mathbf{c}_s \cdot \mathbf{t}_s)^2 - n\bar{\mathbf{t}}_s^2(\mathbf{c}_s \cdot \mathbf{c}_s) - n\bar{\mathbf{c}}_s^2(\mathbf{t}_s \cdot \mathbf{t}_s) + 2n\bar{\mathbf{c}}_s\bar{\mathbf{t}}_s(\mathbf{c}_s \cdot \mathbf{t}_s) \quad (1.6)$$

where $\mathbf{c}_s \cdot \mathbf{c}_s = \sum_i (c_{s,i})^2$, $\mathbf{c}_s \cdot \mathbf{t}_s = \sum_i (c_{s,i}t_{s,i})$, $\mathbf{c}_s \cdot \mathbf{y} = \sum_i (c_{s,i}y_i)$, $\mathbf{t}_s \cdot \mathbf{t}_s = \sum_i (t_{s,i})^2$, and $\mathbf{t}_s \cdot \mathbf{y} = \sum_i (t_{s,i}y_i)$ are scalar products and where $c_{s,i}$, $t_{s,i}$ and y_i denote the values of C_s , T_s , and Y for the i th execution, respectively.

From 1.2.1, we know that there are three possible (T_s, C_s) pairs: $(T_s = 0, C_s = 0)$, $(T_s = 0, C_s = 1)$, and $(T_s = 1, C_s = 1)$. However, when an execution has $(T_s = 0, C_s = 0)$, its corresponding $(c_{s,i})^2$, $c_{s,i}t_{s,i}$, $c_{s,i}y_i$, $(t_{s,i})^2$, and $t_{s,i}y_i$ values are all equal to 0, so that it makes no contribution to the values of the scalar products $\mathbf{c}_s \cdot \mathbf{c}_s$, $\mathbf{c}_s \cdot \mathbf{t}_s$, $\mathbf{c}_s \cdot \mathbf{y}$, $\mathbf{t}_s \cdot \mathbf{t}_s$, and $\mathbf{t}_s \cdot \mathbf{y}$. Such an execution makes no contribution to either the numerator (1.5) or the denominator (1.6) of the quotient in equation (2.3). This implies that the value of the estimator $\hat{\beta}_1$ is determined solely by executions with $(T_s = 0, C_s = 1)$ and $(T_s = 1, C_s = 1)$. Provided that each of these pairs occurs for at least one execution, positivity holds for the stratum (group) of executions with $C_s = 1$, since $P(T_s = 0|C_s = 1) > 0$ and $P(T_s = 1|C_s = 1) > 0$. In this case $\hat{\beta}_1$ estimates the effect of the treatment variable T_s on the outcome variable Y , given

that C_s is restricted to be 1. That is, $\hat{\beta}_1$ estimates the effect of covering s on the occurrence of failures when $pred(s)$ is covered.

1.3.2 Analysis of RQ2

In this section, we will discuss how random violations of positivity influence the performance of Baah et al's CSFL model (2.1) and how to handle them. As discussed in Section 1.2, random nonpositivity occurs when a statement s is always executed ($T_s = 1$) or is never executed ($T_s = 0$) given that its forward control predecessor $pred(s)$ is covered ($C_s = 1$). In this case, the estimator $\hat{\beta}_1$ is not an unbiased estimator of the average failure-causing effect of and may perform poorly as an SFL metric. The problem of random nonpositivity can be resolved by running additional test cases to increase code coverage. In case that is not practical, however, we consider what should be done instead.

Assume that for statement s , the treatment indicator T_s is always equal to 1 given that $C_s = 1$. Since $pred(s)$ is, by assumption, the unique forward control dependence predecessor of s , it must dominate s in the program's control flow graph (lie on all paths to s). Hence, if $pred(s)$ is not covered then s cannot be covered either. Consequently, $T_s = C_s$ for all test cases. This will cause a collinearity problem [24] with the linear model (2.1). A standard way to address this problem is to remove the variable C_s from model (2.1) to obtain the following model:

$$Y = \beta_0 + \beta_1^* T_s + \epsilon \quad (1.7)$$

The estimate $\widehat{\beta}_1^*$ plays the role of causal effect estimator. It is known that $\widehat{\beta}_1^* \approx P(Y = 1|T_s = 1)$ [7]. Since $T_s = C_s$, we also have that $\widehat{\beta}_1^* \approx P(Y = 1|C_s = 1)$. Thus, under random non-positivity, $\widehat{\beta}_1^*$ estimates the probability of failure given $C_s = 1$.

Since model (1.7) does not adjust for confounding bias, $\widehat{\beta}_1^*$ may deviate from the

Statements	Sample Code
	double foo(int a , int b, int c) {
s_1	int x = 0, int y = 0;
s_2	if (c > 0){
s_3	$x = x + 1; //fault$
s_4	if(a > 0) {
s_5	y = x + 2;
s_6	if(b > 0) {
s_7	output(y + 1);
	}
	else {
s_{10}	output(y + 2);
	}
	}
	else{
s_{11}	output(y + 3);
	}
	}
	}

Figure 1.3: Erroneous Program

failure causing effect of covering statement s . For example, consider the program in Figure 1.3, which contains a faulty statement s_3 , which should be $x = x + 1$. Suppose that we want to estimate the failure causing effect of covering statement $s = s_7$. Assume that none of the observed executions cover statement s_{10} . This is a random violation of positivity, because $(T_{s_7} = 0, C_{s_7} = 1)$ is not observed. The estimator $\widehat{\beta}_1^*$ will be equal to $P(Y = 1|C_{s_7} = 1)$, where $pred(s_7) = s_6$. Because the faulty statement s_3 always executes before statement s_6 is executed, we have $P(Y = 1|C_{s_7} = 1) = 1$, even though both s_7 and s_6 are correct.

To address random nonpositivity involving a target statement s and $pred(s)$, we propose assigning the suspiciousness score of $pred(s)$ to statement s , provided that the causal effect estimator for $pred(s)$ adjusts for confounding. When random non-

positivity occurs, s and $\text{pred}(s)$ have the same coverage information and thus their coverage-based suspiciousness scores should be same. Referring again to Figure 1.3, the suspiciousness score of s_7 would be made equal to the suspiciousness score of s_6 , which is estimated by model (2.1) with $T_s = s_6$ and $C_s = s_4$. We empirically evaluate this idea in Section 1.4.2.

1.3.3 Analysis of RQ3

In this section, we will derive a probabilistic interpretation for causal effect estimator $\hat{\beta}_1$. We first define some notation for different numbers of executions: $N_{T_s} = 1$ is the number of executions with $T_s = 1$; $N_{C_s} = 1$ is the number with $C_s = 1$; $N_{C_s=1, T_s=1}$ is the number with $C_s = 1$ and $T_s = 1$; $N_{C_s=1, Y=1}$ is the number with $C_s = 1$ and $Y = 1$; and $N_{T_s=1, Y=1}$ is the number with $T_s = 1$ and $Y = 1$. Because $\text{pred}(s)$ dominates s in the program's control flow graph, we have

$$N_{C_s=1, T_s=1} = N_{T_s=1} \quad (1.8)$$

In addition, since C_s, T_s are binary variables we have:

$$\mathbf{c}_s \cdot \mathbf{c}_s = \sum_i (c_{s,i})^2 = N_{C_s=1} \quad (1.9)$$

$$\mathbf{c}_s \cdot \mathbf{t}_s = \mathbf{t}_s \cdot \mathbf{t}_s = \sum_i (t_{s,i})^2 = N_{T_s=1} \quad (1.10)$$

$$\mathbf{c}_s \cdot \mathbf{y} = \sum_i c_{s,i} y_i = N_{C_s=1, Y=1} \quad (1.11)$$

$$\mathbf{t}_s \cdot \mathbf{y} = \sum_i t_{s,i} y_i = N_{T_s=1, Y=1} \quad (1.12)$$

With equations (1.8)-(1.12) we can rewrite the numerator (1.5) of the quotient in

equation (2.3), as

$$\begin{aligned}
& N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{C_s=1,Y=1} - n\bar{\mathbf{c}}_s^2N_{T_s=1,Y=1} + n\bar{\mathbf{c}}_s\bar{\mathbf{t}}_sN_{C_s=1,Y=1} \\
& = N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{C_s=1,Y=1} - \frac{N_{C_s=1}^2N_{T_s=1,Y=1}}{n} + \frac{N_{C_s=1}N_{T_s=1}N_{C_s=1,Y=1}}{n} \\
& = N_{C_s=1}N_{T_s=1,Y=1}\left(1 - \frac{N_{C_s=1}}{n}\right) - N_{T_s=1}N_{C_s=1,Y=1}\left(1 - \frac{N_{C_s=1}}{n}\right) \\
& = (N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{C_s=1,Y=1})\left(1 - \frac{N_{C_s=1}}{n}\right)
\end{aligned} \tag{1.13}$$

Applying equations (1.8)-(1.12) to the denominator (1.6) in equation (2.3), we can rewrite it as

$$\begin{aligned}
& N_{C_s=1}N_{T_s=1} - N_{T_s=1}^2 - n\bar{\mathbf{t}}_s^2N_{C_s=1} - n\bar{\mathbf{c}}_s^2N_{T_s=1} + 2n\bar{\mathbf{c}}_s\bar{\mathbf{t}}_sN_{T_s=1} \\
& = N_{C_s=1}N_{T_s=1} - N_{T_s=1}^2 - \frac{N_{T_s=1}^2N_{C_s=1}}{n} - \frac{N_{C_s=1}^2N_{T_s=1}}{n} + \frac{2N_{C_s=1}N_{T_s=1}}{n} \\
& = N_{C_s=1}N_{T_s=1} - N_{T_s=1}^2 + \frac{N_{T_s=1}^2N_{C_s=1} - N_{C_s=1}^2N_{T_s=1}}{n} \\
& = N_{T_s=1}(N_{C_s=1} - N_{T_s=1})\left(1 - \frac{N_{C_s=1}}{n}\right)
\end{aligned} \tag{1.14}$$

Given the derivations in (1.13) and (1.14), equation (2.3) can be rewritten as follows:

$$\begin{aligned}
\hat{\beta}_1 & = \frac{(N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{C_s=1,Y=1})(1 - \frac{N_{C_s=1}}{n})}{N_{T_s=1}(N_{C_s=1} - N_{T_s=1})(1 - \frac{N_{C_s=1}}{n})} \\
& = \frac{N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{C_s=1,Y=1}}{N_{T_s=1}(N_{C_s=1} - N_{T_s=1})} \\
& = \frac{N_{C_s=1}N_{T_s=1,Y=1} - N_{T_s=1}N_{T_s=1,Y=1}}{N_{T_s=1}(N_{C_s=1} - N_{T_s=1})} - \frac{N_{T_s=1}N_{C_s=1,Y=1} - N_{T_s=1}N_{T_s=1,Y=1}}{N_{T_s=1}(N_{C_s=1} - N_{T_s=1})} \\
& = \frac{N_{T_s=1,Y=1}}{N_{T_s=1}} - \frac{N_{C_s=1,Y=1} - N_{T_s=1,Y=1}}{N_{C_s=1} - N_{T_s=1}}
\end{aligned} \tag{1.15}$$

Thus, the causal effect estimator $\hat{\beta}_1$ is a difference of two terms:

$$\frac{N_{T_s=1,Y=1}}{N_{T_s=1}} \tag{1.16}$$

and

$$\frac{N_{C_s=1,Y=1} - N_{T_s=1,Y=1}}{N_{C_s=1} - N_{T_s=1}} \tag{1.17}$$

Let $N_{T_s=0, C_s=1}$ be the number of executions with $(T_s = 0, C_s = 1)$, and let $N_{T_s=0, C_s=1, Y=1}$ be the number of executions with $(T_s = 0, C_s = 1, Y = 1)$. Considering the relationship between s and $\text{pred}(s)$, we see that

$$N_{T_s=0, C_s=1} = N_{C_s=1} - N_{T_s=1} \quad (1.18)$$

$$N_{T_s=0, C_s=1, Y=1} = N_{C_s=1, Y=1} - N_{T_s=1, Y=1} \quad (1.19)$$

Recall that $N_{C_s=1, T_s=1} = N_{T_s=1}$. Similarly, we have $N_{T_s=1, Y=1} = N_{C_s=1, T_s=1, Y=1}$. Rewriting term (1.16), we see that

$$\begin{aligned} \frac{N_{T_s=1, Y=1}}{N_{T_s=1}} &= \frac{\frac{N_{C_s=1, T_s=1, Y=1}}{n}}{\frac{N_{T_s=1}}{n}} \\ &\approx \frac{P(T_s=1, C_s=1, Y=1)}{P(T_s=1, C_s=1)} \\ &= P(Y = 1 | T_s = 1, C_s = 1) \end{aligned} \quad (1.20)$$

Applying equations (1.18) and (1.19) to term (1.17), we see that

$$\begin{aligned} \frac{N_{C_s=1, Y=1} - N_{T_s=1, Y=1}}{N_{C_s=1} - N_{T_s=1}} &= \frac{\frac{N_{T_s=0, C_s=1, Y=1}}{n}}{\frac{N_{T_s=0, C_s=1}}{n}} \\ &\approx \frac{P(T_s=0, C_s=1, Y=1)}{P(T_s=0, C_s=1)} \\ &= P(Y = 1 | T_s = 0, C_s = 1) \end{aligned} \quad (1.21)$$

Hence,

$$\hat{\beta}_1 \approx P(Y = 1 | T_s = 1, C_s = 1) - P(Y = 1 | T_s = 0, C_s = 1) \quad (1.22)$$

This demonstrates that Baah et al's AFCE estimator $\hat{\beta}_1$ actually approximates the *associational risk difference* [14] within the stratum of executions with $C_s = 1$. This measure is equal to the *causal risk difference* [11] within the stratum $C_s = 1$ if the treatment effect of T_s on Y is unconfounded in that stratum. Whether or not the last condition is true, $\hat{\beta}_1$ is not an unbiased estimator of the AFCE over the whole population of executions. This is consistent with our conclusions about structural

nonpositivity in Section 1.3.1. Note that if a random violation of positivity occurs, one of the two probability terms in equation (1.22) will be undefined, so $\widehat{\beta}_1$ will be undefined.

1.4 Empirical Study

We also conducted an empirical study of research questions RQ2 and RQ3. We first describe the study platform and subject programs and then present the study results.

1.4.1 Study Platform and Subject Programs

Platform: Our study platform is based on the JavaPDG dependence analysis tool [20] and the ASM Java bytecode manipulation framework [1]. To obtain the data required to use Baah et al’s model (2.1), we first instrument a Java subject program’s class files using ASM, to record statement coverage information at runtime. Then JavaPDG is used to generate a program dependence graph (PDG) of the subject program. Each PDG node is mapped back to a source code statement. For each statement , the PDG records the statement ID of *preds*, if the latter exists.

Subject Programs: We selected three subject programs written in Java: NanoXML, Rome, and Xerces2. NanoXML [2] (version 1) is an XML parser from Software-artifact Infrastructure Repository (SIR) [4]. Rome (revision 840) is a open source library for parsing, generating, and publishing RSS and Atom feeds [3]. Apache Xerces2(v.2.9.1) is a processor for parsing, validating, serializing, and manipulating XML [5].

Tests and Faults: NanoXML comes with test suites. To test Xerces2, XML files were collected from the system directories of an Ubuntu Linux 7.04 machine. For Rome, test cases were obtained by downloading Atom and RSS files with a custom

Table 1.1: Subject programs, tests, and faults

Subject Program	LOC	Number of Tests	Faults
NanoXML (SIR v1)	4.4K	1,000	4
Rome (revision 840)	24K	2,000	5
Xerces2 (v.2.9.1)	167K	1536	5

web crawler. A sample of faults was selected randomly from the repository for each subject program: 4 for NanoXML, 5 for Rome, and 5 for Xerces2. A summary of our subject programs and tests is shown in Table 1.1.

1.4.2 Evaluation of RQ2

To evaluate our conclusions about RQ2, we designed two sub-studies. The first sub-study was done to check whether random violations of positivity happen in practice. For a statement s , such violations might occur in two ways: (1) no test executions have $(T_s = 0, C_s = 1)$, which means s is always covered given $C_s = 1$ and (2) no test executions have $(T_s = 1, C_s = 1)$, which means s is never covered given $C_s = 1$. Note that in case (2), statement s is never executed and so will not be assigned a suspiciousness score. Thus, in our study we considered only case (2). We also considered *only* statements s for which preds exists. Then we determined, for each subject program, which such statements were covered. For each covered statement s , we checked if there were executions with $(T_s = 0, C_s = 1)$. If not, a random violation of positivity, denoted RVP, occurred for s . Table 2.8 shows the proportion of RVP statements among all covered statements for each subject program. It shows that 4% to 7% of covered statements had random violations of positivity.

The second sub-study for RQ2 was done to determine if random violations of positivity affect the suspiciousness scores of statements. The performance of Baah et al's causal effect estimator $\hat{\beta}_1$ was measured by the number of RVP statements

Table 1.2: Proportion of RVP statements among Covered statements with forward control dependence predecessor

Subject Program	Number of RVP statements	Covered Statements with $\text{pred}(s)$	Proportion
NanoXML	19	315	6.03%
Rome	95	1353	7.02%
Xerces2	232	5545	4.18%

Table 1.3: Comparison between Baah et al's Original estimator and the "Adjusted" estimator

Subject Program	Number of RVP statements	Baah et al's estimator-bad scores	Adjusted estimator-bad scores
NanoXML	19	19	3
Rome	95	29	23
Xerces2	232	207	102

assigned a "bad" suspiciousness score. We considered an RVP statement to have a bad suspiciousness score if its score was larger than but the statement was not faulty or if its score was at most but the statement was faulty. In Section 1.3.2, we proposed assigning the suspiciousness score of preds to an RVP statement s . Hence, we also checked if this "adjusted" estimator performed better than $\hat{\beta}_1$ under random violations of positivity. Table 2.9 shows the number of RVP statement assigned "bad" suspiciousness scores by each estimator. All the RVP statements of NanoXML had "bad" suspiciousness scores. For Xerces2, 207 out of 232 RVP statements had bad suspiciousness scores. For Rome, RVP statements do not cause big problem: only 29 out of 95 RVP statements had bad suspiciousness scores. When we applied the adjusted causal effect estimator, the numbers of RVP statements with bad suspiciousness scores dropped to 3 for NanoXML, to 23 for Rome, and to 102 for Xerces2. The results suggest that the adjusted estimator performs better than the original one under random violations of positivity.

Table 1.4: Comparison between Baah et al's Original estimator and the "Adjusted" estimator

Subject Program	Mean	Variance	P-value
NanoXML	1.68E-16	1.25E-29	1
Rome	5.68E-16	8.05E-29	1
Xerces2	1.79E-16	7.64E-29	1

Table 1.5: Average execution times of regression-based causal effect estimator and probability-based causal effect estimator

Subject Program	Regression	Probability
NanoXML	8.049 sec	4.354 sec
Rome	135.809 sec	44.308 sec
Xerces2	143.235 sec	54.578 sec

1.4.3 Evaluation of RQ3

In Section 1.3.3, we have derived equation (1.22), which is a probabilistic characterization of Baah et al's estimator $\hat{\beta}_1$. An alternative estimator can be computed based directly on the right side of this equation, by replacing each probability by the corresponding sample proportion. The two estimators should produce nearly identical suspiciousness scores. To evaluate the correctness of equation (1.22), we applied both estimators to the data from each of the subject programs. We then computed the mean difference between these resulting scores, over all the statements of each subject program. The result is shown in Table 2.10. We see that the mean difference is extremely small for each program, as is the variance of the difference. Table 2.10 also shows the P-values of Student's tests of the null hypothesis of no difference in the score distributions, which are all 1 for each program. This indicates the means of each two groups of suspiciousness scores are statistically indistinguishable.

We also measured the computation time for both estimators. The results are shown in Table 2.11. The probability-based causal effect estimator required substantially less computation time than the regression-based estimator, especially for the large subject program Xerces2.

1.5 Related Work

The most closely related work is on causal statistical fault localization techniques. Baah et al [8] extended their original CSFL model by also controlling for confounding bias caused by data flow dependences, and they found this reduced localization costs. Gore et al [13] proposed an improved version of Baah et al’s original approach by providing a model that also addresses what they call *failure flow confounding bias*. Shu et al [21] proposed a CSFL technique for localizing faulty *methods* in large programs, which exploits dynamic call graph and dependence information and addresses nonpositivity.

Other related work examines positivity violations in causal inference generally. Westreich, et al [23] pointed out that positivity is important for making valid inferences from observational data but is often overlooked in practice, and they discussed general ways of dealing with nonpositivity. Wang, et al [22] analyzed the bias of an inverse-probability-of-treatment-weighted estimator in the face of positivity violations. Petersen, et al [19] systematically reviewed how violations of positivity influence different types of causal-effect estimators.

Some recent studies have investigated methods for estimating causal effects in the presence of positivity violations. A “trimming” technique is used in [11] is to discard units whose probability of treatment, conditional on covariates, is outside of a specified interval. Another method proposed by Bembom et al [10] is to exclude the confounders involved in positivity violations from the adjustment sets.

1.6 Conclusion

Causal statistical fault localization techniques such as Baah et al’s CSFL regression technique can be biased when the positivity condition is violated. In this paper,

we have analyzed two types of violations of positivity: structural violations and random violations. We established that structural violations do occur with Baah et al's technique but are not harmful. We proved that random violations also occur and that they can distort suspiciousness scores. To address the problem of random nonpositivity, we proposed a modification to the way suspiciousness scores are assigned with Baah et al.'s technique. Empirical results were presented that indicate it improves the technique's performance. We also presented a probabilistic characterization of Baah et al's estimator and showed that it provides a more efficient way to compute the same scores.

Since Baah et al's CSFL regression technique is based on a causal graph which omits data dependences, and since it characterizes program states only in terms of statement coverage, it does not eliminate all confounding bias in fault localization. Nevertheless, it seems to perform well, and with our suggested improvements it is computationally efficient.

Chapter 2

Causal Inference Based Fault Localization for Numerical Software with NUMFL

2.1 Introduction

Numerical software plays a very important role in science, industry, and defense, and failures of numerical software have been reported as the cause of several well-publicized “disasters” [?, ?]. However, automated techniques intended specifically for localizing numerical faults based on execution data have received relatively little attention from researchers, although there has been substantial research on general *statistical fault localization* (SFL) techniques (e.g. [?, ?, ?]) and on other general automated debugging techniques (see Section 2.6).

Typical SFL techniques take data characterizing a set of both passing and failing program executions, including PASS/FAIL labels (provided by testers or end users) and recorded profiles of internal program dynamics, and they compute statistical measures of the strength of the association, if any, between the occur-

rence of software failures and the occurrence of certain runtime events at particular program locations. These measures are then used to help guide the search for the causes of observed failures, typically by ranking program statements by the strengths of their associations with failures. When SFL techniques are evaluated they are generally used as the sole source of information about possible fault locations. However, it seems more realistic to envision them ultimately being used in combination with other sources of information, such as programmer hunches and *fault prediction models* [?] based on static code properties and project history. Potentially, SFL techniques provide a relatively inexpensive way to maximize the information obtained by testing.

In the vast majority of research on SFL, execution dynamics have been characterized either purely by *code-coverage profiles* (also called “spectra”), indicating which statements, branches, or paths were covered by each execution (e.g., [?]), or by indicators of the outcomes of *predicates* (e.g., [?]) – both existing branch predicates and predicates inserted specifically to enhance SFL (e.g., ones that compare the values of numeric variables to zero). Although the outcomes of such predicates reflect the *values* of program variables, they may do so inadequately for SFL, e.g., because predicates or conditions are omitted mistakenly, because they are hidden in library code or microcode, or because few predicates are actually required in the program. These facts make typical SFL techniques *poorly suited* for localizing faults in numerical programs and subprograms having relatively few conditional branches. Even predicates inserted in a program to enhance SFL are likely to characterize the values of numeric variables inadequately, unless application-specific information is available that indicates which predicates should be inserted.

Although purely numerical programs, and numerical components of other programs, are often relatively small, the intricacy of their computations can make them very difficult to debug manually. In order to provide automated fault local-

ization assistance to developers who need to debug numerical programs or components, we present a new approach to SFL, denoted by *NUMFL*, that is designed specifically to localize faults in numerical code. *NUMFL*, like some other recent work on SFL [?, ?, ?, ?], is based on *causal inference methodology* [?], which seeks to mitigate biases like confounding bias that can badly distort SFL scores used to guide the search for faults. However, in contrast to previous work, *NUMFL* is based on generalized forms of *propensity scores* [?, ?], which are a fairly recent development in causal inference that provide a means of reducing confounding bias when estimating the causal effect of a numeric *treatment* or *exposure* variable on an outcome variable.

In this chapter, each value of the “treatment” variable T_e is the result of evaluating a numerical expression or subexpression with a *unique program location* identified by e , and the outcome variable Y represents the error (possibly zero) in the output of the numerical program or component under consideration. The causal effect of T_e on Y is characterized by a function $r_e(t)$, which in medical research is called a *dose-response function* (DRF) [?]. To enable localization of faults, *NUMFL* summarizes the behavior of $r_e(t)$ over a set of evaluations of expression e , with a single quantity $susp(e)$ called a *suspiciousness score*. It employs generalized propensity scores to make it less likely that a correct expression will receive a high suspiciousness score because it used variables whose values were erroneous due to faults in *other* expressions. Note that we do *not* use propensity scores themselves as suspiciousness scores; the two kinds of scores have very different purposes.

We assume that (in most cases) users of *NUMFL* have a set of program or component inputs that induces multiple failing and multiple passing runs. For these inputs, *NUMFL* requires corresponding *expected outputs* (not just PASS/FAIL labels) and execution profiles characterizing variable values. The expected outputs are provided by testers or end-users, and the profiles are recorded automatically by

program instrumentation. To compute the suspiciousness score $susp(e)$, NUMFL requires, in addition to values of the treatment variable T_e and the output-error variable Y , corresponding values of the set of variables *used* in expression e . Although the value-profiles used by NUMFL are more detailed than basic coverage profiles used by typical SFL techniques, the potential cost of recording and analyzing value profiles is offset by the relatively small size of many numerical programs. Moreover, we assume that developer-time is a more critical resource in debugging than is computation time, because developers usually can do other work while an SFL algorithm runs.

The main contributions of this chapter are:

- NUMFL, a new, value-based approach to SFL for numerical programs, which is based on sound causal inference methodology
- A new, value-based approach to SFL for numerical programs, named NUMFL, that is based on sound causal inference methodology, and two variants of NUMFL, denoted NUMFL-GPS and NUMFL-CBPS, based on alternative forms of generalized propensity scores
- The first use of generalized propensity scores to reduce confounding bias in SFL
- An implemented platform to profile the variables used and defined by numerical expressions in Java programs
- An empirical comparison of NUMFL to five competing SFL techniques on components from four widely-used Java numerical libraries, which indicates that NUMFL is more effective overall than the other techniques
- Empirical evaluations of NUMFL on programs with single faults, with multiple faults, with both passing and failing executions, and with only failing executions

- An empirical comparison of NUMFL-GPS and NUMFL-CBPS to each other

The rest of the chapter is organized as follows: we present a motivating example in Section 2.2; background for our approach is presented in Section 2.3; NUMFL is described in detail in Section 2.4; we report on its empirical evaluation in Section 2.5; related work is surveyed in Section 2.6; and Section 2.7 concludes the chapter.

2.2 Motivating Example

Figure 2.1 shows a short function *harmean*, which correctly calculates the harmonic mean of two floating point numbers, in the middle column and shows a faulty version of *harmean* in the rightmost column. (In real fault localization scenarios only the faulty code is usually available.) We injected a fault into statement s_3 by adding a floating point number c to the original expression $a * b$. Given a pair of inputs (a, b) , the faulty version of s_3 produces an erroneous value for the variable x . This value may propagate to statement s_8 and, via the variable r , cause an incorrect return value at statement s_9 . We use $r_{correct}$ and r_{faulty} to denote the return value of the correct code and faulty code, respectively. Let us assume that the faulty version of *harmean*, like many numerical programs, is considered to fail if the output error exceeds a predefined threshold ϵ , that is, if

$$outerr = |r_{correct} - r_{faulty}| > \epsilon$$

Our goal is to automatically localize faults in numerical expressions, given variable-value profiles and expected outputs. In the faulty code of Figure 2.1, there are three numerical expressions, in statements s_2 , s_3 and s_8 , which define variables k , x , and r . A simple approach to detecting which expressions contain numerical faults is to obtain a “suspiciousness” score for each numerical expression by calculating a measure of the statistical association between the values of the expression

Statements	Correct Code	Faulty Code
s_1	<code>double harmean(a ,b)</code>	<code>double harmean(a,b,c)</code>
s_2	<code>k=a+b;</code>	<code>k=a+b;</code>
s_3	<code>x=a*b;</code>	<code>x=a*b+c; //bug</code>
s_4	<code>if (x==0) {</code>	<code>if (x==0) {</code>
s_5	<code> return null;</code>	<code> return null;</code>
s_6	<code>}</code>	<code>}</code>
s_7	<code>else {</code>	<code>else {</code>
s_8	<code>r=2*x/k +k;</code>	<code>r=2*x/k +k;</code>
s_9	<code>return (r);</code>	<code>return (r);</code>
	<code>}</code>	<code>}</code>

Figure 2.1: Motivating Example

and the output error. This naïve approach has two potential problems, however. First, erroneous values due to a fault in one expression may propagate to other, correct expressions, causing them to receive high suspiciousness scores. For example, in Figure 2.1 the fault in statement s_3 causes variable x to have erroneous values that propagate to statement s_8 and cause variable r to have erroneous values. Consequently, the output error of *harmean* is associated with the values computed by both s_3 and s_8 , even though s_8 is correct. This problem, which is an instance of *confounding bias* (or *confounding*), is due to the fact that the computation of x at s_3 is a *common cause* of program failure and of the computation of r at s_8 . A naïve measure of the association of r with the output error, which does not account for confounding, will reflect both the true causal effect of r on failure and the biasing effect of the confounder x on r and *outerr*.

The second problem with the naïve approach is that common association measures like Pearson’s correlation coefficient [?] are often inadequate to measure the causal effect of a numerical expression on a program’s output error, even without confounding. For the example in Figure 2.1, $outerr = |r_{correct} - r_{faulty}| = |2c/(a+b)|$. If $a = 1$ and $b = 0$, then $outerr = 2|c|$ and $x = c$. By definition, the correlation be-

tween x and $outerr$ is:

$$\text{corr}(x, outerr) = \frac{\text{cov}(x, outerr)}{\sigma_x \sigma_{outerr}} = \frac{\text{cov}(c, 2|c|)}{\sigma_x \sigma_{outerr}}$$

where $\text{cov}(x, outerr)$ is the covariance between x and $outerr$ and where σ_x and σ_{outerr} are the standard deviations of x and $outerr$, respectively. Using basic covariance identities, we find that $\text{cov}(c, 2|c|) = 2\text{cov}(c, |c|) = 2E[(c - \mu_c)(|c| - \mu_{|c|})]$, where μ_c and $\mu_{|c|}$ are the means of c and $|c|$ respectively. If the distribution of variable c is symmetric about 0, $\text{cov}(c, |c|)$ is equal to 0, and so is $\text{corr}(x, outerr)$. Therefore, $\text{corr}(x, outerr)$ can be 0, even though the statement defining x contains a fault.

NUMFL is intended to address the aforementioned problems and to provide less-biased estimates of the *failure-causing effect* of a numerical expression. We now map the causal variables defined in the Introduction to the variables in our example:

1. Treatment variable T_e is the variable defined in a numerical expression e . In Figure 2.1, variables k , x and r are the treatment variables associated with statements s_2 , s_3 and s_8 , respectively.
2. Outcome variable Y is the absolute difference between the output of the faulty program and the expected (correct) output. For the example, Y is $outerr$.
3. X represents the confounding variables, which are each causes of both treatment T_e and outcome Y . For example, in the numerical expression $r = 2*x/k$, the variables x and k are confounders because they each influence the values of both the treatment $T_e = r$ and the outcome $Y = outerr$.

Figure 2.2 shows the causal relationships between treatment, outcome, and con-

founding variables.

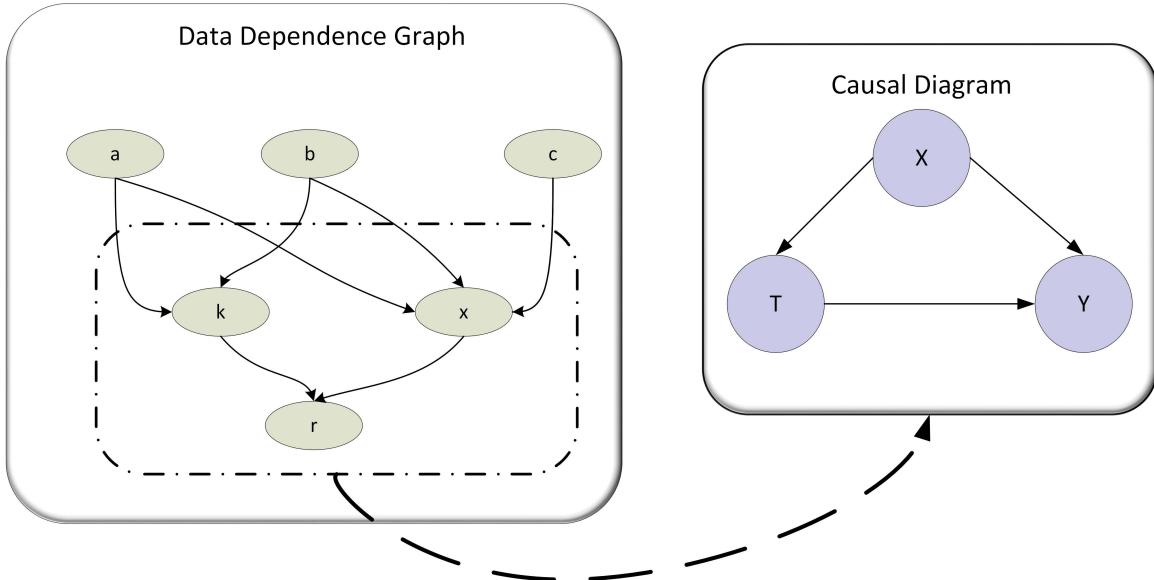


Figure 2.2: Causal diagram of treatment, outcome, and confounder.

2.3 BACKGROUND

2.3.1 Causal Inference Methodology

Causal inference methodology [?] has emerged in recent decades from research in a number of applied fields, to provide a basis for making valid inferences, from experimental or observational data, about the causal effects of specified treatments or exposures upon outcomes of interest. Data about study variables is augmented with background knowledge about the causal relationships among variables, which is represented as *causal DAG*: a directed acyclic graph, in which nodes correspond to variables and in which there is an edge $A \rightarrow B$ if A is an actual or assumed cause of B . Causal inference theory establishes graph-theoretic conditions, such as Pearl's Backdoor Criterion [?], under which a given causal effect can be estimated statistically without confounding or other forms of bias such as selection bias and measurement bias.

2.3.2 Ordinary Propensity Scores

Consider a treatment variable T with two possible values 1 and 0. (These values may indicate “treated” and “untreated”, respectively, or they may indicate alternative treatments.) One of the reasons that ideal randomized experiments, when they are feasible, are often considered the “gold standard” for the design of causal inference studies [?] is that randomization makes it likely that the joint distribution of the covariates of the units with $T = 1$ is similar to the covariate distribution of the units with $T = 0$. Such similarity, which is called *covariate balance* [?], implies that the two groups of units are comparable with respect to the values of confounding covariates, so that any difference in average outcomes of the groups is likely to be due to the treatment variable and not to confounding. In randomized experiments, covariate balance is a consequence of the fact that the randomized treatment variable is *independent* of the covariates.

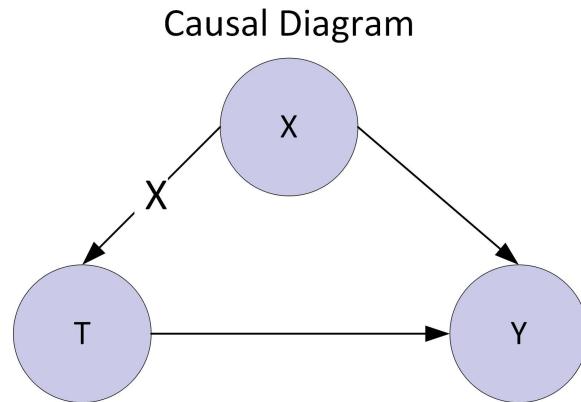


Figure 2.3: Matching units based on their propensity scores breaks the link between confounding variables and treatment.

An important approach to achieving covariate balance in observational studies is the use of (ordinary) *propensity scores* [?]. For a binary treatment variable T and a vector of covariates \mathbf{X} , the propensity score $Pr(T = 1|\mathbf{X} = \mathbf{x})$ is the conditional probability of treatment $T = 1$ given that the observed value of \mathbf{X} is \mathbf{x} . It has been shown that the propensity score is a *balancing score* in the sense that comparison

groups with similar propensity scores tend to have similar covariate distributions [?]. True propensity scores are generally unknown, but they can be estimated from data about study units' actual treatment and covariate values.

Suppose that for each unit i examined in an observational study, we have recorded the values of a binary treatment variable $T_i \in \{0, 1\}$ and a vector of covariates \mathbf{X}_i . We can use a parametric model $\pi_{\beta}(\mathbf{X}_i)$ to estimate the propensity score for unit i . One choice is the logistic model:

$$\pi_{\beta}(X_i) = Pr(T_i = 1 | \mathbf{X}_i) = \frac{\exp(\mathbf{X}_i' \boldsymbol{\beta})}{1 + \exp(\mathbf{X}_i' \boldsymbol{\beta})}$$

We can estimate the parameter β using maximum likelihood estimation [?], which involves maximizing the log-likelihood function:

$$\hat{\boldsymbol{\beta}}_{MLE} = \arg \max \sum_{i=1}^N T_i \log \{\pi_{\beta}(\mathbf{X}_i)\} + (1 - T_i) \log \{1 - \pi_{\beta}(\mathbf{X}_i)\} \quad (2.1)$$

With the fitted model, we can estimate the ordinary propensity score $\pi_{\beta}(\mathbf{X}_i)$ for each observed unit.

After the propensity score model is estimated, covariate balance may be achieved by matching units based on their estimated propensity scores [?]. For example, each unit with $T = 1$ can be matched to a unit with $T = 0$ that has a similar estimated propensity score, if such a unit exists. As illustrated in Figure 2.3, matching units based on their propensity scores breaks the link between the confounding variables and the treatment variable.

Ordinary propensity scores are not applicable to continuous treatment variables, however. To address confounding of SFL scores for numerical expressions, we consider two variants of ordinary propensity scores that can accommodate continuous (and integer) treatment variables. The first variant is the Generalized Propensity Score (GPS) proposed by Imai and Van Dyk [?]. The second variant is

the Covariate Balancing Propensity Score (CBPS) proposed by Imai and Ratkovic [?]. Since CBPS is quite new, it has not been established whether it is superior to GPS. Hence, we shall present and evaluate two versions of NUMFL, denoted NUMFL-GPS and NUMFL-CBPS, which are based on GPS and CBPS, respectively. First, though, we briefly describe GPS and CBPS in the next two subsections.

2.3.3 Generalized Propensity Score (GPS)

The *Generalized Propensity Score* proposed by Imai and van Dyk [?] is intended for use with any kind of treatment variable, including continuous ones. Let $p_{\psi}(T|\mathbf{X})$ be a model, with parameters ψ , of the *conditional probability density function* (p.d.f.) of the treatment variable T given the covariate vector \mathbf{X} . The GPS for a specific unit with treatment level $T = t$ and covariate values $\mathbf{X} = \mathbf{x}$ is the density value $r = p_{\psi}(T = t|\mathbf{X} = \mathbf{x})$. Imai and van Dyk [?] require that the model $p_{\psi}(T|\mathbf{X})$ has a *unique parameter* $\theta = \theta_{\psi}(\mathbf{X})$ such that $p_{\psi}(T|\mathbf{X})$ depends on \mathbf{X} only through θ . For example, if the treatment is represented by a *linear Gaussian model* $T|\mathbf{X} \sim \mathcal{N}(\mathbf{X}'\beta, \sigma^2)$ with mean $\mathbf{X}'\beta$ (the scalar product \mathbf{X} -transpose times β) and variance σ^2 , so that $\psi = (\beta, \sigma^2)$, then $\theta = \mathbf{X}'\beta$ (here θ is scalar). The model parameters ψ , r , θ , β , etc. are estimated from data; the corresponding estimates are denoted with by $\hat{\psi}$, \hat{r} , $\hat{\theta}$, $\hat{\beta}$, etc.. In Imai and van Dyk's approach, it is the values of the parameter estimate $\hat{\theta}_{\hat{\psi}}(\mathbf{X})$ that are used to control confounding, rather than the values of $p_{\hat{\psi}}(T|\mathbf{X})$ themselves.

Table 2.1 lists 10 test cases of faulty code in the motivating example. The three inputs a , b and c are generated randomly in the range $[-5, 5]$. Table 2.1 also shows the values of intermediate variables values of k and x which are defined in expressions s_2 and s_3 respectively. The variable r in expression s_8 is the faulty code's output and the variable r_c represents the output of the correct code in motivating example with the same inputs. Outcome variable Y is equal to $|r - r_c|$, so all the

values of Y are positive in the table. All the values in the table are rounding to three decimals. We use expression s_8 as an example to demonstrate generalized propensity score is estimated. For expression s_8 , the treatment variable T_e is variable r and the confounding variables X are covariates x and k . We first fit a linear regression model $T_e = \beta_0 + \beta_1 x + \beta_2 k$ with r as response, x and k as predictors. Given the data in Table 2.1, the fitted regression model is $T_e = 0.614x + 1.212k - 1.462$. Then we estimate GPS $\hat{\theta}_{\hat{\psi}}(x, k)$ by inputting observed value of x and k into the fitted regression model. The estimated GPS for expression s_8 is denoted by $\hat{\theta}_{s_8}$ and is shown in the last column of the table.

The confounding variables' effect on treatment variable can be controlled if conditioned on GPS. This can be proved with the data in Table 2.1. For the confounding variable x 's effect on treatment variable r , we fit two regression models: the first model uses r as respond and x as predictor; the second model uses r as respond, but uses both x and GPS $\hat{\theta}_{s_8}$ as predictors. Given the data in Table 2.1, the first model is fitted as $r = 0.487x - 1.729$ and the second model is fitted as $r = -2.271E^{-16}x + 1.0\hat{\theta}_{s_8} - 1.461$. In the first model, the coefficient of x means the variable r will increase 0.487 if x increased 1 unit. In the second model, the coefficient of x is close to 0, while the coefficient of propensity score $\hat{\theta}_{s_8}$ is 1. This means the variable value of r is mostly depend on the value of $\hat{\theta}_{s_8}$. Similarly, we can have another two fitted model for the other confounding variable k : $r = 0.999k - 1.415$ and $r = -2.755E^{-16}k + 1.0\hat{\theta}_{s_8} - 1.461$. The coefficient of k is also reduced to 0 in the second model. Thus, given GPS, the effect of confounding variables on treatment variable is significantly reduced, which can also be illustrated by Figure 2.3

2.3.4 Covariate Balancing Propensity Score (CBPS)

Section 2.3.2 explained that the ordinary propensity score is a balancing score and that it can be estimated from data using a parametric statistical model. However,

Table 2.1: VARIABLE VALUES AND GPS OF THE MOTIVATING EXAMPLE

Test #	1	2	3	4	5	6	7	8	9	10
a	-1.697	4.088	0.242	-0.269	-3.495	-2.081	-2.063	-2.896	3.839	-3.412
b	-1.430	0.660	4.843	-1.803	-3.352	1.282	-1.520	4.568	1.796	0.325
c	-3.990	3.778	-2.242	-0.347	-1.678	-0.358	3.766	-4.690	-2.535	-1.645
k	-3.127	4.748	5.084	-2.072	-6.847	-0.799	-3.583	1.672	5.636	-3.088
x	-1.564	6.478	-1.071	0.138	10.036	-3.025	6.902	-17.919	4.362	-2.752
r	-2.127	7.477	4.663	-2.205	-9.778	6.777	-7.436	-19.768	7.184	-1.305
r_c	-4.679	5.885	5.545	-2.540	-10.268	5.881	-5.334	-14.157	8.083	-2.371
Y	2.552	1.592	0.882	0.335	0.490	0.896	2.102	5.611	0.900	1.065
$\hat{\theta}_{ss}$	-4.749	9.731	5.502	-2.426	-2.132	-2.825	-0.102	-8.978	9.506	-5.431

if the propensity score model $\pi_{\beta}(\mathbf{X}_i)$ is *misspecified*, matching on the estimated propensity scores (and related techniques) may fail to balance the covariates, yielding biased estimates of causal effects. To address this problem, Imai and Ratkovic proposed the *Covariate Balancing Propensity Score* (CBPS), which is robust to mild misspecification of the propensity score model [?]. The CBPS optimizes covariate balance by modifying the estimation procedure for parameter β . Differentiating equation (2.1), equating the result to zero, and taking expectations, we have [?]

$$E \left\{ \frac{T_i \pi'_{\beta}(\mathbf{X}_i)}{\pi_{\beta}(\mathbf{X}_i)} - \frac{(1 - T_i) \pi'_{\beta}(\mathbf{X}_i)}{1 - \pi_{\beta}(\mathbf{X}_i)} \right\} = 0, \quad (2.2)$$

where $\pi'_{\beta}(\mathbf{X}_i) = \partial \pi_{\beta}(\mathbf{X}_i) / \partial \beta$. Equation (2.2) is called a *balancing condition* or a *moment condition* [?]. (The mean of a random variable is its “first moment” [?].) In CBPS, the balancing condition is generalized as

$$E \left\{ \frac{T_i \tilde{\mathbf{X}}_i}{\pi_{\beta}(\mathbf{X}_i)} - \frac{(1 - T_i) \tilde{\mathbf{X}}_i}{1 - \pi_{\beta}(\mathbf{X}_i)} \right\} = 0, \quad (2.3)$$

where $\tilde{\mathbf{X}}_i = f(\mathbf{X}_i)$ represents a vector-valued function of the covariates \mathbf{X}_i . To ensure that the first moment of each covariate is balanced, even when the model is misspecified, we can set $\tilde{\mathbf{X}}_i = \mathbf{X}_i$. CBPS employs a parameter estimation frame-

work called the *generalized method of moments* (GMM) [?], which is based on solving moment-condition equations for the parameters of interest and substituting sample moments for unknown population moments. Imai *et al.* extended CBPS to treatments with $K > 2$ integer values, using a *multinomial model* for the conditional probability of treatment given the covariates. We adapted this approach slightly to make it applicable to value-based fault localization (see Section 2.4.2), and we evaluate CBPS in NUMFL as an alternative to GPS .

2.4 TWO VERSIONS OF NUMFL

In this section, we define two versions of NUMFL, NUMFL-GPS and NUMFL-CBPS, and explain how they are used to reduce confounding bias during estimation of a numerical expression’s *average failure-causing effect* (AFCE). Intuitively, an aggregate measure of the failure-causing effect of a numerical expression e should summarize the effects on output errors of evaluating e over a sample of program runs that each cover or reach e . Accordingly, in causal inference the designated “treatment” variable T_e should reflect the values produced by individual evaluations of e . (Of course e may be evaluated repeatedly in a single program run, due to iteration.) Runs that do not reach e are *not relevant* to such a measure. This is unlike measures of the failure-causing effect of covering a statement s at least once during a run (e.g., [?]), which contrast runs that cover s with runs that don’t cover s . With such measures, the treatment variable indicates whether or not s was covered during a given run.

Recall that confounding of the causal effect of a treatment variable T upon an outcome variable Y is bias that is due to the presence of one or more common causes of T and Y . The influence of such a common cause X can make the effect of T on Y , as reflected by a naïve measure of statistical association, appear

to be stronger or weaker than it really is. As mentioned in Section 2.3.2, ordinary propensity scores cannot be used in causal inference to control confounding when the treatment variable is continuous. Since the “treatments” that NUMFL deals with are the values of numeric program variables, we instead define and evaluate two versions of NUMFL, namely NUMFL-GPS and NUMFL-CBPS, that are based respectively on GPS and CBPS, the two generalizations of ordinary propensity scores described in Sections 2.3.3 and 2.3.4.

2.4.1 NUMFL-GPS

As with ordinary propensity scores, GPS is used to control for statistical associations between the treatment variable and confounding covariates, which in the case of NUMFL are variables used (read) in a numeric expression e whose AFCE we wish to estimate. In general, these program variables are potential confounders because they may contain erroneous values just before expression e is evaluated, due to faults in previously evaluated expressions. If these erroneous values cause program failures (that is, “coincidental correctness” does not occur) the result of evaluating e may be strongly associated with failures even if e is correct, unless steps are taken to control confounding. In NUMFL, therefore, when estimating the AFCE of T_e on the output error Y , we control for the values of the variables used in e . (Those familiar with Pearl’s Backdoor Adjustment Criterion [?] should note that this breaks any backdoor paths between T_e and Y in the acyclic data flow graph induced by a program execution.)

Control of Confounding.

For a given numerical expression e in a program, NUMFL-GPS currently fits a linear Gaussian GPS model $\mathbf{T}_e | \mathbf{X}_e \sim N(\mathbf{X}'_e \boldsymbol{\beta}_e, \sigma^2_e)$, where the treatment variable T_e represents the result of evaluating e (once) and where the possibly confounding

covariates in the vector \mathbf{X}_e represent the corresponding values of the program variables used in evaluating e . Observe that one program run may generate multiple values of T_e and \mathbf{X}_e , due to iteration. To reduce profiling overhead, these may be sampled rather than recorded exhaustively. We currently sample only the values from the *last iteration* of a loop.

Applying GPS in NUMFL entails the following three steps:

1. Given a sample of observed values for the treatment variable T_e and for the covariates \mathbf{X}_e , fit a linear regression model $T_e = \mathbf{X}'_e \boldsymbol{\beta}_e$ to obtain the estimated parameter vector $\hat{\boldsymbol{\beta}}_e$.
2. For each observed value $\mathbf{x}_{e,i}$ of \mathbf{X}_e , compute the estimate $\hat{\theta}_{e,i} = \mathbf{x}_{e,i}' \hat{\boldsymbol{\beta}}_e$.
3. Group observations with the same or similar values of $\hat{\theta}_{e,i}$ into m subclasses of roughly equal size.

The regression model fitted in the first step characterizes how the values of the covariates in \mathbf{X}_e influence the value of the treatment variable T_e . In the second step, $\hat{\theta}_{e,i}$ estimates this influence for a particular value $\mathbf{x}_{e,i}$ of \mathbf{X}_e . The scalar $\hat{\theta}_{e,i}$ summarizes the influence of the vector value $\mathbf{x}_{e,i}$ on the treatment, and hence $\hat{\theta}_{e,i}$ may be used in place of $\mathbf{x}_{e,i}$ for confounding control. Accordingly, in the third step, each subclass of observations with similar $\hat{\theta}_{e,i}$ values corresponds to a set of $\mathbf{x}_{e,i}$ values that influence the treatment similarly. Thus, within each subclass, there is little or no association between confounders and the treatment variable T_e .

To illustrate this procedure, we refer again to the faulty version of the function *harmean* in Figure 2.1. Statement s_8 is $r = 2 * x/k + k$. To control possible confounding of the average failure-causing effect of r by the variables x and k , we first fit a linear model $r = \beta_1 z + \beta_2 k$, where $z = x/k$, using a sample of corresponding observed values (r_i, x_i, k_i) . Second, we apply the fitted model to each pair (x_i, k_i) to obtain a predicted value $\hat{\theta}_i$. Third, we group the observations with similar $\hat{\theta}_i$

values into subclasses. This can be done by sorting the $\hat{\theta}_i$ into descending order and partitioning the sorted values into m roughly equal-size bins.

Although GPS can control confounding bias caused by multiple confounding covariates, there is one challenge to applying it in NUMFL-GPS. If the dimension of X_e is high, the first step of GPS requires a large number of observations to fit a suitable regression model. In practice, a numerical expression defined by a statement could contain more than 10 confounders, but the number of tests may not be large enough to fit the regression parameters with adequate precision. Thus, to apply GPS, we need to control the dimension of confounding variables.

To address this problem, we *decompose* a complex numerical expression into several subexpressions, each involving operators with the same precedence level. For example, a numerical statement $a = (b + c + d) * e$ will be decomposed into two subexpressions: (1) $temp = b + c + d$ and (2) $a = temp * e$. Here, $temp$ is a temporary variable that plays the role of the treatment variable for subexpression (1) and the role of a possible confounder for subexpression (2). Thus, each subexpression has fewer confounding variables and a relatively simple structure. For each subexpression, we use GPS to control confounding bias and then estimate the subexpression's AFCE.

Failure-causing Effect Estimation.

Within each of the subclasses created by grouping observations with similar $\hat{\theta}_i$ values, the treatment values $T_{e,i}$ should be largely independent of the covariate values $X_{e,i}$, provided that the GPS model is adequate. Hence, the relationship between the treatment variable T_e and the outcome variable Y should be nearly unconfounded in each subclass. If this relationship is roughly linear in each subclass, we can estimate the expected dose-response function $E[Y|T_e]$ *within a particular*

subclass using a simple linear regression model [?]:

$$Y = \gamma_e T_e + b \quad (2.4)$$

Recall that Y is the absolute difference between the output of the faulty program and the expected (correct) output. In equation (2.4), b is a constant intercept. The coefficient γ_e is the slope of $E[Y|T_e]$. It indicates how much the expected value of the outcome variable changes when the treatment value increases by one unit. The slope coefficient γ_e can be estimated by the least-squares estimator $\hat{\gamma}_e$:

$$\hat{\gamma}_e = (\mathbf{t}'_e \mathbf{t}_e)^{-1} \mathbf{t}'_e \mathbf{y}, \quad (2.5)$$

where \mathbf{t}'_e is the transpose of the vector of treatment values and where \mathbf{y} is the vector of outcome values (output errors).

Intuitively, an association measure used as an SFL suspiciousness metric for numerical programs should, when applied to a numerical expression e , reflect the likelihood that e is faulty. Although the coefficient estimate $\hat{\gamma}_e$ summarizes the dose-response function, it is not an adequate SFL metric, because of the *symmetry* of many numerical errors. For example, suppose that $Y = |T_e|$. Since the output error Y is completely determined by T_e , expression e should receive a high suspiciousness score. However, if the value of T_e is distributed symmetrically around zero, then $\hat{\gamma}_e$ will be close to zero, which suggests misleadingly that e has no causal effect on program failures.

To derive a better suspiciousness metric, we first analyze the relationship between a numeric fault and the DRF slope estimator $\hat{\gamma}_e$. Assume that the numeric expression e has a fault, which results in erroneous treatment values represented by the treatment variable $T_e^f = T_e$. Let the treatment variable T_e^c represent the corresponding treatment values in the correct program. Then we have $T_e^f = T_e^c + \varepsilon_e$,

where ε_e is a treatment error term. Then $\hat{\gamma}_e$ may be decomposed as follows:

$$\begin{aligned}\hat{\gamma}_e &= (\mathbf{t}_e^f \mathbf{t}_e^f)'^{-1} (\mathbf{t}_e^c + \varepsilon_e)' \mathbf{y} \\ &= (\mathbf{t}_e^f \mathbf{t}_e^f)'^{-1} \mathbf{t}_e^c' \mathbf{y} + (\mathbf{t}_e^f \mathbf{t}_e^f)'^{-1} \varepsilon_e' \mathbf{y} \\ &= \hat{\gamma}_e^c + \hat{\gamma}_e^f,\end{aligned}\tag{2.6}$$

where \mathbf{t}_e^f , \mathbf{t}_e^c , and ε_e are the vectors of sample values for T_e^f , T_e^c , and ε_e , respectively, and where $\hat{\gamma}_e^c = (\mathbf{t}_e^f \mathbf{t}_e^f)'^{-1} \mathbf{t}_e^c' \mathbf{y}$ and $\hat{\gamma}_e^f = (\mathbf{t}_e^f \mathbf{t}_e^f)'^{-1} \varepsilon_e' \mathbf{y}$. The component $\hat{\gamma}_e^f$ of $\hat{\gamma}_e$ characterizes the causal relationship between the treatment error ε_e and the output error Y . If ε_e is symmetrically distributed then the contributions to $\hat{\gamma}_e^f$ of the positive and negative values of ε_e will tend to cancel each other, since Y is an absolute value, leaving $\hat{\gamma}_e^f$ close to zero.

We have considered two possible approaches to this problem. We call the first of these a *dual linear regression model* (DLRM). The basic idea of DLRM is simple: compute $|\hat{\gamma}_e^f|$ separately for positive ε_e and for negative ε_e and then add the two resulting values. (Using the absolute values of the two estimates ensures that they do not cancel each other.) However, although the values of T_e are known, the values of T_e^c and ε_e are unknown, so $|\hat{\gamma}_e^c|$ and $|\hat{\gamma}_e^f|$ cannot be estimated individually. This issue can be addressed given the following assumptions:

Assumption 1: If expression e is faulty then within each GPS subclass the variance of T_e^c is much smaller than the variance of ε_e .

Assumption 2: If expression e is faulty then within each GPS subclass, ε_e is symmetrically distributed about zero.

Assumption 1 implies that the error ε_e is responsible for most of the variance of treatment variable T_e within a subclass. We have observed that this is often the case. Assumption 2 asserts that the previously mentioned issue with symmetri-

cally distributed treatment errors pertains generally.

Given these two assumptions, using DLRM involves the following steps, which are applied separately to each GPS subclass:

1. Sort the values of the treatment variable T_e into descending order. Then split the data into two subsets which contain the values that are larger and smaller than the median value, respectively.
2. Estimate the slope of $E[Y|T_e]$ in each subset separately using linear regression model (1).
3. Summarize the failure-causing effect of T_e by adding the two estimated slopes' absolute values.

Under Assumption 1, if expression e is faulty then T_e^c can be viewed as a constant relative to ε_e within a subclass, so that a large value of T_e corresponds to a large ε_e . This implies that T_e and ε_e have the same sorted order. Assumption 2 implies that splitting the treatment data at its median value separates the treatments with positive ε_e values from the treatments with negative ε_e values. Step 3 prevents the two causal effect estimates from cancelling each other out. Figure 2.4 (a) shows the DRF curve of the DLRM.

In practice, the distribution of ε_e is usually unknown, so it is quite uncertain whether Assumption 2 holds. To address this issue, we have used an alternative to DLRM based on a *quadratic regression model* [18], which we shall refer to as QRM. QRM is more flexible than DLRM, because it does not require sorting and splitting the data within subclasses. It is based on the following alternative to Assumption 2:

Assumption 3: Executions with large absolute treatment errors $|\varepsilon_e|$ have larger output errors Y than executions with small values of $|\varepsilon_e|$.

We have observed that this assumption often holds. If both Assumption 1 and Assumption 3 hold, the failure-causing effect of T_e on Y can be estimated by fitting a quadratic regression model $Y = \zeta T_e^2 + \eta T_e + c$. Figure 2.4 (b) shows the dose-response curve of QRM, which clearly reflects Assumption 3. We use the fitted value $\hat{\zeta}$ of the coefficient ζ as the AFCE estimate within each subclass.

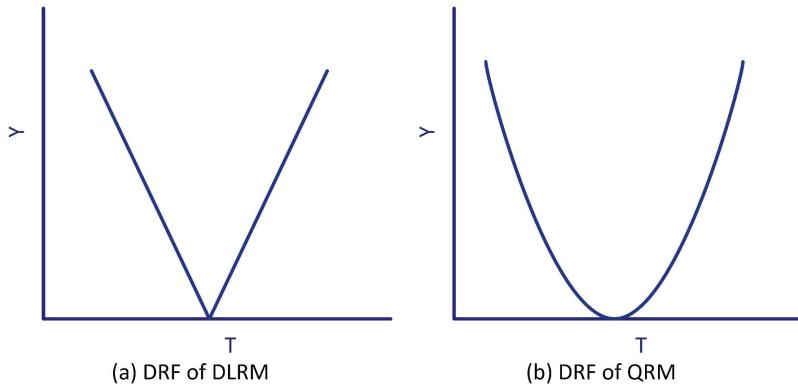


Figure 2.4: Matching units based on their propensity scores breaks the link between confounding variables and treatment.

Finally, we chose to use the absolute value of fitted a regression coefficient's t -statistic [19] as a suspiciousness score, rather than the coefficient itself, because we wish to "penalize" coefficients with large standard errors. We use $|t|$ to denote the absolute value of the t -statistic for a fitted coefficient $\hat{\beta}$: $|t| = |\hat{\beta}/\text{std}(\hat{\beta})|$, where $\text{std}(\hat{\beta})$ is the standard error of $\hat{\beta}$. Thus, for DLRM the failure-causing effect of treatment T_e is estimated by the summation of two linear regression models' $|t|$ values for the fitted slope coefficient $\hat{\gamma}_e$. For QRM, this effect is estimated by the $|t|$ value of the estimated coefficient $\hat{\zeta}$ of the quadratic term of the regression model.

Figure 2.5 shows the NUMFL-GPS algorithm. Note that all input values are standardized ($x \rightarrow \frac{x-\mu}{\sigma}$) to adjust for differences in scale between variables. NUMFL-GPS processes each numeric expression or subexpression e in three stages. In the first stage (lines 2-5 and 10-14), it fits a linear propensity score model regressing the treatment variable T_e on the confounding variables X_e , then uses the fitted model

Figure 2.5 NUMFL Algorithm

Input: Subexpression value table $E = [T_e, \mathbf{X}_e]$, with all values standardized, and type of model M

Output: Suspiciousness scores $\tau(e)$ of subexpressions, sorted in descending order

```

1: for each subexpression  $e$  do
2:    $T_e \leftarrow$  treatment variable of  $i$ th subexpression
3:    $\mathbf{X}_e \leftarrow$  confounding variables of  $i$ th subexpression
4:   if using GPS then
5:     Fit linear regression model  $T_e = \mathbf{X}_e' \boldsymbol{\beta}_e$ 
6:   else if using CBPS then
7:     Fit models for  $Pr(T_e = k | \mathbf{X}_e)$ ,
8:      $k = 1 \dots K$ , using multinomial logistic regression
9:   end if
10:  for each  $x_{e,j}$  do
11:    Estimate the propensity score for  $x_{e,j}$  using fitted GPS or
12:    CBPS model(s).
13:  end for
14:  Group the observations into  $m$  roughly equal-size subclasses.
15:  for each subclass  $k$  do
16:    if  $M$  is DLRM then
17:      Fit two linear regression models:
18:       $Y = \gamma_{e,1} T_e + b$  for observations  $T_e > median(T_e)$ 
19:       $Y = \gamma_{e,2} T_e + b$  for observations  $T_e \leq median(T_e)$ 
20:       $\tau_1 = t\text{-value of } \gamma_{e,1}$ 
21:       $\tau_2 = t\text{-value of } \gamma_{e,2}$ 
22:       $\tau^k = |\tau_1| + |\tau_2|$ 
23:    end if
24:    if  $M$  is QRM then
25:      Fit quadratic regression model  $Y = \zeta T_e^2 + \eta T_e + c$ 
26:       $\tau^k = |t\text{-value of } \hat{\zeta}|$ 
27:    end if
28:  end for
29:   $\tau(e) =$  weighted average of  $\tau^k$  across  $m$  subclasses
30: end for
31: Sort  $\tau(e)$  values in descending order.

```

to calculate the generalized propensity score for each observation. The scores are grouped into m roughly equal-sized subclasses. In the second stage (lines 15-28), the algorithm estimates the “penalized” AFCE of T_e on Y separately in each subclass. If DLRM is employed, the data within a subclass is split into two equal-size groups. The algorithm fits a linear model for each group, and it records the t -statistics τ_1 and τ_2 for the coefficients of T_e in the two models. The penalized AFCE for subclass k is given by the sum $\tau^k = |\tau_1| + |\tau_2|$. If QRM is employed, the algorithm fits a quadratic model and records the coefficient $\hat{\zeta}$ of the quadratic term. The penalized AFCE for subclass k is estimated by the absolute value of the t -statistic for $\hat{\zeta}$. In the third stage, the overall AFCE or suspiciousness score $\tau(e)$ for subexpression e is computed as a weighted average of τ^k over all subclasses k (line 29). Finally, the suspiciousness scores for all subexpressions are sorted in descending order (line 31). The developer uses the sorted list to guide fault localization.

2.4.2 NUMFL-CBPS

NUMFL-CPBS differs from NUMFL-GPS in that the former employs the Covariate Balancing Propensity Score instead of GPS for confounding control. Recall from Section 2.3.4 that the CBPS seeks to optimize covariate balance by employing the Generalized Method of Moments (GMM), which solves balance equations for the parameters of interest.

Control of Confounding.

In Imai and Ratkovic’s extension of CBPS to treatment variables with $K > 2$ discrete values [?], a multinomial logistic regression model is used to estimate the conditional probability $\pi_{\beta}^k(\mathbf{x}) = Pr(T = k | \mathbf{X})$ of treatment k . To handle a continuous treatment variable T_e associated with a numerical expression e , we discretize the values of T_e by partitioning them into ordered bins. For each k , $1 \leq k < K$, the

probability that the original value of T_e belongs in bin k is modeled by

$$\Pr(T_e = k \mid \mathbf{X}_e) = \frac{e^{\beta_k \mathbf{x}_e}}{1 + \sum_{i=1}^{K-1} e^{\beta_i \mathbf{x}_e}}$$

and

$$\Pr(T_e = K \mid \mathbf{X}_e) = \frac{1}{1 + \sum_{i=1}^{K-1} e^{\beta_i \mathbf{x}_e}}$$

The CBPS can be estimated using the open source R package “CBPS” created by Fong, *et al* [?].

The whole process of applying CBPS in NUMFL involves the following three steps:

1. Given a sample of observed values for the discretized treatment variable T_e and for the covariates \mathbf{X}_e , use the R package “CBPS” to estimate the coefficients of a multinomial logistic propensity score model $\pi_\beta^k(\mathbf{x}_{e,i}) = P(T_{e,i} = k \mid \mathbf{x}_{e,i})$ for each k .
2. For each observed value $\mathbf{x}_{e,i}$, estimate propensity score $\hat{\pi}_{e,i}$ with the fitted propensity score model.
3. Group observations with the same or similar values of $\hat{\pi}_{e,i}$ into m subclasses of roughly equal size.

Here $\hat{\pi}_{e,i}$ represents the calculated propensity score for each observed value. Similar $\hat{\pi}_{e,i}$ values correspond to a set of $\mathbf{x}_{e,i}$ values that influence the treatment similarly, so we group the observations into subclasses as we did in NUMFL-GPS. Propensity score estimation and grouping in NUMFL-CBPS corresponds to lines 6-14 in the algorithm of Figure 2.5.

Failure-causing Effect Estimation.

Failure-causing-effect estimation in NUMFL-CBPS follows the same process followed in NUMFL-GPS, which is shown in lines 15-29 of Figure 2.5. For a given subexpression e , QRM or DLRM is used to estimate the “penalized” AFCE of T_e on Y within each subclass individually. Then the failure-causing effect is calculated as a weighted average the penalized AFCEs over all subclasses. Finally, the results for all subexpressions are sorted.

Table 2.2: STANDARDIZED VARIABLE VALUES OF THE MOTIVATING EXAMPLE

Test #	1	2	3	4	5	6	7	8	9	10
a	-0.166	0.876	0.183	0.091	-0.490	-0.235	-0.232	-0.382	0.831	-0.475
b	-0.364	0.023	0.797	-0.433	-0.720	0.138	-0.381	0.746	0.233	-0.039
c	-0.523	0.834	-0.218	0.113	-0.119	0.111	0.832	-0.646	-0.269	-0.114
k	-0.336	0.580	0.619	-0.213	-0.769	-0.065	-0.389	0.222	0.683	-0.331
x	-0.110	0.404	-0.079	-0.001	0.631	-0.204	0.431	-1.156	0.269	-0.186
r	-0.027	0.517	0.358	-0.031	-0.460	0.478	-0.328	-1.027	0.501	0.020
Y	2.552	1.592	0.882	0.335	0.490	0.896	2.102	5.611	0.900	1.065

We will use the expression s_3 and s_8 in the faulty code of motivating example shown in Figure2.1 to demonstrate the NUMFL algorithm in Figure2.5 step by step. The variable values are come from Table2.1. In the motivating example, we know that the bug exists in expression s_3 , so the estimated suspiciousness score of s_3 should be larger than the estimated suspiciousness score of s_8 . In practice, running the NUMFL algorithm requires decomposing complex numerical expression in to several subexpressions , which has relatively simple structure. But the expressions s_3 and s_8 already have simple structure, so we choose to estimate the AFCE of the expressions without decomposing them into subexpressions.

For expression s_3 , the first step is to identify the treatment variable and confounding variables. In the expression s_3 , the treatment variable T_e is variable x and the confounding variables are a , b and c . Then we adjust the differences in scale between variables by standardizing the variables’ values. Table2.2 shows all

the variables values after standardization. Note that the outcome variable Y is not standardized. Next we estimate propensity scores for each observations. To estimate GPS $\hat{\theta}_{s_3}$, we can fit a linear regression model as described in section2.3.3. If NUMFL-CBPS is used, we need to fit a multinomial logistic regression model, which is some what complex. Here we use R package "CBPS" to estimate the CBPS which can automatically fit a multinomial regression model with the treatment variables and confounding variables and then estimate the propensity score. For the detail of the package "CBPS", the reader should refer to [?]. Table2.3 shows expression s_3 's estimated GPS $\hat{\theta}_{s_3}$ and CBPS $\hat{\pi}_{s_3}$ for each observation. With the estimated propensity scores, we group observations with same or similar propensity scores into m subclasses. For simplicity, we use $m = 2$ for the motivating example. We rank the tests according to their propensity scores in descending order. The first 5 tests are in subclass 1 and the last 5 tests are in subclass 2. The last two columns of Table2.3 shows the subclass index of each test for NUMFL-GPS and NUMFL-CBPS. From Table2.3, we can see there is some difference between the subclassification results of NUMFL-GPS and NUMFL-CBPS. In NUMFL-GPS, test 4 and test5 are in subclass 2 , while in NUMFL-CBPS, test4 and test5 belong to subclass1. Similarly, we calculate GPS and CBPS for expression s_8 , which is summarized in Table2.4.

The suspiciousness score of expression is estimated by the average of failure-causing effect in two subclasses. Assume we use QRM to estimate failure-causing effect, a quadratic regression model $Y = \zeta T_e^2 + \eta T_e + c$ is fitted in each subclass. The $|t\text{-value}|$ of the coefficient ζ is the estimated failure-causing effect. Table2.5 shows the estimated failure-causing effect in each subclass when NUMFL-GPS is used. In Table2.5, $|t - value|_1$ denotes the estimated failure-causing effect in subclass1 and $|t - value|_2$ denotes the estimated failure-causing effect in subclass2. The estimated suspiciousness score (AFCE) is equal to $(|t - value|_1 + |t - value|_2)/2$. For

comparison, we also fit a quadratic regression model with full sample without subclassification and the estimated failure-causing effect is denoted by $|t - value|_0$. In Table2.5, $|t - value|_0$ of s_8 is close to $|t - value|_0$ of s_3 , even though s_8 is not faulty. This is because the faulty variable x in s_3 is confounder of variable r in s_8 and make s_8 associate to program failure. When NUMFL-GPS is applied, the estimated AFCE of s_8 is significantly smaller than the estimated AFCE of s_3 . The estimated suspiciousness scores of NUMFL-CBPS are shown in Table2.6. In Table2.6, the difference between s_3 and s_8 's suspiciousness score is larger than the difference between their $|t - value|_0$ s. This means both GPS and CBPS are effective in controlling confounding bias.

Table 2.3: ESTIMATED GPS AND CBPS OF EXPRESSION s_3

Test #	$\hat{\theta}_{s_3}$	$\hat{\pi}_{s_3}$	Subclass index	
			GPS	CBPS
1	0.057	0.847	2	2
2	0.364	0.716	2	2
3	-0.606	5.65E-11	1	1
4	0.310	5.05E-06	2	1
5	0.692	1.60E-09	2	1
6	-0.143	5.872	1	2
7	0.637	2.570	2	2
8	-1.119	5.22E-06	1	1
9	-0.113	0.130	1	1
10	-0.079	5.694	1	2

2.5 EMPIRICAL EVALUATION

To evaluate the effectiveness of NUMFL, we conducted an empirical study involving several subject programs, in which the performance of NUMFL was compared with the performance of several baselines techniques. In the study, we investigated four main research questions: (1) What is the performance of NUMFL compare to baseline techniques when each subject program version contains only one fault?

Table 2.4: ESTIMATED GPS AND CBPS OF EXPRESSION s_8

Test #	$\hat{\theta}_{s_8}$	$\hat{\pi}_{s_8}$	Subclass index	
			GPS	CBPS
1	-0.258	0.521	1	2
2	0.562	3.156	2	2
3	0.323	3.878	2	2
4	-0.127	3.099	1	2
5	-0.110	0.004	2	1
6	-0.149	1.14E-07	1	1
7	0.005	0.008	2	1
8	-0.498	1.51E-06	1	1
9	0.549	3.079	2	2
10	-0.297	0.069	1	1

Table 2.5: ESTIMATED AFCE WITH NUMFL-GPS

Expression	$ t - value _1$	$ t - value _2$	Suspiciousness score	$ t - value _0$
s_3	13.861	0.228	7.045	2.763
s_8	1.045	0.515	0.78	2.601

Table 2.6: ESTIMATED AFCE WITH NUMFL-CBPS

Expression	$ t - value _1$	$ t - value _2$	Suspiciousness score	$ t - value _0$
s_3	4.034	2.219	3.127	2.763
s_8	1.898	0.325	1.112	2.601

- (2) What is the performance of NUMFL compare to the baselines when each subject program version contains two faults?
- (3) Given data from only failing executions, is NUMFL effective?
- (4) Which is most effective, NUMFL-GPS or NUMFL-CBPS?

2.5.1 Experimental Platform and Data Collection

We developed a data collection and analysis platform for numerical fault localization studies involving Java programs. The platform is based on a modified Java parser [?] and the ASM Java bytecode manipulation framework [1]. We first parse the source code of a subject program. Each complete numerical expression is decomposed into a set of subexpressions as described in Section 2.4.1. The ASM compiler is used to instrument the bytecode files of the subject program to record variable values used and produced by the evaluation of each subexpression. Information is recorded to permit the recorded values to be mapped back to the corresponding source-code subexpressions. Each instrumented subject program is executed on a test suite and the induced variable values are recorded. For a subexpression within a loop, we currently record the associated values only for the last iteration of the loop, in order to reduce overhead.

The data collection algorithm is implemented in Java and can be downloaded from [?]. The NUMFL algorithm and other baseline techniques were implemented using the R statistical computing environment [?]. In this study, the number of propensity score subclasses used in the NUMFL algorithm was set to 10.

2.5.2 Subject Programs, Faults, and Tests

Subject Programs. For the empirical study, we selected 16 subject programs from four Java numerical libraries: (1) Apache Common Math (versions 2.1 and 3.1.1), which is a popular Java library for scientific computing [?]; (2) the Oj! Algorithms

library Ojalgo (version 33.0), which is an open source Java library for mathematics, linear algebra and optimization [?]; (3) JAMA, which is a basic linear algebra package for Java [?]; and (4) SciMark 2.0, which is a Java benchmark for measuring the performance of numerical codes occurring in scientific applications [?]. We chose subject programs whose purpose we understood (so that we would be able to write tests for them if necessary) and having as many numerical expressions as possible. We chose four large (≥ 1500 SLOC) and eight small subject programs (< 1500 SLOC) from Apache Common Math; for Ojalgo, we wrote a subject program to calculate the Schur decomposition of a matrix that uses two Ojalgo classes (PrimitiveDenseStore and HermitianEVD32); for JAMA, we created one subject program that uses four different matrix decomposition algorithms; we used two of SciMark's five computation kernels as subject programs, FFT and LU factorization. A summary of our subject programs is shown in Table 2.7.

Table 2.7: SUMMARY OF SUBJECT PROGRAMS

Subject Program	SLOC	# of Sub-expressions	# of Tests	# Faulty versions
Apache_EigenDecompose	1858	611	8000	10
Apache_DSCompiler	1774	220	5000	10
Apache_BigMatrix	1580	244	3000	10
Apache_Rotation3D	1704	504	3000	10
Ojalgo_SchurDecompose	2129	649	5000	10
Jama_MatrixDecompose	1952	578	5000	10
SciMark_LU	295	35	3000	2
SciMart_FFT	197	59	3000	2
Apache_SymmLQ	1226	57	5000	2
Apache_SplineInterpolator	130	45	5000	2
Apche_SimpleRgress	869	61	5000	2
Apache_SchurTransformer	458	154	3000	2
Apache_MillerUpdatRgress	1110	152	1000	2
Apache_HarmonicFitter	385	50	3000	2
Apache_FastSine	197	66	5000	2
Apache_FastCosine	188	77	5000	2

Faults. To evaluate NUMFL, we required faulty versions of subject programs. After much searching, we were able to find few well documented faults (including

fixes) that produced numerical output that was sometimes, but not always, incorrect. Hence, we *injected* three types of simulated numerical faults into the subject programs: (1) adding a small random number to a numerical expression (the number varied between and within runs); (2) multiplying a numerical expression by a random number; (3) randomly changing one of the operators of a numerical expression (once only). Each faulty version of a subject program contained one bug. We generated 12 faulty versions of each subject program whose number of lines of source code was larger than 1500. For each subject program with fewer than 1500 SLOC, we generated two faulty versions. Except for SciMark, every subject program came with a unit test suite which provided a predefined error tolerance; we chose a tolerance of 1.0E-5 for SciMark. We ran the faulty versions of the subject programs and the original correct versions with the same inputs. If the output error Y exceeded the tolerance, the execution was considered to be failure. If the subject program's output was a scalar variable, the output error Y was the absolute difference between the correct and faulty programs' outputs. If the subject program's output was an array, we calculated the difference between each element in the faulty program's output and the corresponding element in correct program's output. The output error Y was taken to be the first difference encountered that was larger than the tolerance or zero if no such difference was found.

Tests. Since a number of our subject programs came with very few test cases, it was necessary to create test cases for them. We first analyzed the subject programs and the test cases provided by their developers. Then we randomly generated inputs similar to those of the test cases. Note that for NUMFL, we did not generally use the total number of tests shown in Table 2.7, though we did so for the baseline techniques. Instead, we first selected all N tests of the smaller of the set of failed tests and the set of passed tests, and we then randomly selected N tests from the larger set. (See Section 2.5.5 for an exception.)

2.5.3 Baseline SFL Metrics and Cost Measure

Baselines. We compared NUMFL to four baseline SFL metrics. Two are coverage-based metrics that have performed well in comparisons with other such metrics: Ochiai [?] and DStar (with $star = 2$) [?]. The Ochiai metric estimates the suspiciousness of a statements s with the equation

$$O(s) = f_s / \sqrt{f(f_s + p_s)} \quad (2.7)$$

where: f_s is the number of failed tests that cover statement s ; p_s is number of passed tests that cover s ; and f is the total number of failed tests. The Dstar metric (with $star = 2$) is

$$D(s) = f_s^2 / (p_s + f - f_s) \quad (2.8)$$

where $f - f_s$ is the number of failed tests that do not cover s .

The other two baselines are predicate-level SFL metrics, SOBER [?] and the Exploratory Software Predictor (ESP) [?]. SOBER computes the probability $\pi(P)$ that a predicate P evaluated to be true in an execution. If the distribution of $\pi(P)$ in passing runs differs significantly from its distribution in failing runs then P is considered to be related to the fault. In this study, for a treatment variable T_e we use these predicates [20]: $T_e > 0$, $T_e = 0$ and $T_e < 0$.

ESP employs “elastic predicates” to partition the value space for each variable x at each assignment to x . ESP provides two instrumentation schemes: single variable and scalar pairs. The single variable scheme uses execution profiles to compute the mean μ_x and standard deviation σ_x for a variable x . These statistics are then used in nine predicates (e.g., $x < \mu_x + \sigma_x$) that collectively partition the values of x for three standard deviations above and below μ_x . ESP then computes an importance score for each predicate. The suspiciousness of each assignment to x is taken to be the highest importance score among the corresponding elastic

predicates. In a similar way, the scalar pair [31] scheme addresses differences in the values of pairs of variables (e.g., $x - y > \mu_{x-y} + \sigma_{x-y}$).

Cost Measure. We measured the costs of applying NUMFL and the baseline metrics by the percentage of *subexpressions* that need to be examined, in decreasing order of suspiciousness scores, to find the fault, assuming the fault is recognized when it is encountered. This contrasts with most SFL techniques, which localize faults at the statement level. There are two reasons that we chose to have NUMFL compute suspiciousness scores for subexpressions rather than for statements. First, the location of a faulty subexpression not only implies the location of the numerical statement that contains the subexpression, but it also indicates which part of the statement is problematic. Second, in this study we collected data only for floating point variables involved in numerical expressions. As a result, the number of subexpressions was usually smaller than the number of lines of code. To ensure a fair comparison between NUMFL and the predicate-level baseline metrics, predicates were associated with subexpressions. In comparing NUMFL to the statement-level, coverage-based baseline metrics, subexpressions belonging to same statement received the *same suspiciousness score*. To compare NUMFL fairly to the latter metrics, if multiple subexpressions got the same suspiciousness score as the faulty subexpression, we considered the faulty subexpression to rank in the middle of them.

2.5.4 Comparative Performance of NUMFL vs. Baselines

Table 2.8 shows, for NUMFL-GPS and the baseline metrics and for each subject program, the average percentage of subexpressions that had to be examined to find the fault, computed across all the faulty versions. Here we show the results for QRM but not for DLRM, which QRM outperformed. (Nevertheless, DLRM outperformed the 5 baseline metrics.) For 14 of 16 subject programs, NUMFL-

GPS-QRM performed better than Ochiai, DStar ($star = 2$), and SOBER. NUMFL-GPS-QRM performed better than ESP-SIV (single variable) and ESP-SCP (scalar pair) for all 16 subject programs. Overall, NUMFL-GPS-QRM was more effective in localizing numerical faults than any of the baseline metrics.

Table 2.8: AVERAGE FAULT LOCALIZATION COSTS OF NUMFL-GPS-QRM AND BASELINE METRICS ON SINGLE-FAULT PROGRAM VERSIONS

Subject Program	Technique					
	NUMFL-GPS-QRM	Ochiai	Dstar	ESP(SIV)	ESP(SCP)	SOBER
Apache_EigenDecompose	12.3%	9.2%	9%	22.2%	17.2%	7.8%
Apache_DScompiler	11%	19.9%	16.5%	22.9%	18.9%	24.2%
Apache_BigMatrix	11.4%	51.8%	51.8%	37.9%	31.8%	28.9%
Apache_Rotation3D	8%	30.5%	30.5%	20.1%	23.6%	28.5%
Ojaljo_SchurDecompose	11.4%	22.7%	22.7%	20.2%	27.3%	30.9%
Jama_MatrixDecompose	14.2%	11.4%	11.4%	24.3%	27%	46.4%
SciMark_LU	15.3%	38.9%	68.1%	27.8%	18.8%	12.5%
SciMart_FFT	9.5%	48.3%	75%	68.1%	36.6%	12.5%
Apache_SymmLQ	2.6%	37.7%	85.1%	7%	10.5%	32.9%
Apache_SplineInterpolator	31.7%	51.1%	47.8%	65%	64.4%	56.1%
Apache_SimpleRegress	4.3%	49.2%	29.9%	7.3%	7.2%	7.9%
Apache_SchurTransformer	3.3%	8.2%	8.2%	36.2%	10.2%	44.4%
Apache_MillerUpdatRegress	7.5%	12.7%	12.7%	37.6%	19.6%	14.5%
Apache_HarmonicFitter	27.3%	45%	58.5%	39.5%	41.7%	49.3%
Apache_FastSine	1.5%	30.2%	87.1%	41.9%	3.8%	26.7%
Apache_FastCosine	1.3%	33.2%	94.9%	79.7%	41.4%	31.2%
Average Cost	10.8%	31.3%	44.3%	34.9%	25%	28.4%

We also compare the performance of NUMFL-GPS-QRM to that of each baseline SFL metric graphically. The comparison measure is the difference between the cost for the baseline metric and the cost for NUMFL-GPS-QRM. Since the two costs are percentages, the difference is the percentage reduction in cost obtained by using NUMFL-GPS-QRM, which may be positive or negative. For example, if the cost of using NUMFL-GPS-QRM is 10% and the cost of using the baseline metric is 40%, then the improvement is 30%. Figure 2.6 shows the results of comparisons of NUMFL-GPS-QRM with each of the baseline metrics. In each graph, the vertical axis represents the percentage improvement (reduction) in cost. The horizontal-axis represents different subject-program versions for which there are cost differences between the metrics, with each version represented by a vertical bar. Bars above the zero-line represent versions for which NUMFL-GPS-QRM performed better than the baseline metric and bars below zero represent versions for

which NUMFL-GPS-QRM performed worse. The length of each bar represents the magnitude of the corresponding cost difference.

NUMFL-GPS-QRM vs. Ochiai. Over all 92 faulty subject-program versions, NUMFL-GPS-QRM performed better than the Ochiai metric on 67 versions but NUMFL-GPS-QRM performed worse on 25 versions. There were 38 versions for which NUMFL-GPS-QRM performed at least 20% better than the Ochiai metric. There were just 5 versions for which the latter performed better than NUMFL-GPS-QRM.

NUMFL-GPS-QRM vs. DStar. NUMFL-GPS-QRM performed better than DStar on 70 subject-program versions but NUMFL-GPS-QRM performed worse than DStar on 22 versions. NUMFL-GPS-QRM performed at least 20% better than DStar on 42 versions, whereas DStar performed at least 20% better than NUMFL-GPS-QRM on just 5 versions.

NUMFL-GPS-QRM vs. ESP-SIV. NUMFL-GPS-QRM performed better than ESP-SIV on 70 subject-program versions but NUMFL-GPS-QRM performed worse than ESP-SIV on 22 versions. NUMFL-GPS-QRM performed at least 20% better than ESP-SIV on 31 versions, whereas ESP-SIV performed at least 20% better than NUMFL-GPS-QRM on just 5 versions.

QRM vs. ESP-SCP. NUMFL-GPS-QRM performed better than ESP-SCP on 61 subject-program versions but NUMFL-GPS-QRM performed worse than ESP-SCP on 31 versions. NUMFL-GPS-QRM performed at least 20% better than ESP-SIV on 27 versions, whereas ESP-SCP performed at least 20% better than NUMFL-GPS-QRM on just 3 versions.

QRM vs. SOBER. NUMFL-GPS-QRM performed better than SOBER on 64 subject-program versions but NUMFL-GPS-QRM performed worse than SOBER on 28 versions. NUMFL-GPS-QRM performed at least 20% better than SOBER on 32 versions, whereas SOBER performed at least 20% better than NUMFL-GPS-

QRM on just 7 versions.

2.5.5 NUMFL-GPS Applied only to Failing Runs

Conventional, coverage-based and predicate-based SFL techniques require profiles and PASS/FAIL labels from both passing and failing runs, in order to rank statements based on estimates of quantities like $Pr[\text{failure} \mid s\text{covered}]$ [?] that vary between statements only if the data come from a mix of passing and failing runs. However, because many numerical programs have few conditional branches, a particular fault may be executed and cause erroneous values to occur on every run that is observed. If these values propagate to the program output, a failure may occur on every run, depending on the numerical accuracy required.

Even if it is applied to data from only failing runs, NUMFL can still produce different AFCE estimates for different statements, because the causal outcome of interest is a continuous variable—the output error of a numerical program. To evaluate whether NUMFL-GPS is actually effective when it is applied to data from only failing runs, we redid the study just described, after creating a new data set by removing the data from passing runs. Table 2.9 and Figure 2.7 compare the performance of QRM with such data to its performance with the original data from both passing and failing runs. Figure 2.7 shows that over all 92 faulty subject-programs versions, QRM performed better with data from only failing runs on 43 program versions and it performed worse on 49 versions. There were only 8 versions for which QRM performed at least 20% worse with data from only failing runs.

From Table 2.9 and Figure 2.7, we can see that NUMFL works fairly well for most subject programs when used with data from only failing runs, although its performance is generally better with data from both passing and failing runs. Note that with many numerical programs the tolerance for output errors is very small

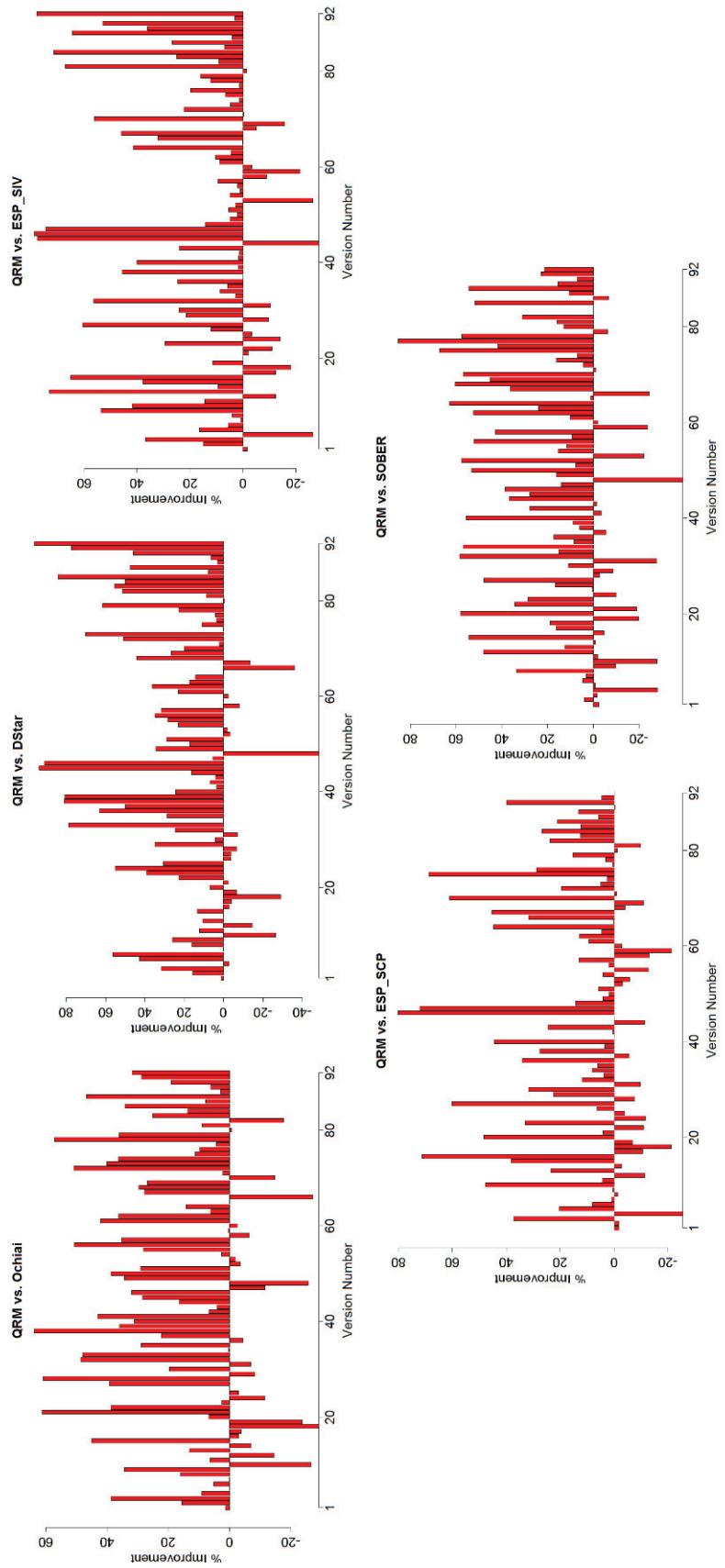


Figure 2.6: Performance of NUMFL-GPS-QRM relative to baseline metrics on individual single-fault program versions.

Table 2.9: AVERAGE FAULT LOCALIZATION COSTS OF NUMFL-GPS-QRM WITH AND WITHOUT DATA FROM PASSING RUNS, ON SINGLE-FAULT PROGRAM VERSIONS

Subject Program	Input	
	Pass and Fail	Fail only
Apache_EigenDecompose	12.3%	11.4%
Apache_DScompiler	11%	11%
Apache_BigMatrix	11.4%	8%
Apache_Rotation3D	8%	18.9%
Ojaljo_SchurDecompose	11.4%	17.7%
Jama_MatrixDecompose	14.2%	24.5%
SciMark_LU	15.3%	54.1%
SciMart_FFT	9.5%	17.2%
Apache_SymmLQ	2.6%	2.6%
Apache_SplineInterpolator	31.7%	21.7%
Apche_SimpleRgress	4.3%	3.4%
Apache_SchurTransformer	3.3%	8.2%
Apache_MillerUpdatRgress	7.5%	12.7%
Apache_HarmonicFitter	27.3%	47.5%
Apache_FastSine	1.5%	1.5%
Apache_FastCosine	1.3%	1.3%
Average Cost	10.8%	16.4%

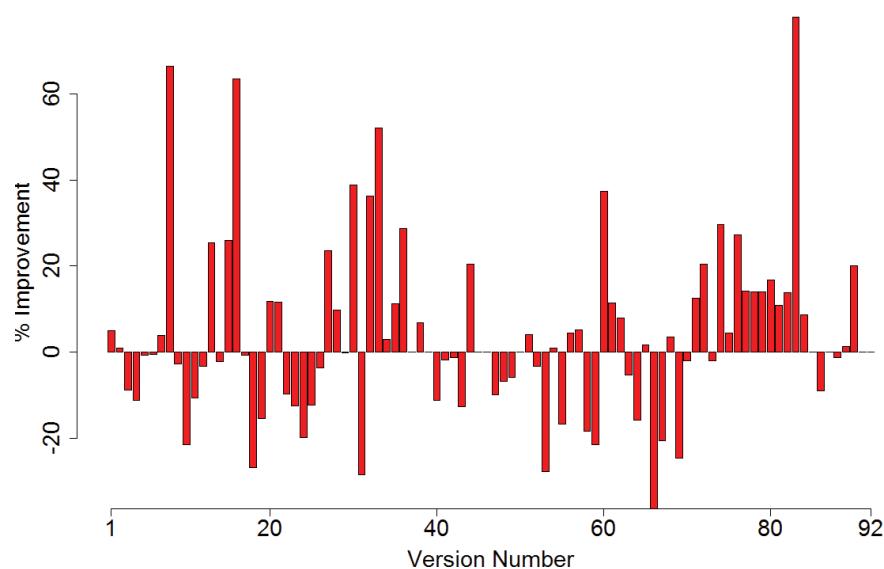


Figure 2.7: Relative performance of NUMFL-GPS-QRM with and without data from passing runs, on individual single-fault program versions.

(between 1.0E-5 and 1.0E-12). For such programs, the output errors from passing runs are clustered around 0, while output errors from failing runs are larger and more varied. Consequently, the data from failing runs carries more information about the dose-response function than does the data from the passing runs. Hence, using only data from failing runs to estimate the DRF does not necessarily result in severe bias.

2.5.6 Application of NUMFL-GPS to Programs with Multiple Faults

The empirical results presented in Section 2.5.4 indicate that NUMFL-GPS performs better than the baseline techniques on the subject program versions containing a single fault. This section reports on the application of NUMFL-GPS to subject program versions with multiple faults. For this sub-study, we selected five of the larger subject programs (shown in Table 2.10) and generated 5 faulty versions of each for a total of 25 faulty versions. To create each faulty version, we randomly injected two simulated faults. (Injecting a larger number of faults in our programs tended to make them fail badly on all inputs). Table 2.10 shows the average cost, over the faulty versions of each subject program, of localizing the first fault to be found, for NUMFL-GPS-QRM and each of the baseline techniques. The table shows that NUMFL-GPS-QRM outperformed the other baseline techniques on average, although SOBER and Ochiai each performed better on one of the subject programs.

Table 2.10: AVERAGE FAULT LOCALIZATION COSTS OF NUMFL-GPS-QRM AND BASELINE METRICS ON MULTIPLE-FAULT PROGRAM VERSIONS

Subject Program	Technique					
	NUMFL-GPS-QRM	Ochiai	Dstar	ESP(SIV)	ESP(SCP)	SOBER
Apache_EigenDecompose	10.3%	20%	19.4%	28.3%	25.8%	6.3%
Apache_DScompiler	4.5%	31.5%	23.2%	19.9%	10.4%	9%
Apache_Rotation3D	7%	3.6%	33.6%	17.5%	17.9%	25.8%
Ojaljo_SchurDecompose	5.4%	22.7%	27.1%	8.4%	9.6%	27.1%
Jama_MatrixDecompose	14.1%	26.3%	16.5%	26.3%	26.2%	15.5%
Average Cost	8.3%	20.8%	24%	20.1%	18%	16.7%

Figure 2.8 graphically contrasts the performance of NUMFL-GPS-QRM on the individual two-fault program versions with that of the baseline metrics. It is evident that SOBER’s performance is the second best after NUMFL-GPS-QRM. Overall 25 faulty subject-program versions, NUMFL-GPS-QRM performed better than SOBER on 15 versions but performed worse on 10 versions. There were 8 versions for which NUMFL-GPS-QRM performed at least 10% better than SOBER but only one version for which SOBER performed at least 10% better than NUMFL-GPS-QRM. Both Ochiai and ESP-SCP performed better than NUMFL-GPS-QRM on 8 versions but performed worse on 17 versions. NUMFL-GPS-QRM performed better than ESP-SIV on 19 versions and performed better than DStar on 21 versions.

2.5.7 Comparison of NUMFL-GPS and NUMFL-CBPS

In this section, we report the results of empirically comparing the performance of NUMFL-GPS-QRM with that of NUMFL-CBPS-QRM. We applied the two techniques to the subject program versions with single faults as well as to the versions with two faults. The average fault localization costs on the single fault versions is shown in Table 2.11. There were 13 versions for which NUMFL-GPS-QRM performed better than NUMFL-CBPS-QRM. There were only 3 versions for which NUMFL-CBPS-QRM performed better than NUMFL-GPS-QRM. Figure 2.9 graphically contrasts the performance of the two methods on the single fault versions. NUMFL-GPS-QRM performed better on 61 versions, while NUMFL-CBPS-QRM performed better on 31 versions. NUMFL-GPS-QRM performed at least 20% better than NUMFL-CBPS-QRM on 15 versions, whereas NUMFL-CBPS-QRM performed at least 20% better than NUMFL-GPS-QRM on just 4 versions.

Table 2.12 shows the average cost, over the faulty versions of each subject program into which two faults were injected, of localizing the first fault to be found, for both NUMFL-GPS-QRM and NUMFL-CBPS-QRM. NUMFL-GPS-QRM

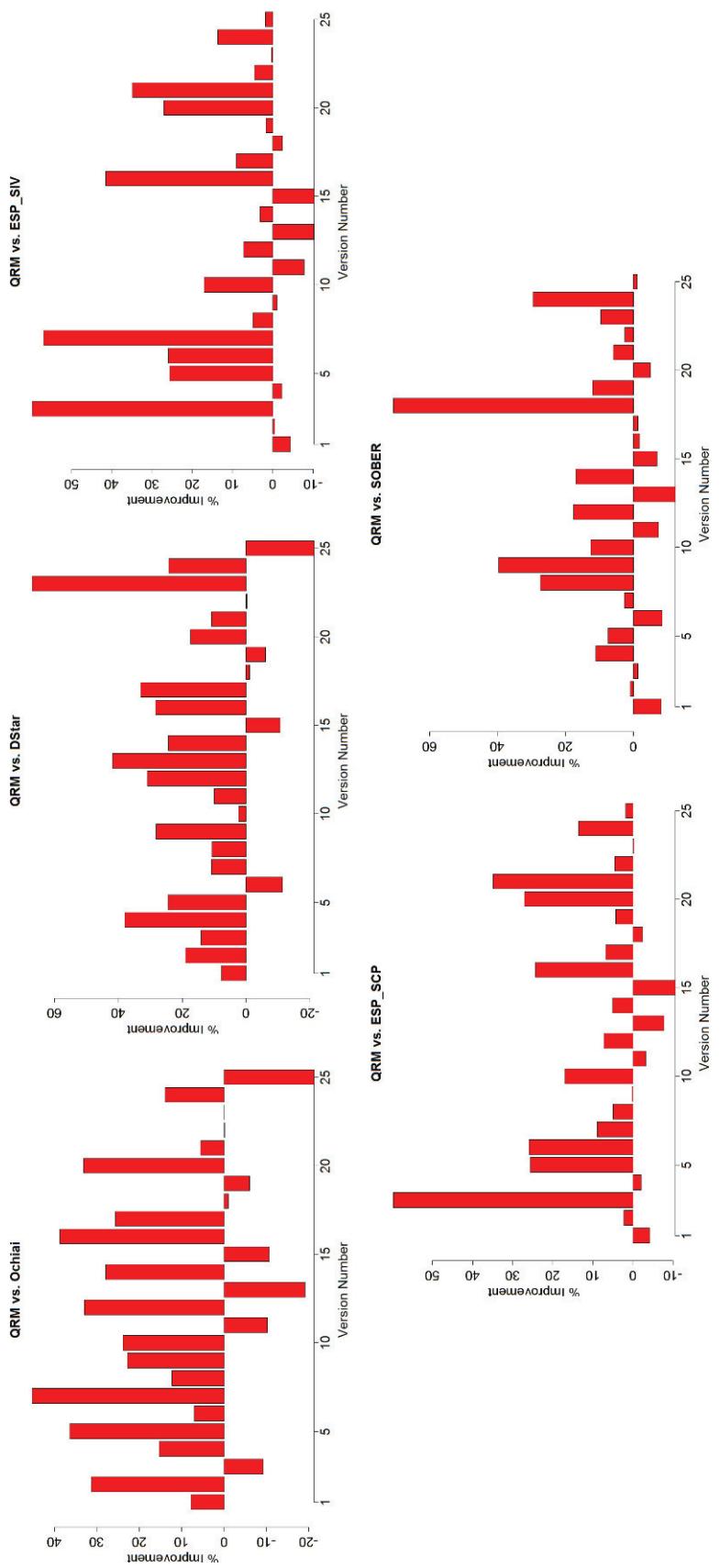


Figure 2.8: Performance of GPS-QRM relative to baseline metrics on individual two-fault program versions .

Table 2.11: AVERAGE FAULT LOCALIZATION COSTS OF NUMFL-GPS-QRM AND NUMFL-CBPS-QRM ON SINGLE-FAULT PROGRAM VERSIONS

Subject Program	NUMFL	
	GPS-QRM	CBPS-QRM
Apache_EigenDecompose	12.3%	8.8%
Apache_DScompiler	11%	12%
Apache_BigMatrix	11.4%	9.9%
Apache_Rotation3D	8%	18.9%
Ojaljo_SchurDecompose	11.4%	14%
Jama_MatrixDecompose	14.2%	23%
SciMark_LU	15.3%	27.8%
SciMart_FFT	9.5%	19.8%
Apache_SymmLQ	2.6%	4.4%
Apache_SplineInterpolator	31.7%	35%
Apache_SimpleRgress	4.3%	17%
Apache_SchurTransformer	3.3%	14.9%
Apache_MillerUpdatRgress	7.5%	9.9%
Apache_HarmonicFitter	27.3%	32%
Apache_FastSine	1.5%	13%
Apache_FastCosine	1.3%	1.2%
Average Cost	10.8%	16.4%

performed better than NUMFL-CBPS-QRM on the two-fault versions of 4 subject programs. NUMFL-GPS-QRM performed worse than NUMFL-CBPS-QRM on the versions of 1 subject program. Figure 2.10 graphically contrasts the performance of the two methods on the individual two-fault versions. NUMFL-GPS-QRM performed better than NUMFL-CBPS-QRM on 13 versions and NUMFL-GPS-QRM performed worse on 12 versions. NUMFL-GPS-QRM performed at least 10% better than NUMFL-CBPS-QRM on 7 versions, whereas NUMFL-CBPS-QRM performed at least 10% better than NUMFL-GPS-QRM on just 1 version.

In summary, NUMFL-GPS-QRM performed better than NUMFL-CBPS-QRM on both single-fault and two-fault programs. The generalized propensity score model $\theta = X'\beta$ achieved better covariate balance than the multinomial logistic regression model used with CBPS. This may be due to the composition of the data collected from our subject program versions. The performance of NUMFL-

CBPS was poorest with versions that had no more than about 150 failing executions. However, although NUMFL-CBPS performed worse than NUMFL-GPS in our study, the former's average fault localization cost was still lower than those of the baseline techniques.

Table 2.12: AVERAGE FAULT LOCALIZATION COSTS OF NUMFL-GPS-QRM AND NUMFL-CBPS-QRM ON MULTIPLE-FAULT PROGRAM VERSIONS

Subject Program	NUMFL	
	GPS-QRM	CBPS-QRM
Apache_EigenDecompose	10.3%	11.1%
Apache_DScompiler	4.5%	5.9%
Apache_Rotation3D	7.0%	3.0%
Ojaljo_SchurDecompose	5.4%	19.8%
Jama_MatrixDecompose	14.1%	23.4%
Average Cost	8.26%	12.64%

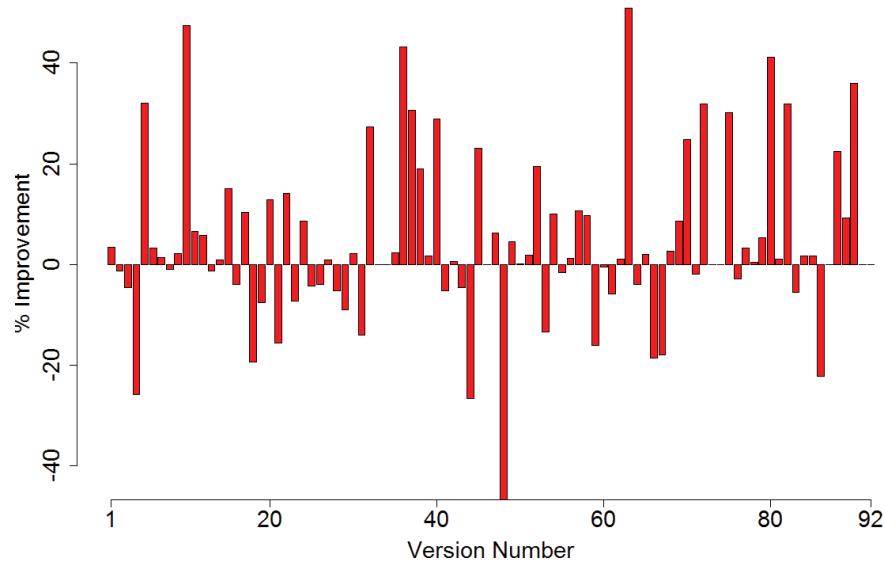


Figure 2.9: . Relative performance of NUMFL-GPS-QRM and NUMFL-CBPS-QRM on individual single-fault program versions .

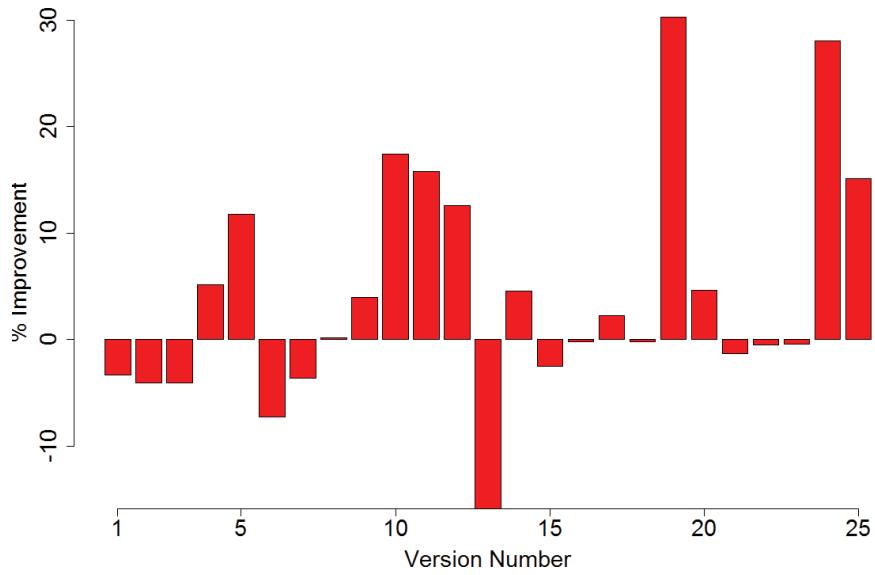


Figure 2.10: Relative performance of NUMFL-GPS-QRM and NUMFL-CBPS-QRM on individual two-fault program versions .

2.5.8 Computation Time

We used two machines for this study: (1) a Dell Precision T5600 with two 2.30 GHz intel Xeon CPUs and 64 GB RAM; and (2) a Dell PowerEdge T300 with a 2.83 GHz Intel Xeon CPU and 24GB RAM. The computation time required to apply any of the non-causal baseline techniques was less than 1 minute per program version. The computation time for NUMFL-QRM and NUMFL-CBPS per version are summarized in table 2.13

From table 2.13, The NUMFL is mildly slower than baseline techniques. The NUMFL's computation time is between 7 minutes and 8 minutes for large subject programs and is between 20 seconds to 100 seconds for small subject programs. It is important to mention that we did not attempt to parallelize the computation of AFCE estimates, even though AFCE estimates for different sub-expression can be computed independently.

Table 2.13: AVERAGE COMPUTATION TIME OF NUMFL-GPS-QRM AND NUMFL-CBPS-QRM ON ONE SINGLE-FAULT PROGRAM VERSIONS

Subject Program	NUMFL	
	GPS-QRM(Seconds)	CBPS-QRM (Seconds)
Apache_EigenDecompose	452.32	8.8%
Apache_DScompiler	104.66	12%
Apache_BigMatrix	122.98	9.9%
Apache_Rotation3D	427.53	18.9%
Ojalvo_SchurDecompose	463.44	14%
Jama_MatrixDecompose	403.72	23%
SciMark_LU	24.72	27.8%
SciMart_FFT	38.20	19.8%
Apache_SymmLQ	64.98	4.4%
Apache_SplineInterpolator	31.7	35%
Apache_SimpleRgress	54.74	17%
Apache_SchurTransformer	73.62	14.9%
Apache_MillerUpdatRgress	97.05	9.9%
Apache_HarmonicFitter	58.94	32%
Apache_FastSine	46.59	13%
Apache_FastCosine	72.75	1.2%
Average Cost	85.79	16.4%

2.5.9 Limitations

NUMFL and its evaluation are subject to several limitations. First, NUMFL employs regression models for two purposes: estimating generalized propensity scores and estimating the causal effect of the treatment on the outcome. We used Gaussian (Normal) linear models for both purposes in NUMFL-GPS, because they are supported by fast and robust software, and they performed well in our empirical study. In NUMFL-CBPS, we use multinomial logistic regression propensity score models. However, other model choices may be more appropriate for applying NUMFL to different numerical software. Determining that would require preliminary analysis of the data. A related issue is that sufficient data must be available to adequately fit each model. We have found that the number of failing tests should at least 100 to fit adequate regression models. This is not a serious problem, since faults in numerical programs are usually not guarded by many branch conditions

that are likely to cause “coincidental correctness.” A limitation of our empirical study is that the seeded faults were of three basic types. In future work, we intend to evaluate NUMFL on subject programs with more varied faults. Finally, validity of NUMFL (with QRM) depends on Assumptions 1 and 3 in section 2.4. These assumptions do not always hold in practice. For example, if the effect of a numerical fault does not propagate to the output (coincidental correctness), then Assumption 3 will be violated.

2.6 RELATED WORK

The seminal SFL research of Jones et al. [?], which is coverage based, and of Libil et al. [?], which is predicate based, has inspired much subsequent research. The use of causal inference methodology in SFL is due to Baah et al. [?]. They showed that estimating the AFCE of covering a statement s using a linear regression model that adjusts for coverage of the direct control dependence predecessor of s is effective for reducing confounding bias that often distorts fault localization scores. Later, Baah et al. [?] extended this work by using covariate matching to control confounding bias involving both control and data dependence predecessors. More recently, Gore et al. [?] extended Baah’s initial approach by providing a model that reduces what they called “failure flow confounding bias,” which involves predicate outcomes. Recently, Shu et al. [?] proposed a method-level causal inference model to localize faulty methods in large programs. The aforementioned techniques, unlike NUMFL, do not use values of program variables in fault localization.

State-altering techniques, such as *cause-transitions* [?] and *value replacement* [?] are among the few fault localization techniques based on values of variables. Cause-transitions employs *delta debugging* [?] to isolate the cause of a program failure.

Value replacement localizes faults by switching program states and re-running the program. Unlike SFL techniques, these techniques actually alter program states, and they require an oracle to determine if alterations cause program failures. On the other hand, they are non-statistical and do not require a sample of both passing and failing executions. The *Daikon* system identifies possible invariant conditions in a program based on a sample of executions [?]. The *DIDUCE* system uses Daikon to report violations of dynamic invariants, which may indicate failures [?]. However, these techniques do not address confounding bias.

Some recent studies have developed techniques to analyze instability in floating-point computations. *CADNA* [?] is a library to estimate round-off errors with Monte-Carlo Arithmetic. Tang et al. [?] proposed a technique to automatically detect such errors by systematically altering the underlying numerical calculation. Lam et al. [?] proposed to use the detection of significant digit cancellation events to test the precision of numerical programs. Later, Zhang et al. [?] extended Lam's work by monitoring the propagation of cancelled bits. These studies focused on detecting accumulated round-off errors due to finite-precision computation, but they do not address the problem of localizing faults in numerical expressions generally.

Other researchers have proposed alternatives to Imai and van Dyk's approach to defining and using the generalized propensity score. Hirano and Imbens estimate the causal effect of a continuous treatment variable by fitting one regression model with the GPS as a predictor [?]. This method requires discretizing the treatment variable when calculating the propensity score. Zhao and Imai extend Hirano and Imbens's work by using a smooth coefficient model (SCM) in the regression, so the model can estimate the dose-response function of the treatment variable instead of average causal effect [?]. In preliminary work (with different subject programs), we found that these GPS methods did not perform as well as

Imai and Van Dyk's approach, which is used in this paper.

2.7 CONCLUSION

In this chapter, we have presented and evaluated a value-based causal model, denoted NUMFL, for localizing faults in numerical software. NUMFL employs generalized propensity scores and covariate balancing propensity scores to control confounding bias involving floating-point program variables that carry erroneous values to correct statements. NUMFL uses a quadratic regression model (QRM) to estimate the average failure-causing effect of a numerical expression. We reported the results of an empirical comparison of NUMFL to several competing techniques on both single-fault subject programs and multiple-fault subject programs. NUMFL performed notably better than the other techniques. We also found that NUMFL-GPS works well with data from failing *runs alone*. Finally, we compared the performance two versions of NUMFL, denoted NUMFL-GPS and NUMFL-CBPS, based on the two aforementioned types of propensity scores. We found that the NUMFL-GPS performed better than NUMFL-CBPS for both single-fault programs and two-fault programs. In the future work, will seek to extend our empirical results to a broader range of subject programs with more varied fault types. We intend eventually to evaluate NUMFL in a user study, but given the difficulty of conducting an unbiased one, we think it is desirable to refine NUMFL as much as possible beforehand. Finally, we will also explore the integration of NUMFL with coverage or predicate based causal SFL techniques.

Chapter 3

Causal Inference Based Fault Localization for Numerical Software with Bayesian Additive Regression Trees

3.1 Introduction

Average failure causing effect estimation is challenging when the outcome Y is not linearly related to the treatment T and confounders X . Previous work like NUMFL estimates AFCE with non linear parametric regression model, which depends on some pre-assumptions of the relationship between T and Y , given the confounding variable X is well controlled. If any assumption does not hold, then the AFCE estimation can be biased. Bayesian Additive Regression Trees(BART), a new causal effect estimation method has been proposed in the past few years. It requires less guess-work in model fitting and handles the large number of predictors.

In this chapter, we proposal a new statistical fault localization method based on

BART model and evaluate it on numerical programs with single or multiple faults.

The motivation for using BART in statistical fault localization is:

- BART can flexibly fit non-linear response surfaces even with a large number of predictors
- BART does not require the researcher to specify the functional form of the relationship between treatment and outcome. The user only need to input the treatment, confounding variable and the outcome, but not need to provide how these variables are parametrically related. Also, comparing to methods such as propensity score matching and subclassification, BART produces coherent posterior predictions.
- The causal inference techniques has been proved to be effective in both coverage based fault localization and value based fault localization. The treatment effect estimated with BART appear to be substantially more accurate than linear regression, and propensity score matching with regression adjustment when the treatment variable is binary. It has potential in estimating failure-causing effect for continuous treatment [].
- BART algorithm software is freely available and easy to use [].

The rest of the chapter is organized as follows: we present the background of single regression tree and BART model in Section 3.2; Using BART model to estimate failure-causing effect is described in detail in Section 3.3; we report on its empirical evaluation in Section 3.4; related work is surveyed in Section 3.5; and Section 3.6 concludes the chapter.

3.2 BART Model Algorithm

The BART model algorithm consists of three pars: a sum of regression trees model, a regularization prior and a fitting algorithm Marcov Chain Mote Carlo (MCMC)

3.2.1 A Single Regression Tree model

Regression tree is one type of decision tree that predicts the value of a target variable based on several input variables. Regression tree handles the situation when the target variable is continuous. Figure 3.1 shows a single regression tree model. All the interior nodes of a regression tree have decision rules which send the input data set to either left or right side. After the input data set go through the interior nodes and reach the bottom of the tree, the data set is divided into several disjoint subgroup. Each group of data is represent by a leaf node.

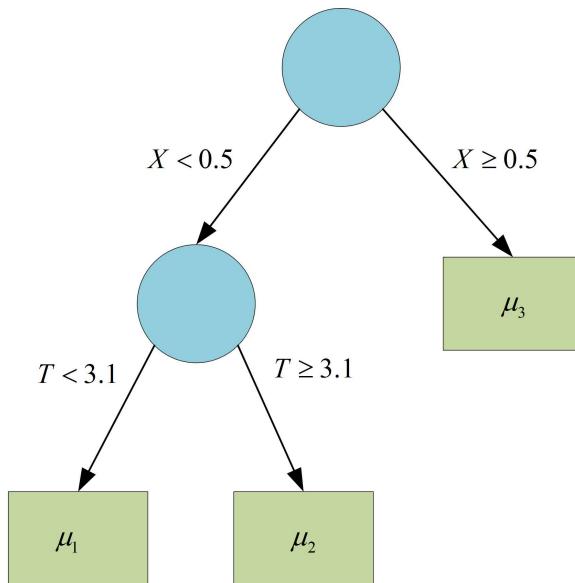


Figure 3.1: Single Regression Tree Structure

A single regression tree model is denoted as:

$$Y = g(Z; R, M) + \epsilon$$

Here $\varepsilon \sim N(0, \sigma^2)$ is a normal distributed error. $\mathbf{Z} = [T, \mathbf{X}]$ denotes all the variables related to the outcome Y , so Z includes both treatment variable T and confounding variables \mathbf{X} . R denotes a binary regression tree consisting a set of interior node decision rules and a set of terminal nodes, and let $M = \{\mu_1, \mu_2, \dots, \mu_b\}$ denotes a set of parameter value associated with each of the b terminal nodes of R . Each terminal node represent a regression model of outcome Y on all the variables Z .

A regression tree model is often used in approximating unknown functions. For example, if the causal effect of treatment T on outcome Y is decided by an unknown function $Y = f(T, \mathbf{X})$, then we can approximate the function $f(T, \mathbf{X})$ by fitting a single regression tree model $g(\mathbf{Z}; R, M)$ on sample data set. The regression tree model divides the value space of $[T, \mathbf{X}]$ in to several subgroups with its tree structure and fit a regression model for each subgroup. When making inference of Y given a specific unit of treatment and confounding variables values $[T = t, \mathbf{X} = \mathbf{x}]$, the regression will first find out which subgroup the unit belongs to and then infer outcome Y with the corresponding linear regression. Regression tree model has two advantages: (1) making prediction is fast. (2) it can handle non-linear function approximation.

3.2.2 A sum of regression trees model

BART model is a sum of trees model. With the definition of a single tree model, the sum of trees model can be expressed as:

$$Y = g(\mathbf{Z}; R_1, M_1) + g(\mathbf{Z}; R_1, M_1) + \dots + g(\mathbf{Z}; R_m, M_m) + \varepsilon$$

where each (R_i, M_i) denotes a single sub-tree model and $\varepsilon \sim N(0, \sigma^2)$. m denotes the number of trees in BART model. We have

$$Y = f(\mathbf{Z}) = f(T, \mathbf{X}) = \left(\sum_{j=1}^m g(T, \mathbf{X}; R_j, M_j) \right) + \varepsilon$$

Comparing to single regression tree model, BART model has two advantages. First BART is more naturally handle the interaction effects . In the sum of trees model, each tree explains part of the overall fit, so there are many different choices of $(R_1, M_1) \cdots (R_m, M_m)$ can lead to an identical function $\sum_{j=1}^m g(T, \mathbf{X}; R_j, M_j)$. Second, BART can scale to large datasets using a parallel MCMC sampler [?]. Thus, fitting BART model does not has much more computation cost than fitting a large single tree model.

3.2.3 A regularization prior

Fitting the BART model requires a prior of all the parameters of the sum of trees model. The prior regularize the fit by keeping the individual tree's effect from being unduly influential. Without such a prior, large tree components would dominate the sum of trees structure. The regularization prior can also help BART avoid overfitting. To simplify the prior specification, the trees in BART model $(R_1, M_1), (R_2, M_2), \dots, (R_m, M_m)$ are considered to be independent of each other and of σ . Also, the terminal node parameters $\mu_{1j}, \mu_{2j}, \dots, \mu_{bj}$ of every tree R_j are independent. So we have:

$$\begin{aligned} P((R_1, M_1), (R_2, M_2) \dots, (R_m, M_m), \sigma) &= \left[\prod_j P(R_j, M_j) \right] p(\sigma) \\ &= \left[\prod_j P(M_j|R_j)P(R_j) \right] p(\sigma) \end{aligned}$$

and

$$P(M_j|R_j) = \left[\prod_i P(\mu_{ij}|R_j) \right]$$

Here $\mu_{ij} \in M_j$ denotes the i th terminal node of the j th regression tree. From the above equations, we can see the independence simplify the prior specification problem to the specification of prior for just $P(\mu_{ij}|R_j)$, $P(R_j)$ and $P(\sigma)$. In [], the specification of prior forms on $P(\sigma)$ is defined as the inverse chi-square distribution. The prior on $P(\mu_{ij}|R_j)$ is defined as conjugate normal distribution. The prior on $P(R_j)$ is complicated which contains 3 aspects:

1. the probability that a nonterminal node at depth d is given by

$$\alpha(1+d)^{-\beta}, \quad \alpha \in (0, 1), \beta \in [0, \infty)$$

2. the prior probability that a variable is selected as the splitting variable at an interior node is $1/k$ and k is the total number of variables including both treatment and confounders.
3. the prior probability that a splitting variable split at value x is $1/N$ and N is the total number of observed values of the splitting variable in the sample data set.

The detail of the prior specification for $P(\mu_{ij}|R_j)$, $P(R_j)$ and $P(\sigma)$ can be referred to [].

3.2.4 Bayesian Backfitting MCMC Algorithm

BART uses a Bayesian backfitting MCMC algorithm to fit the model. The algorithm uses Gibbs sampler []. The Gibbs sampler get m successive draws of (R_j, M_j) conditionally on $(R_{(j)}, M_{(j)}, \sigma)$:

$$(R_j, M_j) | R_{(j)}, M_{(j)}, \sigma, Y$$

$j = 1 \dots m$, followed by a draw of σ from the full conditional:

$$\sigma | R_1, \dots, R_m, M_1, \dots, M_m, Y$$

Here $R_{(j)}$ represents all the trees except R_j , so $R_{(j)}$ will be a set of $m - 1$ trees. $M_{(j)}$ is similarly defined as $R_{(j)}$.

3.3 BART Model with Causal Inference

When apply BART model in estimating average causal effects, we use different algorithms for binary treatment and continuous treatment. For binary treatment, BART model primarily estimate failure-causing effects such as $E(Y(1)|\mathbf{X} = \mathbf{x}) - E(Y(0)|\mathbf{X} = \mathbf{x}) = E(Y|T = 1, \mathbf{X} = \mathbf{x}) - E(Y|T = 0, \mathbf{X} = \mathbf{x}) = f(1, (\mathbf{x})) - f(0, (\mathbf{x}))$. The algorithm contains the following steps:

1. Fit BART model using MCMC algorithm to full sample
2. Get posterior prediction for each unit by setting the treatment variable value $T = 1$ and keep confounding variable value unchanged..
3. Get posterior prediction for each unit by setting the treatment variable value $T = 0$ and keep confounding variable value unchanged.
4. Calculate the difference between the posterior predictions for each unit.
5. Estimate failure-causing effect by averaging all the differences of posterior predictions.

In step 1, the fitted BART model characterized the causal relationship between treatment T and outcome Y given the confounding \mathbf{X} . We can use the fitted model

to predict the outcome Y under different (T, \mathbf{X}) conditions. For a untreated unit ($T = 0, \mathbf{X} = \mathbf{x}$), if we set the treatment variable to 1 and then input $(T = 1, \mathbf{X} = \mathbf{x})$ into the BART model, the output is the estimated outcome for that unit in treated condition. Similarly, we can estimate the outcome of a treated unit in untreated condition by inputing $(T = 0, \mathbf{X} = \mathbf{x})$ into the BART model. Thus, in step2, the BART model is used to predict outcome for each unit at observed treatment condition. In step 3, the fitted BART model is used to estimate posterior predictions for each unit at counterfactual condition. Thus, the difference calculated in step 4 is the causal effect estimation for each unit. The average of these differences is failure-causing effect causal effect which is estimated in step 5.

If the treatment variable is continuous, the causal effect of treatment T on outcome Y is characterized by a function $r_e(T)$, which is called dose-response function in medical research. For the failure-causing effect, the dose response functions of continuous treatments are usually non-linear. For example, in Chapter??, NUMFL use parameterized quadratic model and double linear model to approximate the dose response function within subclasses and get reasonable well result. But the parameterized model has limitations. It usually requires user to make assumptions to specify form of the dose-response function. For example, in NUMFL, we make some assumptions (*Assumption1, 2, 3*). The *Assumption3* is: executions with large absolute treatment errors have larger output errors than executions with small values of treatment errors. Although this assumption is often holds in numeric programs, it is not always to be true. In this case, the dose response curve of treatment T on outcome Y is likely to deviate from the quadratic model $Y = \zeta T_e^2 + \eta T_e + c$, which may result in a bad estimation of failure-causing effect. Comparing to parametric model used in NUMFL, BART model does not require user to make assumptions or specify the functional form of the dose response function. The sum of trees structure of BART model can approximate the non-linearity

of the DRF during the training phone with MCMC.

failure-causing effect estimation is a challenge for BART model. In NUMFL, the failure-causing effect is characterized by the coefficient of the regression model. But in BART model, the sum of trees structure does not such parameters can directly characterize the ACE. To solve this problem, we propose to estimate the treatment causal effect at each unit in the sample. The average of the treatment causal effect on all sample units is the estimated ACE. The causal effect of treatment T on outcome Y for a single unit can be estimated by increasing the treatment variable value of the unit and see how outcome changes. For example, assume a unit i has treatment variable $T = t$ and confounding variables $\mathbf{X} = \mathbf{x}$, we can use the fitted BART model to estimate the outcome of the unit $Y = y$. Then we increase the treatment variable to $t' = t + \varepsilon$, here ε is a small number. We input T' and \mathbf{X} into the fitted BART model and get the estimated posterior $Y = y'$. Then the estimated causal effect of T on Y for unit i is $|y - y'|$. The algorithm is as follows:

1. Fit BART model using MCMC algorithm to full sample
2. Increase the treatment variable value t of each unit by ε . The new treatment value $t' = t + \varepsilon$ and the original confounding variables forms a new data set.
3. For each unit, calculate the difference between the posterior prediction in original data set and the posterior prediction in the new data set.
4. Estimate failure-causing effect by averaging all the differences of posterior predictions.

In the above algorithm, the BART model fitted in first step is used to approximate a function $Y = f(T, (X))$ that specify the dose-response function of the continuous treatment T and confounding variables \mathbf{X} . Step 2 and Step 3 estimate the treatment causal effect for each sample unit. Step 4 estimate the failure-causing effect of treatment on outcome.

One problem in step 2 is how to choose the value of the small number ε . But treatment variables in different numerical expressions have different scale of values, it is hard to find a constant ε which can make $t + \varepsilon$ be a reasonable value for all the treatments. To address this problem, we use the method illustrated by Figure3.2. We sort the original sample data set shown in Figure3.2 (a) in increasing order according to the value of the treatment variables. The sorted data set is shown in Figure3.2 (b). The increased treatment variable value t' in step 2 is equal to the treatment variable value t of the next unit in the list and the last unit in the list will be discarded. Thus, as shown in Figure refbartace (c), for a data set with n observational units, we will have a new data set of $n - 1$ units after increasing the treatment variable. The idea behind this method is that we want the value of treatment after increment is a reasonable value that could be observed in other tests. Also, the value of t' and the value of t are likely to be in the same scale, because they are neighbor in the sorted data set.

Original Data Set			
	Treatment	Confounder	Outcome
Test1	4.88	6	1.1
Test2	3.1	6.1	0.8
Test3	6.75	9.9	2.5
Test4	2.2	1.5	3.3

Sorted Original Data Set			
	Treatment	Confounder	Outcome
Test1	2.2	1.5	3.3
Test2	3.1	6.1	0.8
Test3	4.88	6	1.1
Test4	6.75	9.9	2.5

New Data Set			
	Treatment	Confounder	Outcome
Test1	3.1	1.5	3.3
Test2	4.88	6.1	0.8
Test3	6.75	6	1.1

Figure 3.2: EXAMPLE OF TREATMENT VARIABLE INCREAMENT

3.4 EMPIRICAL EVALUATION

To evaluate the effectiveness of BART model, we conducted the empirical study on the same subject programs as described in chapter 3. The tests suite is also identical to the tests suite in section 2.5. Overall 92 faulty subject-programs versions with single fault and 25 faulty subject-program versions with two faults. Ochiai, Dstar,

SOBER, ESP-SIV are ESP-SCP used as the base line techniques to be compared with BART model. We also compare the performance of BART model with NUMFL-GPS and NUMFL-CBPS which are the proposed in chapter 3. We measured the costs of applying CBPS and the other metrics by the percentage of *subexpressions* that need to be examined, in decreasing order of suspiciousness scores, to find the fault, assuming the fault is recognized when it is encountered.

In the experiment, we use R package "BARTMachine" [] to fit the BART model. We tried 10 trees and 50 trees in the sum of trees structure. The BART model is fitted with both passing and failing tests. The number tests for each subject program is from 3000 to 8000 which shown in table 2.7. We also try to train BART model with fewer data(300 tests). the sensitivity of the BART model to the number of trees and the number of tests are discussed in section 3.4.3.

3.4.1 Comparative Performance of BART vs. Baselines

Figure 2.6 shows the results of comparisons of BART with each of the baseline metrics. In each graph, the vertical axis represents the percentage improvement (reduction) in cost. The horizontal-axis represents different subject-program versions for which there are cost differences between the metrics, with each version represented by a vertical bar. Bars above the zero-line represent versions for which BART performed better than the baseline metric and bars below zero represent versions for which BART performed worse. The length of each bar represents the magnitude of the corresponding cost difference.

BART vs. Ochiai. Over all 92 faulty subject-program versions, BART performed better than the Ochiai metric on 75 versions but BART performed worse on 17 versions. There were 41 versions for which BART performed at least 20% better than the Ochiai metric. There were just 4 versions for which the latter performed better than BART.

BART vs. DStar. BART performed better than DStar on 77 subject-program versions but BART performed worse than DStar on 15 versions. BART performed at least 20% better than DStar on 44 versions, whereas DStar performed at least 20% better than BART on just 4 versions.

BART vs. ESP-SIV. BART performed better than ESP-SIV on 78 subject-program versions but BART performed worse than ESP-SIV on 14 versions. BART performed at least 20% better than ESP-SIV on 30 versions, whereas ESP-SIV never performed at least 20% better than BART.

BART vs. ESP-SCP. BART performed better than ESP-SCP on 75 subject-program versions but BART performed worse than ESP-SCP on 17 versions. BART performed at least 20% better than ESP-SIV on 22 versions, whereas ESP-SCP performed at least 20% better than BART on just 2 versions.

BART vs. SOBER. BART performed better than SOBER on 73 subject-program versions but BART performed worse than SOBER on 19 versions. BART performed at least 20% better than SOBER on 39 versions, whereas SOBER performed at least 20% better than BART on just 5 versions.

Figure 3.4 contrasts the performance of BART on the individual two-fault program versions with that of the baseline metrics. Over all 25 faulty subject-program versions, BART performed better than SOBER on 19 versions but performed worse on 6 versions. There were 8 versions for which BART performed at least 10% better than SOBER but 3 versions for which SOBER performed at least 10% better than BART. Ochiai performed better than BART on 5 versions but performed worse on 20 versions. BART performed at least 10% better than Ochiai on 13 versions. BART performed better than both ESP-SIV and ESP-SCP on 20 versions. BART performed better than DStar on 19 versions.

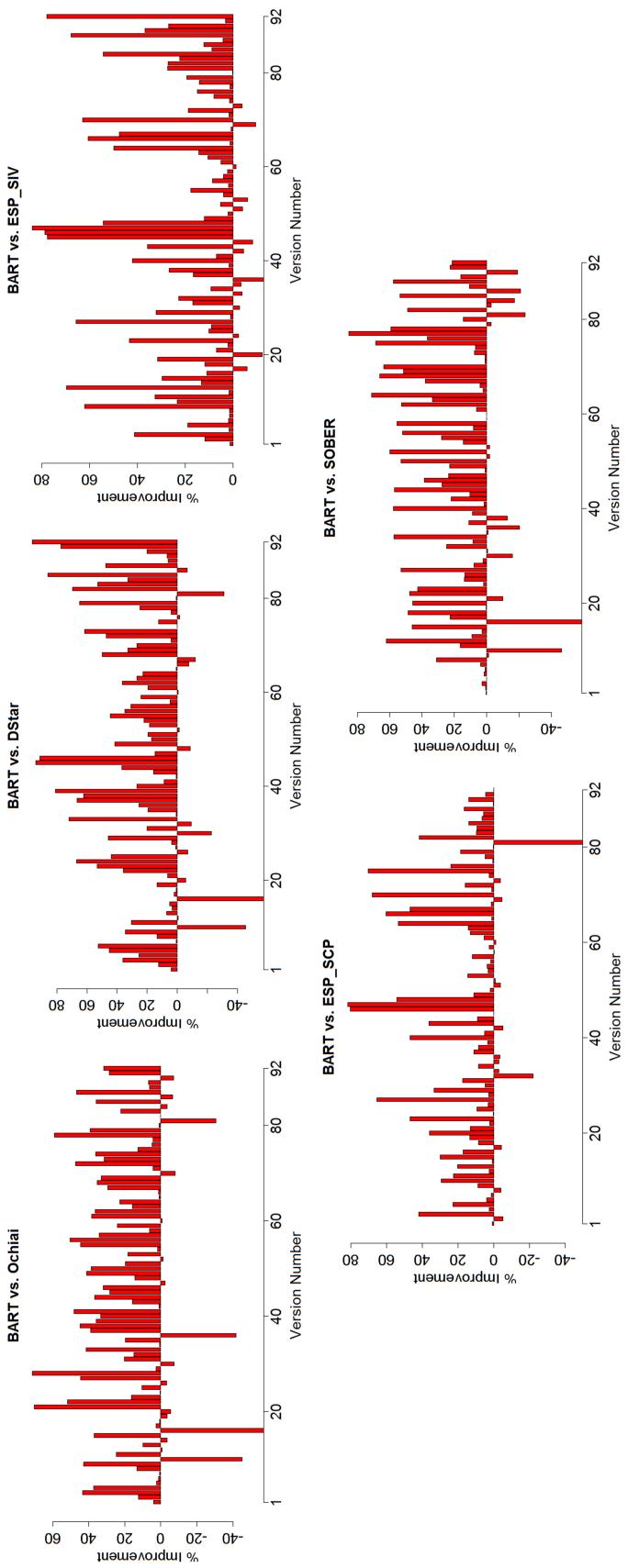


Figure 3.3: Performance of BART relative to baseline metrics on individual single-fault program versions.

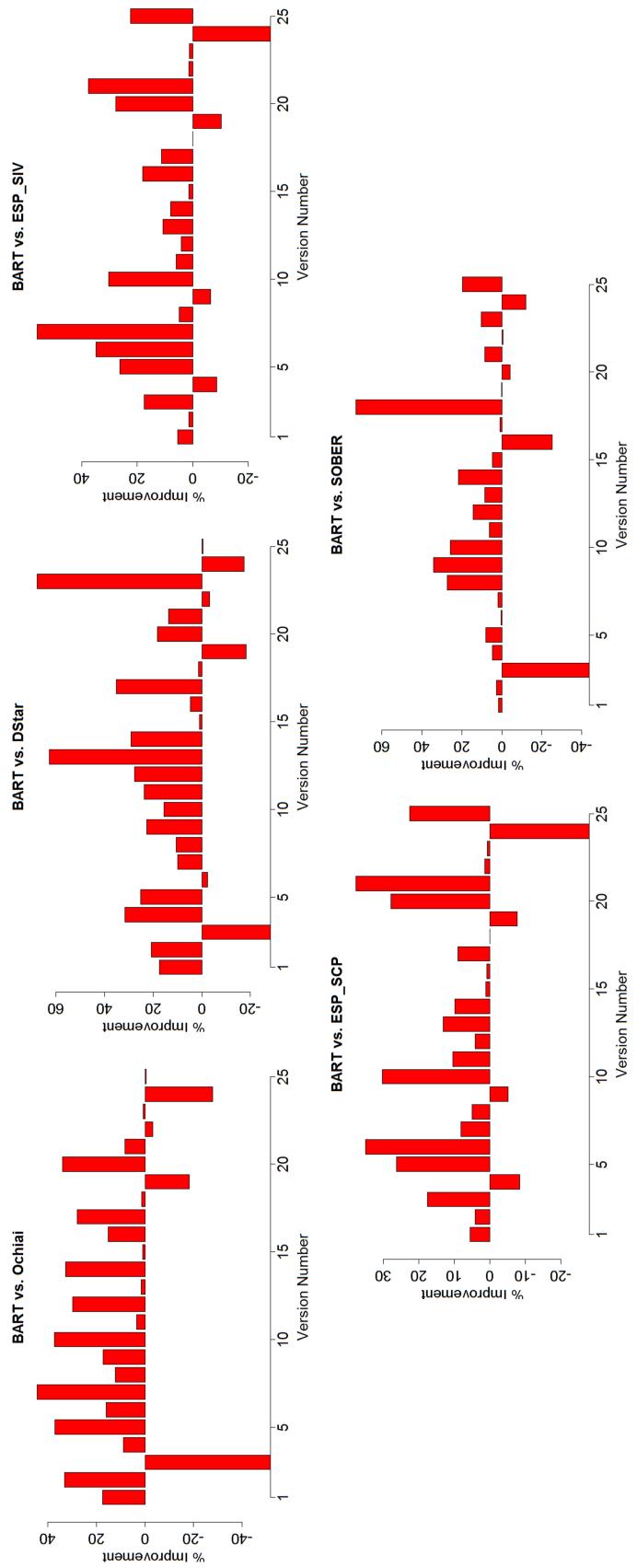


Figure 3.4: Performance of BART relative to baseline metrics on individual single-fault program versions.

3.4.2 BART model vs NUMFL

Table 3.1 shows the average percentage of subexpressions that had to be examined to find the fault, computed across all the faulty versions, for BART model and NUMFL. Here we show the results for NUMFL-GPS-QRM and NUMFL-CBPS-QRM. There were 11 subject programs for which BART performed better than NUMFL-GPS-QRM. There were 5 subject programs for which NUMFL-GPS-QRM performed better than BART. BART performed better than NUMFL-CBPS-QRM on 14 subject programs. There were only 2 subject programs for which NUMFL-CBPS-QRM performed better than BART.

Figure 3.5 graphically contrasts the performance of BART and NUMFL-GPS-QRM on the single fault versions. BART performed better than NUMFL-GPS-QRM on 54 versions, while NUMFL-GPS-QRM performed better on 38 versions. BART performed at least 20% better than NUMFL-GPS-QRM on 9 versions, whereas NUMFL-GPS-QRM performed at least 20% better than BART on 6 versions. Figure 3.6 graphically contrast the performance of BART and NUMFL-CBPS-QRM on the single fault versions. BART performed better than NUMFL-CBPS-QRM on 61 versions, while NUMFL-CBPS-QRM performed better on 31 versions. BART performed at least 20% better than NUMFL-CBPS-QRM on 17 versions, whereas NUMFL-CBPS-QRM performed at least 20% better than BART on just 4 versions.

In summary, BART performed better than both NUMFL-GPS-QRM and NUMFL-CBPS-QRM on single-fault programs. This may be due to the fitted sum of trees structure of BART model well approximate the DRF of treatment variable and thus have more accurate average cause effect estimation than NUMFL techniques.

Table 3.2 shows the average cost, over the faulty versions of each subject program into which two faults were injected, of localizing the first fault to be found, for both BART and NUMFL. From Table 3.2, the average cost of BART is close to that of NUMFL-GPS-QRM on two faults subject programs. BART performed bet-

Table 3.1: AVERAGE FAULT LOCALIZATION COSTS OF BART AND NUMFL METRICS ON SINGLE-FAULT PROGRAM VERSIONS

Subject Program	BART	NUMFL	
		GPS-QRM	CBPS-QRM
Apache_EigenDecompose	2.50%	12.3%	8.8%
Apache_DScompiler	9.72%	11%	12%
Apache_BigMatrix	9.00%	11.4%	9.9%
Apache_Rotation3D	9.07%	8%	18.9%
Ojaljo_SchurDecompose	10.61%	11.4%	14%
Jama_MatrixDecompose	11.62%	14.2%	23%
SciMark_LU	8.33 %	15.3%	27.8%
SciMart_FFT	27.59%	9.5%	19.8%
Apache_SymmLQ	1.75%	2.6%	4.4%
Apache_SplineInterpolator	37.78%	31.7%	35%
Apche_SimpleRgress	1.70%	4.3%	17%
Apache_SchurTransformer	4.56%	3.3%	14.9%
Apache_MillerUpdatRgress	1.24%	7.5%	9.9%
Apache_HarmonicFitter	30.10%	27.3%	32%
Apache_FastSine	1.53%	1.5%	13%
Apache_FastCosine	1.29 %	1.3%	1.2%
Average Cost	10.52%	10.8%	16.4%

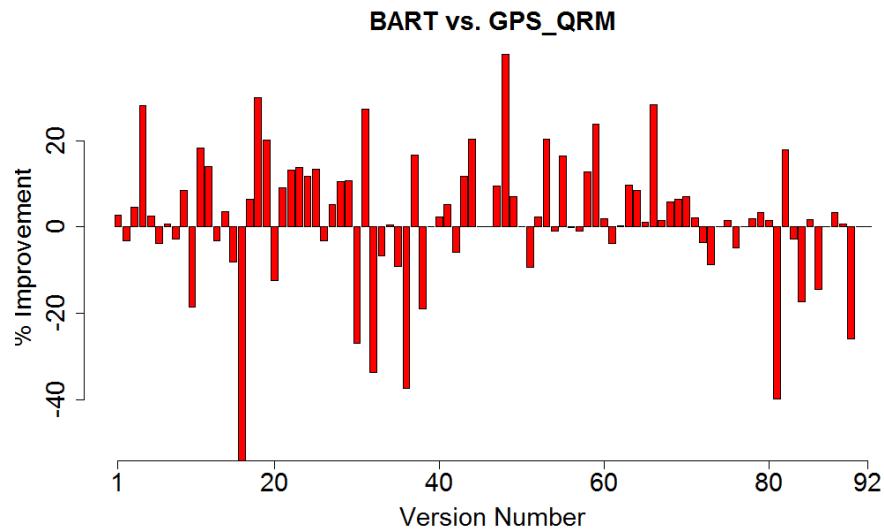


Figure 3.5: Relative performance of NUMFL-GPS-QRM with and without data from passing runs, on individual single-fault program versions.

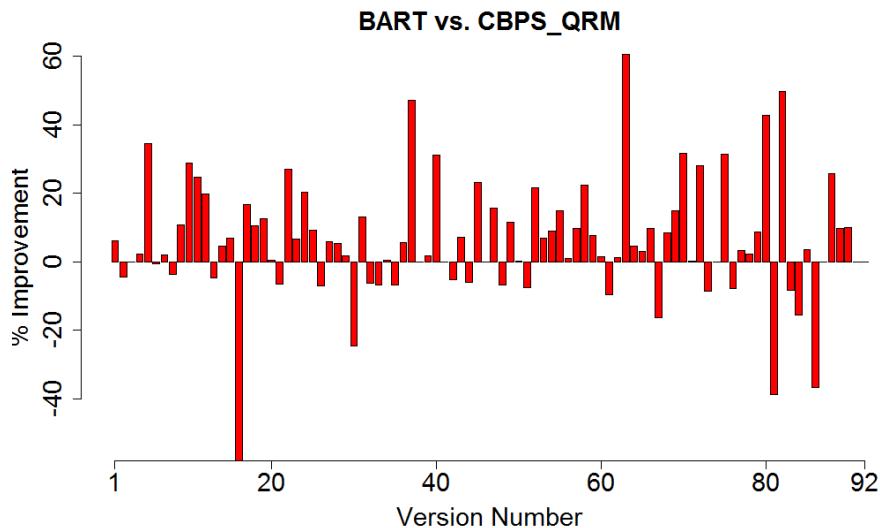


Figure 3.6: Relative performance of NUMFL-GPS-QRM with and without data from passing runs, on individual single-fault program versions.

ter than NUMFL-GPS-QRM on the versions of 2 subject programs, but performed worse than NUMFL-GPS-QRM on the versions of 3 subject program. BART performed better than NUMFL-CBPS-QRM on the versions of 4 subject programs, but performed worse than NUMFL-CBPS-QRM on the versions of only 1 subject program.

Figure 3.7 graphically contrasts the performance of the BART and NUMFL-GPS-QRM on the individual two-fault versions. BART performed better than NUMFL-CBPS-QRM on 13 versions and NUMFL-GPS-QRM performed worse on 12 versions. BART performed at least 10% better than NUMFL-GPS-QRM on 7 versions, whereas NUMFL-CBPS-QRM performed at least 10% better than NUMFL-GPS-QRM on just 1 version. Figure 3.8 graphically contrasts the performance of the BART and NUMFL-CBPS-QRM on the individual two-fault versions. BART performed better than NUMFL-CBPS-QRM on 13 versions and NUMFL-CBPS-QRM performed worse on 12 versions. BART performed at least 10% better than NUMFL-CBPS-QRM on 7 versions, whereas NUMFL-CBPS-QRM performed at least 10% better than NUMFL-GPS-QRM on just 1 version.

Table 3.2: AVERAGE FAULT LOCALIZATION COSTS OF BART AND NUMFL ON MULTIPLE-FAULT PROGRAM VERSIONS

Subject Program	BART	NUMFL	
		GPS-QRM	CBPS-QRM
Apache_EigenDecompose	7.98 %	10.3%	11.1%
Apache_DScompiler	5.13%	4.5%	5.9%
Apache_Rotation3D	10.69%	7.0%	3.0%
Ojaljo_SchurDecompose	17.55 %	5.4%	19.8%
Jama_MatrixDecompose	4.65%	14.1%	23.4%
Average Cost	9.20%	8.26%	12.64%

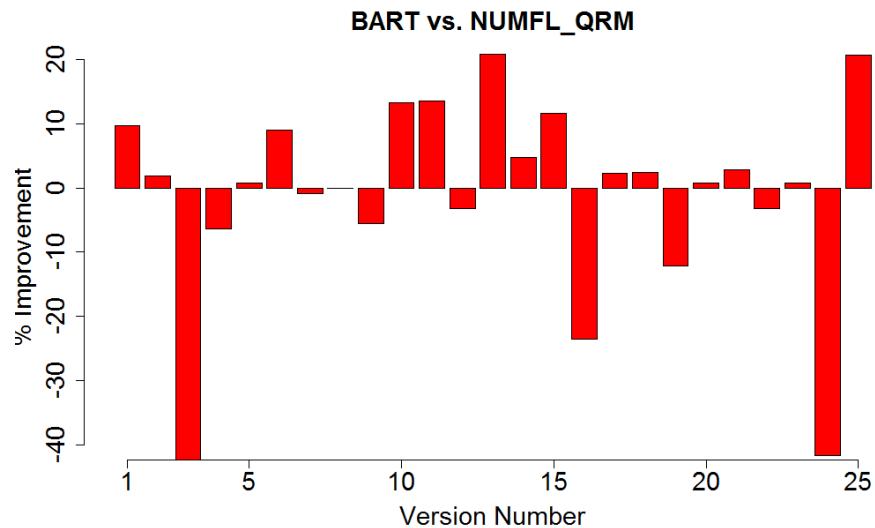


Figure 3.7: Relative performance of NUMFL-GPS-QRM with and without data from passing runs, on individual single-fault program versions.

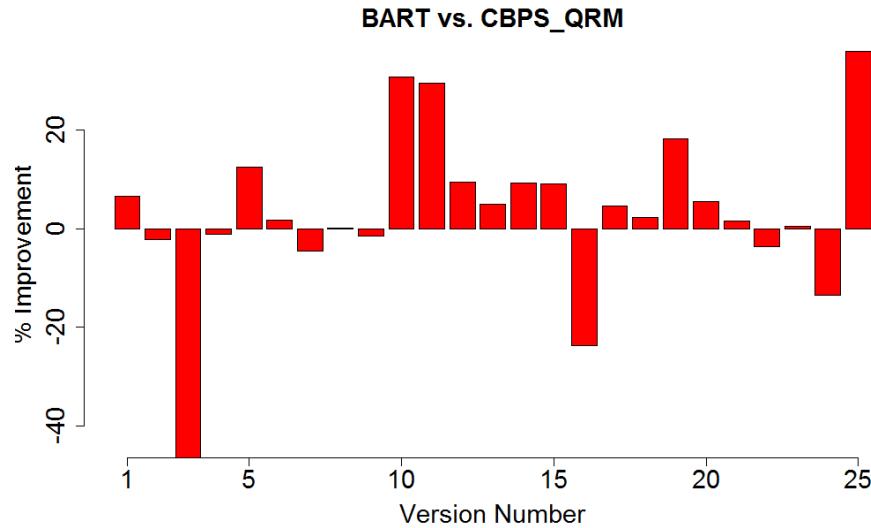


Figure 3.8: Relative performance of NUMFL-GPS-QRM with and without data from passing runs, on individual single-fault program versions.

3.4.3 Sensitivity of BART model on the number of trees and number of tests

In previous sections, we use the full observational data of tests to fit a BART model with 10 trees in the sum of trees structure. In this section, we will analyze if increasing number of trees or decreasing the number of tests would influence the performance of BART. In Table 3.3, the first column of numbers is the fault localization cost of BART model contains 10 trees and fitted with full observational data (3000-8000 tests). The second column of numbers is the fault localization cost of BART model contains 50 trees and fitted with full observational data. The third column of numbers is the fault localization cost of BART model contains 10 trees but fitted with only 300 tests' data. From Table 3.3, when increased the number of trees from 10 to 50, BART model has better performance on 6 subject programs. But there are also 6 subject program where BART model's performance become worse after increasing the number of trees. The average cost across 16 subject programs is roughly same: 10.52% for BART model with 10 trees and 10.58% for BART model

with 50 trees. This means 10 trees are enough to handle the nonlinearity problem in AFCE estimation. When decrease the number of tests to 300, the average cost is slightly increased to 10.74%. This means BART model does not require a large number of tests to localize bugs in numerical software.

Table 3.3: AVERAGE FAULT LOCALIZATION COSTS OF BART MODEL WITH DIFFERENT NUMBER OF TREES AND TESTS ON ONE SINGLE-FAULT PROGRAM VERSIONS

Subject Program	BART Model		
	10 trees	50 trees	300 tests
Apache_EigenDecompose	2.50 %	3.07 %	2.38 %
Apache_DScompiler	9.72 %	8.61 %	9.64 %
Apache_BigMatrix	9.00 %	9.05 %	9.00 %
Apache_Rotation3D	9.07 %	8.73 %	8.16 %
Ojaljo_SchurDecompose	10.61 %	9.89 %	11.44 %
Jama_MatrixDecompose	11.62 %	11.16 %	11.32 %
SciMark_LU	8.33 %	9.72 %	6.94 %
SciMart_FFT	27.59 %	26.72 %	27.59 %
Apache_SymmLQ	1.75 %	1.75 %	1.75 %
Apache_SplineInterpolator	37.78 %	40 %	45.56 %
Apche_SimpleRgress	1.70 %	1.70 %	1.70 %
Apache_SchurTransformer	4.56 %	4.88 %	4.23 %
Apache_MillerUpdatRgress	1.24 %	1.24 %	1.24 %
Apache_HarmonicFitter	30.10 %	30.08 %	28.06 %
Apache_FastSine	1.53 %	1.53 %	1.53 %
Apache_FastCosine	1.29 %	1.29 %	1.29 %
Average Cost	10.52%	10.58%	10.74%

3.4.4 Computation Time Analysis

In this study, we use a Dell Precision T5600 with two 2.30 GHz intel Xeon CPUs and 64 GB RAM. Table 3.4 summarized the average computation time of the three BART models described in last section on each subject program. When the number of trees increased from 10 to 50, the average computation cost nearly doubled. If we reduced number the tests from more than 3000 to 300, the computation cost will reduced more than 50%. From Table 3.4 and Table 3.3, we can conclude that the BART model with 10 trees and fitted with 300 tests get the best cost-performance

ratio among the three BART models fitted with different settings. But we also need to point out that even the BART model is fitted with 300 tests, its computation cost is still about twice of the computation cost of NUMFL. Thus, the computation cost is a weakness of applying BART model on localizing faults in numerical programs.

Table 3.4: AVERAGE COMPUTATION TIME OF NUMFL-GPS-QRM AND NUMFL-CBPS-QRM ON ONE SINGLE-FAULT PROGRAM VERSIONS

Subject Program	Average Computation Time (Secs)		
	10 trees	50 trees	300 tests
Apache_EigenDecompose	2856.73	5530.20	1205.97
Apache_DScompiler	628.31	1243.78	274.88
Apache_BigMatrix	696.58	1337.73	292.28
Apache_Rotation3D	2668.41	5550.45	1082.64
Ojaljo_SchurDecompose	2636.96	5013.37	1313.53
Jama_MatrixDecompose	3134.49	6005.71	1262.88
SciMark_LU	167.94	332.45	121.38
SciMart_FFT	393.26	842.31	234.09
Apache_SymmLQ	908.12	1986.32	245.21
Apache_SplineInterpolator	364.80	747.42	135.00
Apache_SimpleRgress	823.34	1685.88	227.27
Apache_SchurTransformer	768.44	1539.44	315.65
Apache_MillerUpdatRgress	396.10	808.59	198.61
Apache_HarmonicFitter	326.09	673.73	120.28
Apache_FastSine	1006.86	2064.98	259.78
Apache_FastCosine	1089.13	2229.39	294.56

3.5 RELATED WORK

The most related works to this study are those using BART model to estimate treatment causal effect. Hill et al. proposed to apply BART model for causal inference and data science []. In the paper, they designed the method of using BART to estimate average causal effect of binary treatment variable and discussed how to use BART to handle continuous treatment variables and outcome missing data.

Another related work is using tree structure in fault localization. Chen et al [] present a decision tree learning approach to identify the causes of failures in

internet sites. Francis et al [] use tree based method to classify software failures. Kiciman et al [] use decision tree to diagnose which component of large scale systems is the root cause of failure. However, unlike our models, all their works do not localize the fault on statement level.

3.6 CONCLUSION

BART model is a Bayesian non-parametric model which can capture both non-linearities and interactions between variables without knowing the information about how these variables are parametrically related . BART uses a sum of trees structure to approximate the dose response function of continuous treatment variables. The AFCE can be estimated by averaging the causal effect of treatment on outcome at each observation unit. We reported the result of an empirical comparison of BART model to several competing fault localization metrics on both single-fault subject programs and multiple-fault subject programs. BART model performed significantly better than the other techniques. We also compare the BART model with NUMFL, which is introduced in chapter 3. The result shows BART model outperforms NUMFL on single faults localization. In multiple faults localization, BART and NUMFL has similar performances. We also study the sensitivity of the BART model to the number of trees and the number of tests. The result shows BART is robust on the sample size and number of trees. In the future work, will seek to extend BART model to localize faults in non numerical softwares with statement coverage or predicate information.

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