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Using Machine Learning to Guide Architecture Simulation

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Abstract

An essential step in designing a new computer architecture is the careful examination of different design options. It is critical that computer architects have efficient means by which they may estimate the impact of various design options on the overall machine. This task is complicated by the fact that different programs, and even different parts of the *same* program, may have distinct behaviors that interact with the hardware in different ways. Researchers use very detailed simulators to estimate processor performance, which models every cycle of an executing program. Unfortunately, simulating every cycle of a real program can take weeks or months.

To address this problem we have created a tool called SimPoint that uses data clustering algorithms from machine learning to automatically find repetitive patterns in a program's execution. By simulating one representative of each repetitive behavior pattern, simulation time can be reduced to minutes instead of weeks for standard benchmark programs, with very little cost in terms of accuracy. We describe this important problem, the data representation and preprocessing methods used by SimPoint, the clustering algorithm at the core of SimPoint, and we evaluate different options for tuning SimPoint.

Keywords: *k*-means, random projection, Bayesian information criterion, simulation, SimPoint

1. Introduction

Understanding the cycle level behavior of a processor during the execution of an application is crucial to modern computer architecture research. To gain this understanding, researchers typically employ detailed simulators that model each and every cycle of the underlying machine. Unfortunately, this level of detail comes at the cost of speed. Even on the fastest simulators, modeling the full execution of a single benchmark can take weeks or months to complete, and nearly all industry standard benchmarks require the execution of a *suite* of programs. For example, the SPEC benchmark suite consists of 26 different programs, requiring the execution of a combined total of approximately 6 trillion instructions. Still worse, architecture researchers need to simulate each benchmark over a variety of different architectural configurations and design options, to find the set of features that provides an appropriate trade-off between performance, complexity, area, and power. The same program binary, with the exact same input, may be run hundreds or thousands of times to examine how, for example, the effectiveness of a given architecture changes with its cache size. Researchers need techniques which can reduce the number of machine-months required to estimate the impact of an architectural modification without introducing an unacceptable amount of error or excessive simulator complexity. We present a method, distributed as a software package called SimPoint, which can meet this need by exploiting the structured way in which individual programs change behavior over time.

As a program executes its behavior changes. These changes are not random, but rather are often structured as sequences of a small number of recurring behaviors, which we term *phases*. Identifying this repetitive and structured behavior can be of great benefit, since it means we only need to sample each unique behavior once to create a complete representation of the program's execution. This is the underlying philosophy of SimPoint (Sherwood et al., 2001, 2002; Perelman et al., 2003; Biesbrouck et al., 2004; Lau et al., 2004, 2005b). SimPoint intelligently chooses a very small set of samples from an executed program called *simulation points* that, when simulated and weighted appropriately, provide an accurate picture of the complete execution of the program. Simulating in detail only these carefully chosen simulation points can save hours of simulation time over a random sampling of the program, while still providing the accuracy needed to make reliable decisions based on the outcome of the cycle level simulation.

Before we developed SimPoint, architecture researchers would simulate SPEC programs for 300 million instructions from the start of execution, or fast forward 1 billion instructions to try to get past the initialization part of the program. These techniques can result in error rates of up to 3736% in predicting the architecture metrics we wish to measure. SimPoint achieves very low error rates (2% average error, 8% maximum error for the results in this paper) and on average reduces simulation time by a factor of 1,500, compared to simply simulating the whole program. This approach is now used by researchers in the architecture community, and companies such as Intel (Patil et al., 2004). This paper shows how repetitive phase behavior can be found in programs through machine learning and describes how SimPoint automatically finds these phases and picks simulation points.

The rest of the paper is laid out as follows. First, Section 2 describes a summary of the simulation methodology in processor architecture research. Section 3 explains the phase behavior paradigm, and defines terms that are essential in describing the analysis. The correlation between the executing code and performance of a program is described in Section 4, as well as how this code is represented in vector format to capture program behavior. Section 5 describes the machine learning algorithms used to automatically detect phases using the code vectors. Section 6 describes how simulation points are picked from the phases, and the accuracy resulting from representing the entire program execution using the simulation points. Section 7 examines parameters that significantly influence the performance of the SimPoint algorithm in terms of accuracy and run-time. Section 8 examines prior work in phase analysis that uses machine learning. Ongoing and future work is described in Section 9 and our findings are summarized in Section 10.

2. The Application - Simulation

In this section we explain the tools modern computer architects use to evaluate designs and the methods we use to evaluate our solutions.

2.1 Background

Processor architecture research quantifies the effectiveness of a design by executing a program on a software model of the architecture design called an architecture simulator. It is difficult to accurately compare studies that provide results for different sets of programs. To set a standard in the community, the Standard Performance Evaluation Corporation (SPEC) was established to provide a collection of benchmarks to evaluate processor performance. In the same manner, the architecture simulator needs to have a common baseline. SimpleScalar (Burger and Austin, 1997) is a cycle level processor simulator that has become a standard model for architecture research.

2.1.1 SPEC CPU BENCHMARKS

The SPEC CPU2000 benchmark suite has 26 programs, of which 12 are integer programs (primary execution is of integer instructions) and 14 are floating-point programs (primary execution is of floating-point instructions). The benchmark suite is chosen to stress a processor across its many components in a rigorous manner. Each program in the suite has 3 different inputs: *test*, *train*, and *reference*, which respectively correspond to a short test, a more representative training, and a full reference run. The test, train and reference inputs typically execute on the order of a few million, a few billion, and hundreds of billions of instructions respectively. Tables 1 and 2 show all the SPEC CPU2000 benchmarks, divided into integer and floating-point programs. The tables provide a high level description of each benchmark, its source language, and the number of instructions executed (in billions) with the reference and test inputs. These programs were compiled for the Alpha Instruction Set Architecture (ISA) with full optimizations. On average, the reference inputs execute for 223 billion instructions. The program `parser` has the maximum instruction count at 546 billion instructions.

SPEC periodically releases a benchmark suite to evaluate current and future processors. To keep up with the ever increasing rate of processor speeds, SPEC has significantly increased the duration of benchmark execution from the previous suite release in 1995 to the current release of 2000. This is because the reference input needs to run long enough to achieve a valid timing for the benchmark run. This means that with current and future speeds that future releases of the SPEC benchmark suite will need to execute on the order of trillions of instructions for the reference inputs.

2.1.2 SIMPLESCALAR

SimpleScalar is a program that models the cycle level execution of a processor. It takes as input a program-input pair and simulates the execution from beginning to end, while computing relevant statistics for architecture research, such as cycles per instruction (CPI), cache miss rates, branch mispredictions, and power consumption. SimpleScalar has several models to represent different levels of execution detail. At the coarsest level of detail, *sim-fast* models only the functional execution of a program at the instruction level. A more detailed level, *sim-cache*, models the memory hierarchy and computes miss rates for those structures. The level of highest detail, *sim-outorder*, models the cycle-level out-of-order execution of a super-scalar processor. It is a superset of all the other mod-

Benchmark	Ref Length	Test Length	Language	Category
bzip2	143	8.82	C	Compression
crafty	191	4.26	C	Game Playing: Chess
eon	80	0.09	C++	Computer Visualization
gap	269	1.17	C	Group Theory, Interpreter
gcc	46	2.02	C	C Programming Language Compiler
gzip	84	3.37	C	Compression
mcf	61	0.26	C	Combinatorial Optimization
parser	546	4.20	C	Word Processing
perlbmk	111	2.0	C	PERL Programming Language
twolf	346	0.26	C	Place and Route Simulator
vortex	118	9.81	C	Object-oriented Database
vpr	84	0.69	C	FPGA Circuit placement and routing

Table 1: SPEC CPU2000 Integer Benchmarks (lengths in billions of instructions)

Benchmark	Ref Length	Test Length	Language	Category
ammp	326	5.49	C	Computational Chemistry
applu	223	0.18	Fortran 77	Parabolic / Elliptic Partial Differential Equations
apsi	347	5.28	Fortran 77	Meteorology: Pollutant Distribution
art	41	1.48	C	Image Recognition / Neural Networks
equake	131	1.44	C	Seismic Wave Propagation Simulation
facerec	211	4.12	Fortran 90	Image Processing: Face Recognition
fma3d	268	0.00	Fortran 90	Finite-element Crash Simulation
galgel	409	4.34	Fortran 90	Computational Fluid Dynamics
lucas	142	3.71	Fortran 90	Number Theory / Primality Testing
mesa	281	2.88	C	3-D Graphics Library
mgrid	419	16.77	Fortran 77	Multi-grid Solver: 3D Potential Field
sixtrack	470	8.59	Fortran 77	High Energy Nuclear Physics Accelerator Design
swim	225	0.43	Fortran 77	Shallow Water Modeling
wupwise	349	3.63	Fortran 77	Physics / Quantum Chromodynamics

Table 2: SPEC CPU2000 Floating-Point Benchmarks (lengths in billions of instructions)

I Cache	16k 2-way set-associative, 32 byte blocks, 1 cycle latency
D Cache	16k 4-way set-associative, 32 byte blocks, 2 cycle latency
L2 Cache	1Meg 4-way set-associative, 32 byte blocks, 20 cycle latency
Main Memory	150 cycle latency
Branch Pred	hybrid - 8-bit gshare w/ 8k 2-bit predictors + a 8k bimodal predictor
O-O-O Issue	out-of-order issue of up to 8 operations per cycle, 128 entry re-order buffer
Mem Disambig	load/store queue, loads may execute when all prior store addresses are known
Registers	32 integer, 32 floating point
Func Units	8-integer ALU, 4-load/store units, 2-FP adders, 2-integer MULT/DIV, 2-FP MULT/DIV
Virtual Mem	8K byte pages, 30 cycle fixed TLB miss latency after earlier-issued instructions complete

Table 3: Baseline Simulation Model.

els and provides the highest level of execution detail. The architecture research community uses SimpleScalar extensively, and today it is considered a standard architecture simulator.

The different models in SimpleScalar each have a stable execution rate. The fastest model, *sim-fast*, executes on the order of tens of billion instructions per hour on a 1 GHz machine. The slowest yet most accurate model, *sim-outorder*, executes on the order of hundreds of million instructions per hour, which is several orders of magnitude slower than the native hardware. It would take months of computation time to simulate the entire SPEC benchmark suite with *sim-outorder*. What makes matters worse is that researchers need to evaluate many different hardware configurations to measure the effectiveness of a design. This enormous turnaround time for a study makes simulating the full benchmark infeasible, and the majority of researchers only simulate a few hundred million instructions from each benchmark.

2.2 Methodology

For this study, we performed our analysis for the complete set of SPEC CPU2000 programs for multiple inputs using the Alpha binaries from the SimpleScalar website. We collect all of the frequency vector profiles, described in Section 4, using SimpleScalar. To generate our baseline results, we executed all programs from start to completion using SimpleScalar, gathering the hardware metrics. The baseline microarchitecture model is detailed in Table 3.

To examine the accuracy of our approach we provide results in terms of CPI prediction error and *k*-means variance (since SimPoint uses *k*-means clustering). The CPI prediction error is the percent difference between CPI predicted using only simulation points chosen by SimPoint and the baseline (true) CPI of the complete execution of the program. The *k*-means variance is the sum-of-squared distances between every clustered point and its closest center, which is the criterion *k*-means optimizes.

3. Defining Phase Behavior

Since phases are a way of describing the recurring behavior of a program executing over time, we begin by describing phase analysis with a demonstration of the time-varying behavior (Sherwood and Calder, 1999) of two programs from the SPEC 2000 benchmark suite, `gcc` and `gzip`. To characterize the behavior of these programs we have simulated their complete execution from start

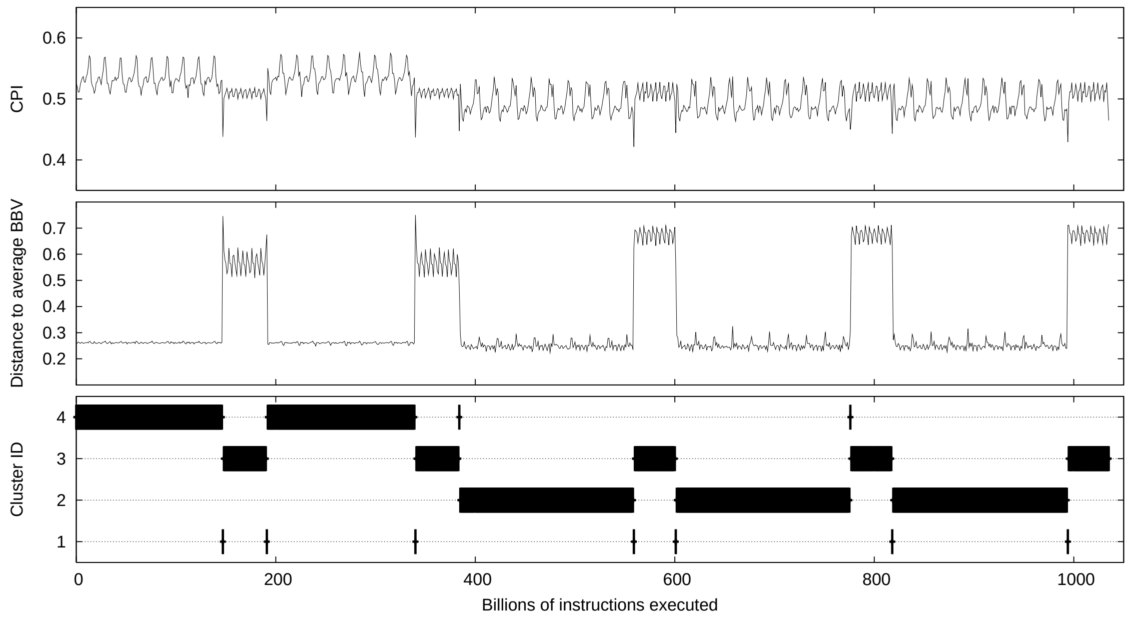


Figure 1: These plots show the relationship between measured performance (CPI) and code usage for the program `gzip-graphic`, and SimPoint's ability to capture phase information by only looking at what code is being executed. For each of the three plots, the horizontal axis represents the execution of the program over time, and each point plotted represents one 10-million instruction interval. The top plot shows the CPI for the executing program. The middle plot shows the distance of each interval's basic block vector (explained in Section 4) to the "target vector", which is a basic block vector that represents the entire program's execution. The target vector is a signature of the program's overall average behavior, and this plot shows how similar the code of each part of the program is to the overall behavior of the program, lower meaning more similar. The bottom plot shows how SimPoint classifies each interval into one of four phases. The phase transitions correspond to changes in the CPI in the top graph, though SimPoint does not use metrics like CPI to classify intervals.

to finish. Each program executes many billions of instructions, and gathering these results took several machine-months of simulation time. The behavior of each program is shown in the top graphs of Figures 1 and 2. Each top graph shows how the CPI rate changes for these two programs over time. CPI is a commonly used metric in the processor architecture community for measuring processor performance. Each point on the graph represents the average CPI taken over a window (we call it an interval) of 10 million executed instructions. These graphs show that programs are fairly complex, changing behaviors frequently.

Note that not only do the behaviors of the programs change over time, they change on the largest of time scales, and even at a large scale one can find repeating behaviors. Programs may have stable behavior for billions of instructions and then change suddenly. In addition to CPI, we have found for the SPEC 95 and 2000 programs that the behavior of *all* of the architecture metrics (branch prediction, cache misses, etc.) tend to change in unison, though not necessarily in the same

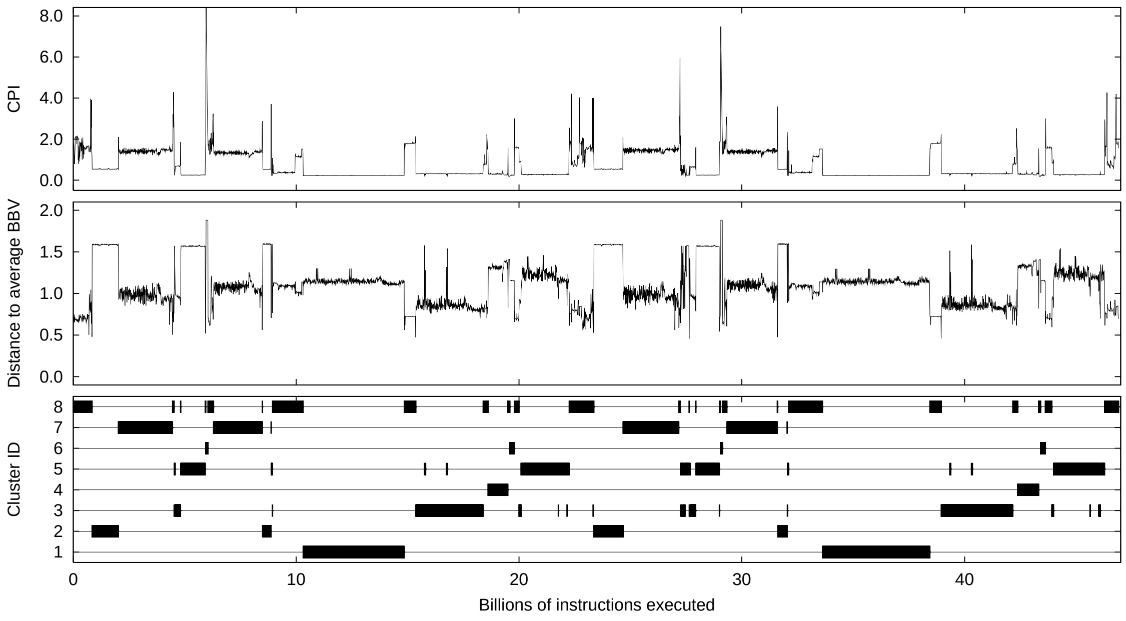


Figure 2: These plots show the relationship between measured performance (CPI) and code usage for the program `gcc-166`, and SimPoint's ability to capture phase information by only looking at what code is being executed. For each of the three plots, the horizontal axis represents the execution of the program over time, and each point plotted represents one 10-million instruction interval. The top plot shows the CPI for the executing program. The middle plot shows the distance of each interval's basic block vector to the "target vector", which is a basic block vector (explained in Section 4) that represents the entire program's execution. The target vector is a signature of the program's overall average behavior, and this plot shows how similar the code of each part of the program is to the overall behavior of the program, lower meaning more similar. The bottom plot shows how SimPoint classifies each interval into one of eight phases. The phase transitions correspond to changes in the CPI in the top graph, though SimPoint does not use metrics like CPI to classify intervals.

direction (Sherwood and Calder, 1999; Sherwood et al., 2002). These corresponding changes are due to underlying changes in program execution.

The underlying methodology used in this work is the ability to automatically identify these underlying program changes *without relying on architectural metrics*. To ground our discussion in a common vocabulary, the following is a list of definitions to describe program behavior and its automated classification.

- Interval – To perform our analysis we break a program's execution up into non-overlapping intervals of execution. An interval is a section of contiguous execution (a time slice) of a program's execution. For example, when using an interval size of 100 million instructions, the first interval of execution starts at instruction 0 and ends at the 100 million instruction executed, the second interval of execution are the instructions 100 million up to 200 million in the program's execution, the third interval represents instructions 200 to 300 million, etc. For the results in this work all intervals are chosen to be the same length, as measured in the number of instructions committed within an interval. This is usually 1, 10, or 100 million instructions, as used by Perelman et al. (2003).

- Similarity – A similarity metric measures the similarity in behavior between two intervals of a program's execution, and is specific to the representation of those intervals.
- Phase – A set of intervals within a program's execution that all have similar behavior, *regardless* of temporal adjacency. A phase may be made up of intervals which are disjoint in time; we would call this a phase with a repeating behavior. A "well-formed" phase should have intervals with similar behavior across various architecture metrics (e.g. CPI, cache misses, branch misprediction). In this paper we consider the terms 'cluster' and 'phase' to be equivalent.
- Phase Classification – Using machine learning to group intervals from a program/input pair into phases (clusters) with similar behavior.

4. The Strong Correlation Between Code and Performance

In this section we describe how we identify phase behavior in an architecture independent fashion.

4.1 Using an Architecture-Independent Metric for Phase Classification

To find program phases, we need a notion of how similar are two different parts of a program's execution. In creating this metric it is advantageous to not rely on hardware-based statistics such as cache miss rates or performance (i.e. CPI), since using these would tie the phases to those statistics which change depending on the architecture configuration. If such statistics were used, the phases would need to be re-analyzed every time there was a change to some architectural parameter (either statically if the size of the cache changed, or dynamically if some policy changes adaptively). This is not acceptable, since our goal is to find a set of samples that can be used across an architecture design space exploration, where many of these parameters may change. To address this, we need a metric that is *independent* of any particular hardware-based statistic, but still relates to the fundamental changes in behavior like those shown in the top graphs of Figures 1 and 2.

An effective way to design such a metric is to base it on the behavior of a program in terms of the code that is executed over time. We have shown that there is a very strong correlation (Lau et al., 2005b) between the set of paths executed in a program and the time-varying architectural behavior observed. The intuition behind this is that the executed code determines the behavior of the program. With this idea it is possible to find the phases in programs using *only* a metric related to how the code is being exercised (i.e. both what code is touched and how often). The central idea behind SimPoint is that it can find the phase behavior shown in the top graphs of Figures 1 and 2 by examining only the frequency with which the code parts (e.g., basic blocks) are executed over time.

4.2 Basic Block Vector

The basic block vector (BBV) (Sherwood et al., 2001) is a structure designed to concisely capture information about how a program is changing behavior over time. A basic block is a section of code (e.g. a contiguous set of instructions) that is executed from start to finish with one entry and one exit. The metric we will use for comparing two time intervals in a program is based on the differences in the execution frequencies for each basic block executed during those two intervals. The intuition behind this is that the behavior of the program at a given time is directly related to the code it is executing during that interval, and basic block vectors provide us with this information.

A program, when run for any interval of time, will execute each basic block a certain number of times. Knowing this information provides a code signature for that interval of execution, and shows where the application is spending its time in the code. The basic idea is that knowing the basic block distribution for two different intervals gives two separate signatures which we can then compare to find out how similar the intervals are to one another. If the signatures are similar, then the two intervals spend about the same amount of time in the same code, and the performance of those two intervals should be similar.

We represent a basic block vector as a one-dimensional array, with one element in the array for each static basic block in the program. Each interval in an executed program is represented by one BBV, and at the beginning of each interval, its corresponding BBV has all zeros. During each interval, we count the number of times each basic block has been entered, and record that number into the corresponding element in the vector. This number is weighted by the number of instructions in the basic block, since we want every individual instruction to have the same influence. Therefore, each element in the array is the count of how many times its corresponding basic block has been entered during an interval of execution, multiplied by the number of instructions in that basic block. For example, if the 50th basic block has one instruction and is executed 15 times in an interval, then bbv[50] = 15 for that interval. At the end of an interval's execution, we normalize the BBV to sum to 1.

We call the vectors used to guide phase analysis *Frequency Vectors*, of which basic block vectors are one type. Frequency vectors can represent basic blocks, branch edges, or any other type of program related structure which provides a representative summary of a program's behavior for each interval of execution. We recently examined frequency vector structures other than basic block vectors for the purpose of phase classification. We have looked at frequency vectors for data, loops, procedures, register usage, instruction mix, and memory behavior (Lau et al., 2004). We found that using register usage vectors, which simply counts for a given interval the number of times each register is defined and used, provides similar accuracy to using basic block vectors. In addition, using only loop and procedure branch execution frequencies performs almost as well as using the full basic block information. We also found, for SPEC 2000 programs, that creating frequency vectors by including both code and data access patterns into the vectors did not improve classification over just using code (Lau et al., 2004).

4.3 Basic Block Vector Difference

In order to find patterns in a program we must first have some way of comparing the similarity of two basic block vectors. The operation should take two basic block vectors and return a single number corresponding to how similar (or different) they are.

There are several ways of measuring the similarity of two vectors, such as taking the dot product between the vectors, finding the Euclidean (2-norm) distance of the connecting vector, or Manhattan (1-norm) distance of the connecting vector. The Euclidean distance has been shown to be effective for off-line phase analysis (Sherwood et al., 2002; Perelman et al., 2003). The SimPoint approach we examine in this paper uses Euclidean distance as the metric for comparing basic block vectors, since it is based on *k*-means. For on-the-fly phase analysis (e.g. predicting phases during computation), the Manhattan distance is more efficiently implemented in hardware. It has been shown to be useful in previous work in online phase prediction (Sherwood et al., 2003; Lau et al., 2005c).

4.4 Showing the Correlation Between Code Signatures and Performance

For a detailed study showing that there is a strong correlation between executed code and real performance, please see Lau et al. (2005b). The top two graphs of Figure 2 give one illustration of this correlation by showing the time-varying CPI and BBV distance graphs next to each other for `gcc-166`. The top graph plots the CPI for each interval executed (at 10M interval length) showing how the program's CPI varies over time. Similarly, the BBV distance graph plots for each interval the Manhattan distance of the BBV (code signature) for that interval from the whole program's target vector. The whole program's target vector is a BBV that comes from viewing the whole program as a single interval. The same information is also provided for `gzip` in the top two graphs of Figure 1. These graphs show that changes in CPI have corresponding changes in code signatures, which is one indication of strong phase behavior for these applications.

These graphs show a strong correlation between code changes and CPI changes even for complex programs like `gcc`. The graphs for `gzip` show that phase behavior can be found even if the intervals' CPIs have small variance. This brings up an important point about classifying intervals based on code similarity rather than based on similarity of CPI or some other hardware metric. Assume we have two intervals with *different code signatures* but they have very *similar CPIs* because both of their working sets fit completely in the cache. During a design space exploration search, as the cache size changes, their CPIs may differ dramatically if one of them no longer fits into the cache. This is why it is important to perform the phase analysis by comparing the code signatures independent of the underlying architecture. We have found that the BBV code signatures correctly identify differences like these, which cannot be seen by looking at just the CPI.

4.5 Basic Block Similarity Matrix

Now that we have methods of comparing program execution intervals, we can use them for finding phase-based behavior. A phase of program behavior can be defined in several ways. Past definitions were built around the idea of a phase being a contiguous interval of execution during which a measured program metric is relatively stable. We extend this notion of a phase to include all similar sections of execution regardless of temporal adjacency. Thus, a phase may appear several times in the execution of a program.

A key observation from this paper is that the phase behavior seen in any program metric is a function of the code being executed. Because of this we can use the comparison between the basic block vectors to get an idea of how closely related any other metrics will be between those two intervals.

To find how all intervals of execution relate to one another we create a *basic block similarity matrix* for a program/input pair. The similarity matrix is an upper-triangular $n \times n$ matrix, where n is the number of intervals in the program's execution. An entry at (x, y) in the matrix represents the Manhattan distance between the basic block vector at interval x and the basic block vector at interval y.

Figures 3 (left and right) and 4 (left) shows the similarity matrices for `gzip`, `bzip`, and `gcc` using the Manhattan distance. The diagonal of the matrix represents the program's execution over time from start to completion. The darker the points, the more similar the intervals are (the Manhattan distance is closer to 0), and the lighter they are the more different they are (the Manhattan distance is closer to the maximum value — which is 2 since each vector is normalized to sum to 1).

Consider the points along the matrix diagonal. The top left corner of each matrix is the start of program execution $(0,0)$, and the bottom right is the point $(n-1,n-1)$ (end of execution). Each interval is perfectly similar to itself, so the points on the diagonal are all dark. Starting from a point on the diagonal, you can compare how its corresponding interval relates to its neighbors forward (backward) in execution by tracing horizontally (vertically) from that point. For example, to compare a given interval x with the interval at $x+m$, start at the point (x,x) on the matrix and trace to the right until you reach $(x,x+m)$.

Let us first examine `gzip` because it has behaviors that are evident at such a large scale that they are easy to see. An interval taken from 70 billion instructions into execution in Figure 3 (left) is directly in the middle of a large phase shown by the triangle of dark points that surround this point. This means that this interval is very similar to its neighbors both forward and backward in time. We can also see that the intervals at 50 billion and 90 billion instructions are also very similar to the program behavior at 70 billion instructions. While it may be hard to see in a printed version, the intervals around 70 billion instructions are similar to the intervals around 10 billion and 30 billion instructions, and even more similar to those around 50 and 90 billion instructions.

Overall, Figure 3 (left) shows that the phase behavior seen in the similarity matrix lines up quite closely with the behavior of the program seen in the top graph of Figure 1, with 5 large regions of self-similar behavior (the first 2 being different from the last 3) each divided by a small region of self-similar behavior. All of the small self-similar regions are also very similar to each other.

The similarity matrix for `bzip` (shown on the right of Figure 3) is very interesting. `Bzip` has complicated behavior, with two large parts to its execution: compression and decompression. This can readily be seen in the figure as the large dark triangular and square patches. The interesting thing about `bzip` is that even within each of these sections of execution there is complex behavior. This, as will be shown later, makes the behavior of `bzip` impossible to capture using only one small contiguous section of execution.

An even more complex case for finding phase behavior is `gcc`, which is shown on the left of Figure 4 (the matrix on the right of that figure will be explained in more detail in Section 5.1.1). The left matrix shows that `gcc` does have regular behavior. Even for such a complex program, we see that there is common code shared between sections of execution, such as the intervals around 13 billion instructions and 36 billion instructions. In fact the strong dark diagonal line cutting through the matrix indicates that there is large-scale repetition between the first half and second half of the program. By analyzing the graph we can see that code at each interval x is very similar to interval (x+23.6B instructions).

5. Automatically Finding Phase Behavior

In this section we describe the algorithms used to automatically detect patterns using the frequency vectors described in the previous section.

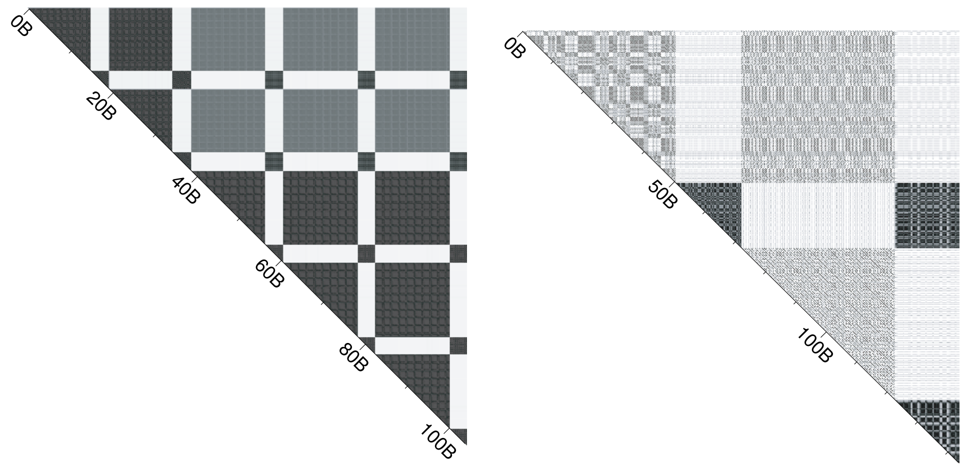


Figure 3: Basic block similarity matrix for the programs `gzip-graphic` (shown left) and `bzip-graphic` (shown right). The diagonal of the matrix represents the program's execution from beginning to end, with units in billions of instructions. The darker the points, the more similar the intervals are (the Manhattan distance is closer to 0), and the lighter the points the more different they are (the Manhattan distance is closer to 2).

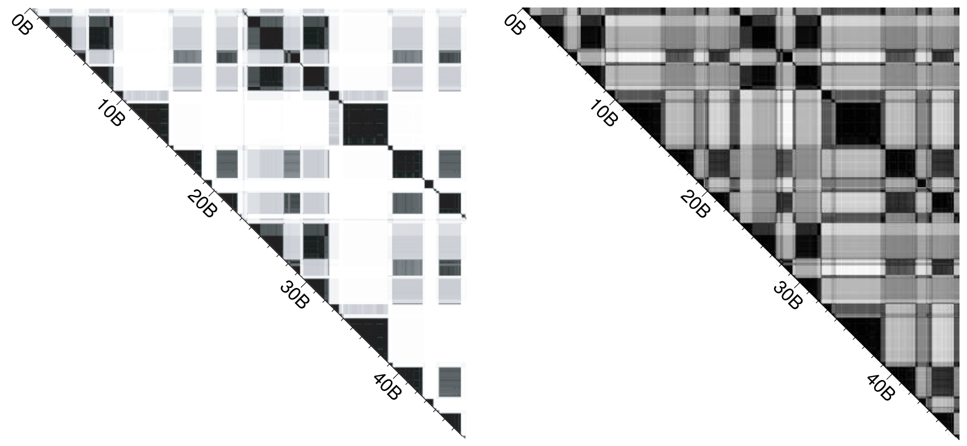


Figure 4: The original similarity matrix for the program `gcc-166` (left), and the similarity matrix for the projection of `gcc-166` (right). The figure on the left uses the original basic block vectors (each of which has over 100,000 dimensions), and uses the Manhattan distance for calculating the difference. The figure on the right uses the same data, but projected down to 15 dimensions, and uses the Euclidean distance for calculating the difference.

5.1 Using Clustering for Phase Classification

A primary goal of SimPoint is to have an automated way of extracting phase information from programs. Data clustering algorithms from unsupervised machine learning have been shown to be very effective at breaking the complete execution of a program into phases that have similar frequency vectors (Sherwood et al., 2002). Because the frequency vectors correlate to the overall performance of the program, grouping intervals based on their frequency vectors produces phases that are similar not only in the distribution of program structures used, but also in every other architecture metric measured, including overall performance.

The goal of clustering is to divide a set of points into clusters such that points within each cluster are similar to one another (by some metric), and points in different clusters are different from one another. We use the machine learning term ‘cluster’ and the architecture term ‘phase’ to express the same concept.

The k-means algorithm (MacQueen, 1967) is an efficient and well-known clustering algorithm, which we use to split program intervals into phases. Prior to clustering, we use random linear projection (Dasgupta, 2000) to reduce the dimension of the input vectors. One drawback of the k-means algorithm is that it requires the number of clusters k as an input to the algorithm, but we do not know beforehand what value is appropriate. To address this, we run the algorithm for several values of k, and then use a penalized likelihood score to guide our final choice for k. Taken to the extreme, if every interval of execution is given its very own cluster, then every cluster will have homogeneous behavior. Our goal is to choose a clustering with a minimum number of clusters which still models the program behavior well.

The following steps summarize the SimPoint phase clustering algorithm at a high level.

1. Profile the program by dividing the program’s execution into contiguous intervals of fixed length (e.g., 1 million, 10 million, or 100 million instructions). For each interval, collect a frequency vector tracking the program’s use of some program structure (basic blocks, branch edges, loops, register usage, etc.). Each frequency vector is normalized so that the sum of all the elements equals 1.

2. Reduce the dimensionality of the frequency vector data to a much smaller number of dimensions using random linear projection. Using projected data speeds up the k-means algorithm significantly and reduces the memory requirements by several orders of magnitude while preserving the essential similarity information.

3. Run the k-means clustering algorithm on the projected data with values of k in the range from 1 to K, where K is a user-prescribed maximum number of phases that can be detected. Each run of k-means produces a clustering, which is a partition of the data into k different phases/clusters. Each run of k-means begins with a random initialization step, which requires a random seed.

4. To compare and evaluate the different clusters formed for different k, we use the Bayesian Information Criterion (BIC) as a measure of the “goodness of fit” of a clustering to a data set. A high BIC score indicates the clustering is a good fit to the data. For each clustering ($k \in \{1, 2, \ldots, K\}$), the fitness of the clustering is scored using the BIC.

5. The final step is to choose the clustering with a small k such that its BIC score is nearly as good as the best observed. The chosen clustering is the final grouping of intervals into phases.

The above algorithm groups intervals into phases. This algorithm has several important parameters: interval length, projected dimension, the maximum number of clusters K, how the BIC is to be used to select the best clustering, etc. Each must be tuned to create accurate and representative simulation points using SimPoint. We discuss these parameters in more detail later in this paper.

5.1.1 RANDOM PROJECTION

For this clustering problem, we have to address the problem of high dimensionality. Many clustering algorithms suffer from the so-called “curse of dimensionality,” which refers to the fact that finding an optimal clustering is intractable as the number of dimensions increases. One problem is that geometric optimizations that give significant speedup in low-dimensional data often have the opposite effect in high dimensions (e.g. k-d trees for speeding up nearest neighbor queries). For basic block vectors, the number of dimensions is the number of executed basic blocks in the program, which ranges from 2,756 to 102,038 for the SPEC benchmark suite, and could grow into the millions for very large programs. For example, one Microsoft application we studied consisted of over 800,000 basic blocks, which is representative of desktop applications. Another practical problem is that the running time and memory requirements of k-means depend on the dimension of the data, making the algorithm slow if the dimension grows too large. Also, we observe that k-means tends to get stuck easily in sub-optimal solutions if the dimension is too high. This is evidenced by the small number of iterations k-means requires to converge on high-dimensional data, as we have observed on this data. The algorithm does not improve much over its initialization.

Two broad methods of reducing the dimension of data are dimension selection and dimension reduction. Dimension selection simply removes some of the dimensions, based on a measure of goodness of each dimension for describing the data. However, this can throw away a lot of information in the dimensions which are ignored. Also, in finding a measure to select useful dimensions is not as clear for unsupervised learning as for supervised learning. Dimension reduction reduces the number of dimensions by creating a new lower-dimensional space and then projecting each data point into the new space (where the new space’s dimensions are not necessarily related to the old space’s dimensions).

For this work we use random linear projection (Dasgupta, 2000) to create a new low-dimensional space into which we orthogonally project the data. This is a simple and fast technique that is very effective at reducing the number of dimensions while retaining the essential structure of the data. There are two steps to projecting a data set down to a lower-dimensional version. Consider a data set X which is represented as a matrix of $n \times d$ real values, where n is the number of vectors, and d is the original dimension. We want a low-dimension version X' which is $n \times d'$, where d' is the projected number of dimensions. To create X', we do the following:

- Create a projection matrix P size $d \times d'$. Fill each entry in the matrix with a random value chosen uniformly in $[-1, 1]$.

- Use a matrix multiplication to obtain $X' = X \times P$.

The analysis given by Dasgupta (Dasgupta, 2000) shows that when using random linear projection for clustering data, there are two primary theoretical benefits. The first is that clusters that are very eccentric will become more spherical in their low-dimensional representation. This is appropriate for the k-means algorithm which searches for spherical clusters. The second is that a mixture of

k Gaussian clusters can be projected into only $O(\log k)$ dimensions while retaining the approximate level of separation between clusters.

Principal components analysis (PCA) is a widely-used method for dimension reduction based on directions of high variance. However, performing PCA on a d-dimensional data set requires $O(d^3)$ operations, which is too expensive for data sets of the size we are considering here that can have hundreds of thousands of dimensions. Constructing the random projection matrix requires only $O(dd')$ time, so it is linear in the original and the new dimension. Dasgupta further showed that there are many simple examples where PCA is not able to reliably reduce k well-separated Gaussian clusters to below $\Omega(k)$ dimensions and keep them well-separated in the low-dimensional projection. Examining the use of PCA for BBV dimension reduction is part of our future research.

For our application, we found that 15 dimensions is low enough to be computationally tractable, but sufficiently high to discover the different phases of execution with clustering. We found this by running experiments which are reported in earlier work (Sherwood et al., 2002). These experiments projected all the data sets we are interested in to a varying number of dimensions and then recorded the number of clusters found by k-means and the BIC. We found that for fewer than 15 dimensions, the number of clusters found dropped off, but for more than 15 dimensions, the number of clusters found did not increase significantly. Similar results were also found using the G-means algorithm to incrementally learn k (without using the BIC) by Hamerly and Elkan (2003). Section 7 evaluates how the choice of dimension affects the accuracy of SimPoint.

Figure 4 shows the similarity matrix for `gcc` on the left using original BBVs, whereas the similarity matrix on the right shows the same matrix but on the data that has been projected down to 15 dimensions. For the reduced dimension data we use the Euclidean distance to measure differences, rather than the Manhattan distance used on the original data. Some information is lost because of the projection, but overall phase behavior we see in the original data is still easily discernible with only 15 dimensions. A scatterplot of the program `gzip` projected to 2 dimensions and clustered into 3 clusters using k-means is shown in Figure 5.

5.1.2 BAYESIAN INFORMATION CRITERION

To compare the different clusterings formed for different k, we use the Bayesian Information Criterion, or BIC (Schwarz, 1978), as a measure of the “goodness of fit” of a clustering to a data set. The BIC is an approximation of the probability of the clustering, given the data that has been clustered. Thus, the larger the BIC score, the higher the probability that the clustering being scored is a “good fit” to the data being clustered. The BIC formulation we use is appropriate for clustering with k-means, however other formulations of the BIC could also be used for other clustering models. The BIC is only one method of choosing a good model from a set of models; other methods such as the Akaike information criterion (AIC) (Akaike, 1974), minimum description length (MDL) (Rissanen, 1978), and Monte-carlo cross-validation (MCCV) (Smyth, 1996) may also be appropriate.

There are two parts of the BIC: the likelihood and the penalty. The likelihood is a measure of how well the clustering models the data. For the k-means likelihood, each cluster’s model is considered a spherical Gaussian distribution (which is the assumption k-means makes). The likelihood of a cluster is the product of the probabilities of each point in the cluster given by the cluster’s Gaussian. The likelihood for the whole model is just the product of the likelihoods for all clusters. However, the likelihood tends to increase without bound as more clusters are added. Therefore the second term is a penalty that offsets the likelihood growth based on the model complexity (i.e. the

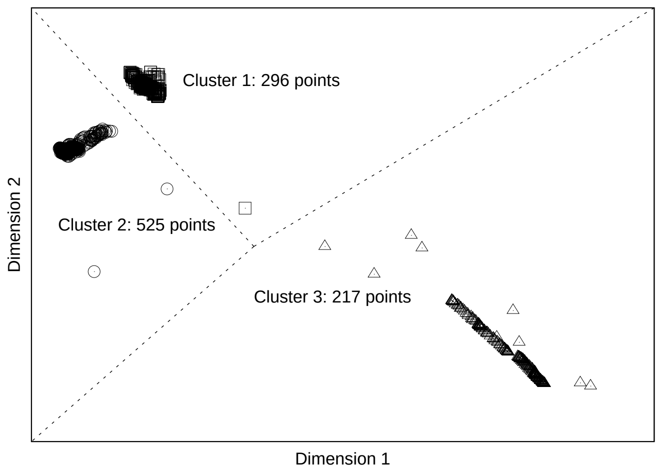


Figure 5: This plot shows a two-dimensional projection of the basic block vectors for the program `gzip`, having 1038 total intervals, and clustered into three clusters with *k*-means. The lines show divisions between the three clusters. Note that SimPoint normally operates in more than two dimensions, but this illustrates the fact that that program behavior does form natural groups that can be found through data clustering.

number of clusters). The BIC is formulated as

$$BIC(X,C_k) = \mathcal{L}(X|C_k) - \frac{p}{2}\log(n)$$

where $\mathcal{L}(X|C_k)$ is the log-likelihood of the clustered data X given the clustering C_k having k clusters, $n = |X|$ is the number of points in the data, and $p = (k-1) + dk + 1 = k(d+1)$ is the number of parameters to estimate: $(k-1)$ cluster probabilities, k cluster center estimates which each requires d mean estimates, and one variance estimate (shared over all clusters). The log-likelihood of the k-means model given the data is

$$\mathcal{L}(X|C_k) \quad = \quad -\frac{nd}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{j=1}^{k}\sum_{i\in C_j}||X_i - c_j||^2 + \sum_{j=1}^{k} n_j \log(n_j/n)$$

where n_j is the number of points in the jth cluster (so n_j/n is the estimated prior probability of cluster j), and σ^2 is the average squared Euclidean distance from each point to its cluster center. The term C_j represents the set of all indexes of X that are members of cluster j, X_i is the ith point in data set X, and $c_j = \frac{1}{n_j}\sum_{i\in C_j} X_i$ is the location of the jth cluster center. The center c_j is the maximum likelihood solution for the cluster's center. The maximum likelihood estimator for σ^2 is

$$\hat{\sigma}^2 \quad = \quad \frac{1}{nd}\sum_{j=1}^{k}\sum_{i\in C_j}||X_i - c_j||^2.$$

For the purposes of calculating the BIC, we can substitute this maximum likelihood estimate for σ^2 into the log-likelihood formulation, to get a simpler version:

$$\mathcal{L}(X|C_k) \quad = \quad -\frac{nd}{2}\log(2\pi\sigma^2) - \frac{nd}{2} + \sum_{j=1}^{k} n_j \log(n_j/n).$$

The BIC formulation we present basically follows that given by Pelleg and Moore (2000).

For a given program and inputs, the BIC score is calculated for each k-means clustering, for K in the range 1 to K. We then choose the clustering that achieves a BIC score that is close to the highest BIC score seen. This is explained more in Section 7.

5.2 Clusters and Phase Behavior

The bottom plots in Figures 1 and 2 show the results of running our phase-finding clustering algorithm on `gzip` and `gcc`. These results use an interval length of 10 million instructions and the maximum number of phases (K) is set to 10. The horizontal axis corresponds to the execution of the program (in billions of instructions), and each interval is classified to belong to one of the clusters (labeled on the vertical axis).

For `gzip`, the program's execution is partitioned into 4 clusters. Looking at the middle plot for comparison, the cluster behavior captured by our algorithm lines up quite closely with the behavior of the program. Clusters 2 and 4 represent the large sections of execution which are similar to one another. Cluster 3 captures the smaller phase that lies in between these larger phases. Cluster 1 represents the phase transitions between the three dominant phases. The intervals in cluster 1 are grouped into the same phase because they execute a similar combination of code, which happens to be part of the code behavior in either cluster 2 or 4 and part of code executed in cluster 3. These transition points in cluster 1 also correspond to the same intervals that have large spikes in CPI seen in the top graph (these spikes are due to increased cache misses for those regions).

The bottom plot of Figure 2 shows how `gcc` is partitioned into 8 clusters. Comparing this to the middle and top plots in the same figure, we see that even the more complicated behavior of `gcc` is captured well by SimPoint. The dominant behaviors in the top two graphs can be seen grouped together in phases 1, 3, 5,and 7.

6. Choosing Simulation Points from the Phase Classification

After the phase classification algorithm has done its job, intervals with similar code usage will be grouped together into the same phases (clusters). Then from each phase, SimPoint chooses one representative interval that will be simulated in detail to represent the behavior of the whole phase. Therefore, by simulating *only* one representative interval per phase, we can extrapolate and capture the behavior of the entire program.

To choose a representative for a cluster, SimPoint picks the interval that is closest (Euclidean distance) to the cluster's k-means center. The center can be viewed as a pseudo-interval which behaves most like the average behavior of the entire phase. Most likely there is no interval that exactly matches the center, so SimPoint chooses the closest interval. The selected interval is called a *simulation point* for that phase (Perelman et al., 2003; Sherwood et al., 2002). We can then perform detailed simulation on the set of simulation points.

As part of its output SimPoint also gives a weight for each simulation point. Each weight is a fraction: it is the total number of instructions represented by the intervals in the cluster from which the simulation point was taken divided by the number of instructions in the program. With the weights and the detailed simulation results of each simulation point, we can compute a weighted average for the architecture metric of interest (CPI, cache miss rate, etc.) for the entire program's execution.

These simulation points are chosen once for a program/input combination because they are chosen based only on how the code is executed, and not based on architecture metrics. Therefore, they only need to be calculated once for a binary/input combination and can be used repeatedly across all of the runs for an architecture design space exploration.

The number of simulation points that SimPoint chooses has a direct effect on the simulation time that will be required for those points. The maximum number of clusters, K, along with the interval length, represents the maximum amount of simulation time that will be needed. When fixed length intervals are used, $(K * \text{interval length})$ is a limit on the number of simulated instructions.

SimPoint allows users to trade off simulation time with accuracy. Researchers in architecture tend to want to keep simulation time to below a fixed number of instructions (e.g., 300 million) for a run. If this is a goal, we find that an interval length of 10 million instructions with $K = 30$ provides very good accuracy (as we show in this paper) with reasonable simulation time (220 million instructions on average). If even more accuracy is desired, then decreasing the interval length to 1 million and setting $K = 300$ performs well for the SPEC 2000 programs, as does setting $K = \sqrt{n}$ (where n is the number of clustered intervals). Empirically we discovered that as the granularity becomes finer, the number of phases discovered increases at a sub-linear rate. The upper bound defined by this square-root heuristic works well for the SPEC benchmarks.

The length of the interval chosen by users of SimPoint depends upon their simulation infrastructure and how much they want to deal with warmup. Warmup is the process of initializing the simulator's state (caches, branch predictor, etc.) at the start of a simulation point so that it is the same as if we simulated from the beginning of the program to that point. For many programs, using a long interval length (e.g., more than 100 million instructions) will make warmup unnecessary. This is the approach used by Intel's PinPoint for simulation (Patil et al., 2004). They simulate intervals of length 300-500 million instructions so they do not have to worry about implementing warmup in their simulation infrastructure. With such long intervals the architecture structures are warmed up sufficiently during the beginning of the interval's execution to provide accurate simulation results. In comparison, short interval lengths can be used, but this requires having an approach for warming up the architecture state. One way to do this is with an architecture checkpoint, which stores the potential contents of the major architecture components at the start of the simulation point (Biesbrouck et al., 2005). This can significantly reduce warmup time, since warmup consists of just reading the checkpoint from a file and using it to initialize the architecture structures.

6.1 Accuracy of SimPoint

We now show the accuracy of using SimPoint for the complete SPEC 2000 benchmark suite and their reference inputs. Figure 6 shows the simulation accuracy results using SimPoint (and other methods) for the SPEC 2000 programs when compared to the complete execution of the programs. For these results we use an interval length of 100 million instructions and limit the number of simulation points to no more than 10. With the above parameters SimPoint finds 4 phases for `gzip`, and 8 for `gcc`. As described above, one simulation point is chosen for each cluster, so this means

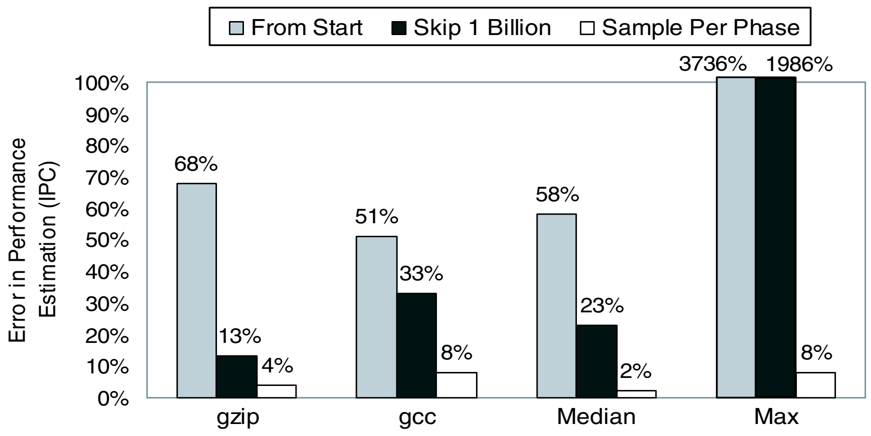


Figure 6: Simulation accuracy for the SPEC 2000 benchmark suite when performing detailed simulation for several hundred million instructions compared to simulating the entire execution of the program. Results are shown for simulating from the start of the program's execution, for fast-forwarding 1 billion instructions before simulating, and for using SimPoint to choose at most ten 100-million-instruction intervals to simulate. The results are shown as percent error of predicted IPC, which is how much the estimated IPC using SimPoint is different from the complete execution of the program. IPC is the inverse of CPI. The median and maximum results are for the complete SPEC 2000 benchmarks.

that a total of 400 million instructions were simulated for `gzip`. The results show that this results in only a 4% error in performance estimation for `gzip`.

For these results, we compare this estimated IPC using SimPoint to the baseline IPC. IPC (Instructions Per Cycle) is the inverse of CPI, and often used instead of CPI when describing performance. The baseline was gathered from spending months of simulation time to simulate the entire execution of each SPEC program. The results in Figure 6 compare SimPoint to how architecture researchers use to choose where to simulate before SimPoint. The first technique was to just simulate the first N million instructions of a benchmark's execution. The second technique was to blindly skip the first billion instructions of execution to get past the initialization of the program's execution, and then simulate for N million instructions. The results show that simulating from the start of execution, for the exact same number of instructions as simulated with SimPoint, results in a median error of 58%. If instead, we fast forwarded for 1 billion instructions and then simulate for the same number of instructions as chosen by SimPoint, we see a median 23% IPC error. When using SimPoint to create multiple simulation points we have a median IPC error of 2%. Note that the maximum error seen for the prior techniques are significant for the SPEC programs, but it is very reasonable (only 8%) for SimPoint.

6.2 Relative Error During Design Space Exploration

The absolute error of a program/input run on one hardware configuration is not as important as tracking the change in metrics across different architecture configurations. There is a lot of discussion and research into getting lower simulation error rates. But what often is not discussed is that a

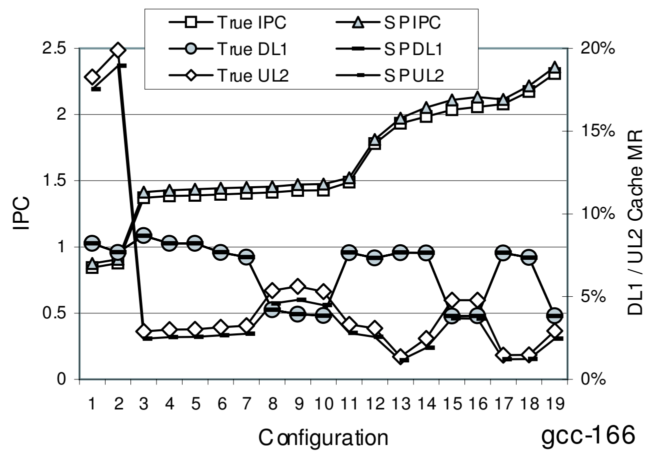


Figure 7: This plot shows the true and estimated IPC and cache miss rates for 19 different architecture configurations for the program `gcc`. The left *y*-axis is for the IPC and the right *y*-axis is for the cache miss rates for the L1 data cache and unified L2 cache. Results are shown for the complete execution of the configuration and when using SimPoint.

low error rate for a single configuration is not as important as achieving the same relative error rates across the design space search and having them all biased in the same direction.

We now examine how SimPoint tracks the relative change in hardware metrics across several different architecture configurations. To examine the independence of the simulation points from the underlying architecture, we used the simulation points for the SimPoint algorithm with an interval length of 1 million instructions and the maximum K set to 300. For the program/input runs examined, we performed full program simulations while varying the memory hierarchy, and for every run we used the same set of simulation points when calculating the SimPoint estimates. We varied the configurations and the latencies of the L1 and L2 caches as described by Perelman et al. (2003).

Figure 7 shows the results across 19 different architecture configurations for `gcc-166`. The left *y*-axis represents the performance in Instructions Per Cycle (IPC) and the *x*-axis represents different memory configurations from the baseline architecture. The right *y*-axis shows the miss rates for the data cache and unified L2 cache, and the L2 miss rate is a local miss rate. For each metric, two lines are shown: "True" for the true metric from the *complete* detailed simulation, and the "SP" for the estimated metric using our simulation points. For the results, the configurations on the *x*-axis are sorted by the IPC of the full run.

This figure shows that the simulation points, which are chosen by only looking at code usage, can be used across different architecture configurations to make accurate architecture design trade-off decisions and comparisons. The simulation points are able to track the relative changes in performance metrics between configurations. This means we are able to make the same decision between two architectures, in terms of which one is better, using SimPoint as the complete simulation of the program. One interesting observation is that although the simulation results from SimPoint have a bias in its predictions, this bias is consistent across the different configurations for a given program/input. This is true for both IPC and cache miss rates. We believe one reason for the bias is that SimPoint chooses the most representative interval from each phase, and intervals that represent phase change boundaries are less likely to be fully represented across the chosen simulation points.

7. Clustering Analysis

In this section we describe the primary parameters that have influence on how SimPoint and the k-means algorithm behave. We first focus on how we achieve a reasonable running time for k-means, and then examine how to search over k to find a good clustering. For the experiments in this section, we use basic block vectors with 100 million instruction intervals. Where it is not specified, we also use $k = 30$ clusters and 15 projected dimensions.

7.1 Methods for Reducing the Run-Time of k-Means

Even though SimPoint only needs to be run once per binary/input combination, we still want a fast clustering algorithm that produces accurate simulation points. To address the run-time of SimPoint, we first look at the three parts which affect most the running time of a single run of k-means. The three parts are the number of intervals to cluster, the dimension of the intervals being clustered, and the number of iterations it takes to perform a clustering.

We first examine how the number of intervals affects the running time of the SimPoint algorithm. Figure 8 shows the time (in seconds) for running SimPoint on different numbers of intervals as we vary the number of clusters. For this experiment, the clustered vectors are randomly generated from uniformly random noise in 15 dimensions. We use random data in these experiments because it does not bias these results based on a particular benchmark and it gives comparable results across a wide range of parameter settings. But more importantly, prior theoretical work by Indyk et al. (1999) suggests that it is most difficult to accelerate (i.e. make more efficient using geometric reasoning) clustering algorithms on data without structure, such as uniformly random data. This is supported by experiments by Moore (2000) and Elkan (2003). So these experiments form a comparable set of challenging results for the per-iteration run-time of SimPoint. The number of iterations will vary depending on the structure of the data, however. For example, using k-means to cluster data from very well-separated clusters is likely to converge in a low number of iterations, while clusters which overlap are likely to require more iterations.

The first graph shows that for 100,000 vectors and $k = 128$, it took about 3.5 minutes for SimPoint 3.0 to perform the clustering. It is clear that the number of vectors clustered and the value of k both have a large effect on the run-time of SimPoint. The run-time changes linearly with the number of clusters and the number of vectors, as expected. Also, we can see that the time per basic operation actually goes down as k increases. This is due to a simple optimization called *partial distance search* (McNames, 2000; Cheng et al., 1984) that allows the algorithm to avoid calculating the full distance from a point (interval) to every cluster center in the first step of k-means. The goal of this step is to find the closest cluster center to the point, so that the interval may be assigned to that center. To find this closest center, a simple loop searches for the cluster center with the minimum squared Euclidean distance. The squared distance calculation sums the squared dimension difference between the point and the cluster center over all dimensions. While searching for the minimum squared distance from a point to all centers, partial distance search keeps the smallest squared distance seen thus far. When calculating the distance to another center, it may find that the intermediate squared distance result (after processing some of the dimensions) is larger than the

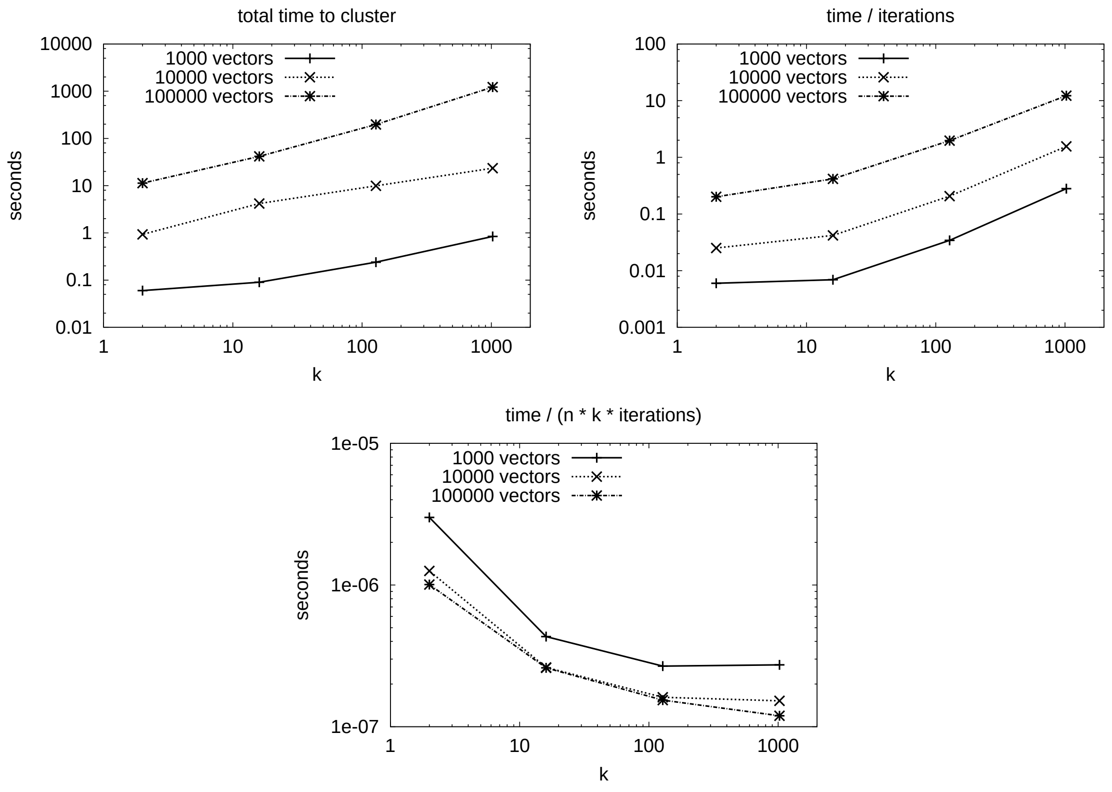


Figure 8: These plots show how varying the number of vectors and clusters affects the amount of time required to cluster with SimPoint 3.0. For this experiment we generated uniformly random data in 15 dimensions. The first plot shows total time, the second plot shows the time normalized by the number of iterations performed, and the third plot shows the time normalized by the number of basic operations performed. Both the number of vectors and the number of clusters have a linear influence on the run-time of *k*-means. The bottom plot shows a decreasing trend due to optimizations in *k*-means which are more beneficial for larger *k*.

smallest squared distance seen to a different center. If this is the case, the distance we are calculating cannot be minimal, so the current calculation is stopped short of calculating the entire squared distance over all of the dimensions. This optimization does not change the correctness of the algorithm. Partial distance search is most beneficial when there are many clusters, since the more centers there are, the more it is likely that there will be a close center that can give a good lower bound for the partial search. Partial distance search is also useful in high dimensional data, since work is saved when computing per-dimension differences, and the more dimensions there are the more computations can potentially be avoided.

Program	# Vecs × # B.B.	SP3-All	SP3-BinS
gcc-166	4692 × 102038	9 min	3.5 min
crafty	19189 × 16970	84 min	10.7 min

Table 4: This table shows the running times (in minutes) by SimPoint 3.0 without using binary search (SP3-All) and SimPoint 3.0 using binary search (SP3-BinS). SimPoint is run searching for the best clustering from *k*=1 to 100, uses 5 random seeds per *k*, and projects the vectors to 15 dimensions. The second column shows how many vectors and the size of the vector (static basic blocks) the programs have.

7.1.1 NUMBER OF INTERVALS AND SUB-SAMPLING

Each iteration of the *k*-means algorithm has a run-time that is linear in the number of clusters, the number of intervals, and the dimensionality. However, since *k*-means is an iterative algorithm, many iterations may be required to reach convergence. We already found in prior work (Sherwood et al., 2002), and revisit in Section 7.1.2 that we can reduce the number of dimensions down to 15 and still maintain SimPoint's accuracy. Therefore, the main influence on execution time for SimPoint is the number of intervals.

To show this effect, Table 4 shows the SimPoint running time for `gcc-166` and `crafty-ref`, which shows the lower and upper limits for the number of intervals and basic block vectors seen in SPEC 2000 with an interval length of 10 million instructions. The second and third columns show the number of intervals and original number of dimensions for each basic block vector. The last two columns show the time it took to execute SimPoint 3.0 searching for the best clustering from *k*=1 to 100, with 5 random initializations (seeds) per *k*. The fourth column shows the time it took to run SimPoint when searching over all *k*, and the last column shows clustering time when using the new binary search described in Section 7.2.3. The results show that increasing the number of intervals by 4 times increased the running time of SimPoint around 10 times. The results also show that the number of intervals clustered has a large impact on the running time of SimPoint, since it can take many iterations to converge, which is the case for `crafty`. We used 15 dimensions during clustering for these results.

The effect of the number of intervals on the running time of SimPoint becomes critical when using very small interval lengths like 1 million instructions or fewer, which can create millions of intervals to cluster. To speed the execution of SimPoint on these very large inputs, we sub-sample the set of intervals that will be clustered, and run *k*-means on only this sample. To sample with SimPoint, the user specifies the number of desired interval samples, and then SimPoint chooses that many intervals (without replacement). The probability of each interval being chosen is proportional to the weight of its interval (the number of dynamically executed instructions it represents). For vectors which all represent the same interval length (as we consider in this paper), this weight is uniform. If vectors represent non-uniform interval lengths (called variable-length intervals, or VLIs), then each vector's weight is proportional to its interval length. We summarize our work with variable length intervals in Section 9.

Sampling is common in clustering for data sets which are too large to fit in main memory (Farnstrom et al., 2000; Provost and Kolluri, 1999). After clustering the data set sample, we have a set of clusters with centers found by *k*-means. SimPoint then makes a single pass through the unclustered intervals and assigns each interval to the cluster that has the nearest center (centroid) to that interval. This then represents the final clustering from which the simulation points are chosen. We originally examined using sub-sampling for variable length intervals (VLI) in Lau et al. (2005a). When using VLIs we had millions of intervals, and had to sub-sample 10,000 to 100,000 intervals for the clustering to achieve a reasonable running time for SimPoint, while still providing very accurate simulation points.

The experiments shown in Figure 9 show the effects of sub-sampling across all the SPEC 2000 benchmarks using an interval length of 10 million instructions, 30 clusters, and 15 projected dimensions. Results are shown for creating the initial clustering using sub-sampling with only 1/8, 1/4, 1/2, and all of the execution intervals in each program, as described above. The first two plots show the effects of sub-sampling on the CPI errors and *k*-means variance, both of which degrade gracefully when smaller samples are used. The average SPEC INT (integer) and SPEC FP (floating point) average results are shown. It is standard to break the results into these two groupings for architecture results. The CPI error is computed in the following manner:

$$\text{CPI Error} = \frac{|\text{True CPI} - \text{SimPoint Estimated CPI}|}{\text{True CPI}}.$$

The average *k*-means variance is the average squared distance between every frequency vector and its closest cluster center. Lower variances are better. When sub-sampling, we still report the variance based on every vector (not just the sub-sampled ones). The *relative* *k*-means variance reported in the experiments is measured on a per-input basis as the ratio of the *k*-means variance for clustering on a sample to that of clustering on the whole input.

As shown in the second graph of Figure 9, sub-sampling a program can cause *k*-means to find a slightly less representative clustering, which results in higher *k*-means variance on average. Note that the *k*-means variance for these experiments are reported on all the input vectors, not just the sampled ones. Even so, when sub-sampling, we found in some cases that it can reduce the *k*-means variance and/or CPI error (compared to using all the vectors), because sub-sampling can remove outliers in the data set that *k*-means may be trying to fit. This is a benefit noted in the work of Fayyad et al. (1998) when they use subsampling to initialize iterative clustering algorithms.

It is interesting to note the difference between floating point and integer programs, as shown in the first two plots. The results shown in the first plot show we can capture the behavior of the SPEC floating point programs more easily, that is, without using all the original data. In addition, the second plot suggests that SPEC floating point programs are also easier to cluster than the SPEC INT, as we can do quite well (in terms of *k*-means variance) even with only small samples. This suggests that they have more regular or uniform code usage patterns than integer programs. The third plot shows the effect of the number of vectors on the running time of SimPoint. This plot shows the time required to cluster all of the benchmark/input combinations and their 3 sub-sampled versions. In addition, we have fit a logarithmic curve with least-squares to the points to give a rough idea of the growth of the run-time. Note that two different data sets with the same number of vectors may require different amounts of time to cluster due to the number of *k*-means iterations required for the clustering to converge.

7.1.2 NUMBER OF DIMENSIONS AND RANDOM PROJECTION

Along with the number of vectors, the other most influential aspect in the running time of *k*-means is the number of dimensions of the data. Figure 10 shows the effect of changing the number of pro-

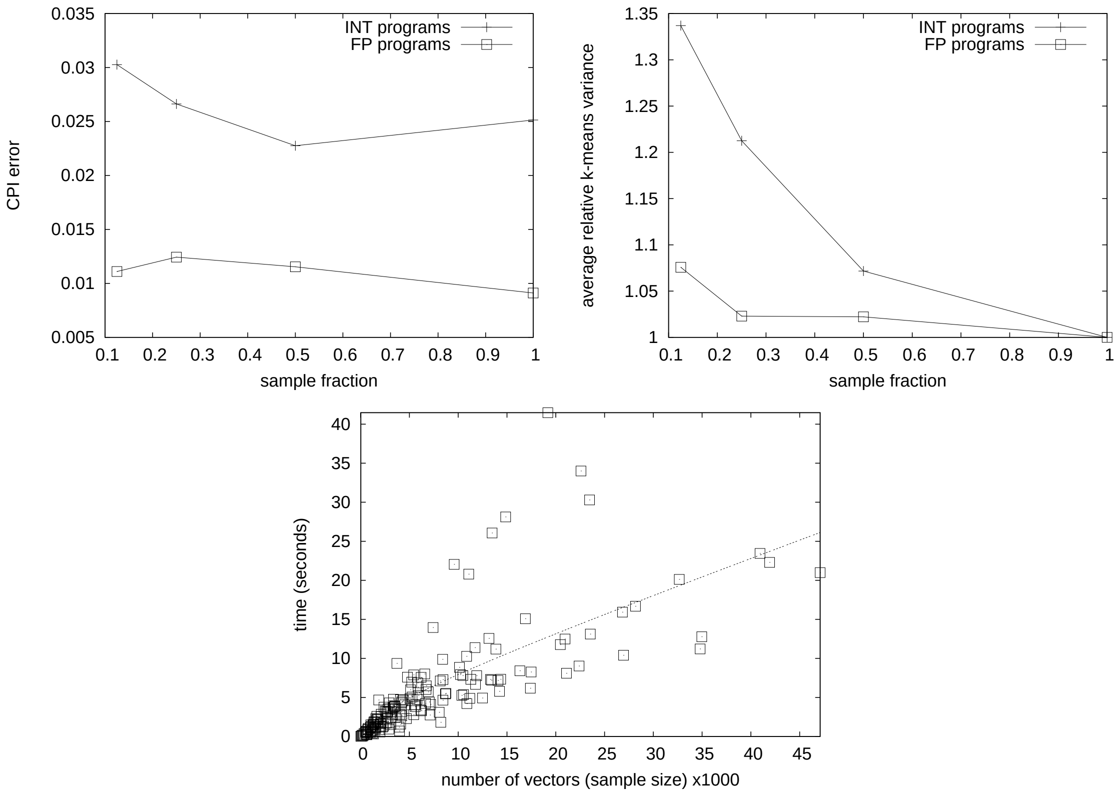


Figure 9: These three plots show how sub-sampling before clustering affects the CPI errors, *k*-means variance, and the run-time of SimPoint. The first plot shows the average CPI error across the integer and floating-point SPEC benchmarks. The second plot shows the average *k*-means clustering variance relative to clustering with all the vectors. The last plot shows a scatter plot of the run-time to cluster the full benchmarks and sub-sampled versions, and a logarithmic curve fit with least squares.

jected dimensions on both the CPI error (left) and the run-time of SimPoint (right). For this experiment, we varied the number of projected dimensions from 1 to 100. As the number of dimensions increases, the time to cluster the vectors increases linearly, as expected. It is more interesting that the run-time also increases for very low dimensions. This is because the points are more "crowded" and the clusters are less well-separated, so *k*-means requires more iterations to converge.

If we use too few dimensions, the data does not retain sufficient information to cluster the data well. This is reflected by the fact that the CPI errors increase rapidly for very low dimensions. However, we can see that at 15 dimensions, the SimPoint default, the CPI errors are quite low, and using a higher number of dimensions does not improve them significantly but requires more computation. Using too many dimensions is also a problem in light of the well-known "curse of dimensionality" (Bellman, 1961), which implies that as the number of dimensions increases, the number of vectors that would be required to densely populate that space grows exponentially. This means that using a higher dimension makes it more likely that a clustering algorithm will converge

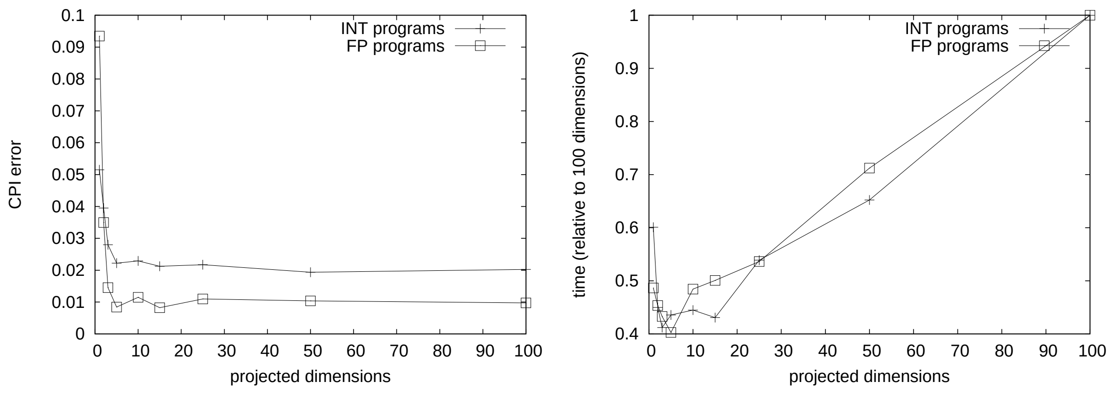


Figure 10: These two plots show the effects of changing the number of projected dimensions when using SimPoint. The default number of projected dimensions SimPoint uses is 15, but here we show results for 1 to 100 dimensions. The left plot shows the average CPI error, and the right plot shows the average time relative to 100 dimensions. Both plots are averaged over all the SPEC 2000 benchmarks, for a fixed $k = 30$ clusters.

to a poor solution, since the input space is not very densely filled. Therefore, it is wise to choose a dimension that is low enough to allow *k*-means to find a good clustering, but not so low that critical information is lost. We find that 15 dimensions works well in these regards.

7.1.3 NUMBER OF ITERATIONS NEEDED

The final aspect we examine for affecting the running time of the *k*-means algorithm is the number of iterations it takes for a run to converge. We provide this analysis to illustrate typical requirements of running SimPoint on a set of benchmarks, and because finding a tight upper-bound on the number of iterations required by *k*-means is an open problem (Dasgupta, 2003), we must rely on evidence to show us what to expect.

The *k*-means algorithm iterates either until it hits a user-specified maximum number of iterations, or until it reaches convergence. In SimPoint, the default limit is 100 iterations, but this can easily be changed. More iterations may be required, especially if the number of intervals is very large compared to the number of clusters. The interaction between the number of intervals and the number of iterations required is the reason for the large SimPoint running time for `crafty-ref` in Table 4.

For our results, we observed that only 1.1% of all runs on all SPEC 2000 benchmarks reach 100 iterations. This experiment was with 10-million instruction intervals, *k*=30, 15 dimensions, and with 10 random initializations of *k*-means. Figure 11 shows the number of iterations required for all runs in this experiment. Out of all of the SPEC program and input combinations run, only `crafty-ref`, `gzip-program`, `perlbmk-splitmail` had runs that had not converged by 100 iterations. The longest-running clusterings for these programs reached convergence in 160, 126, and 101 iterations, respectively. If desired, SimPoint can always run *k*-means to convergence (with no iteration limit).

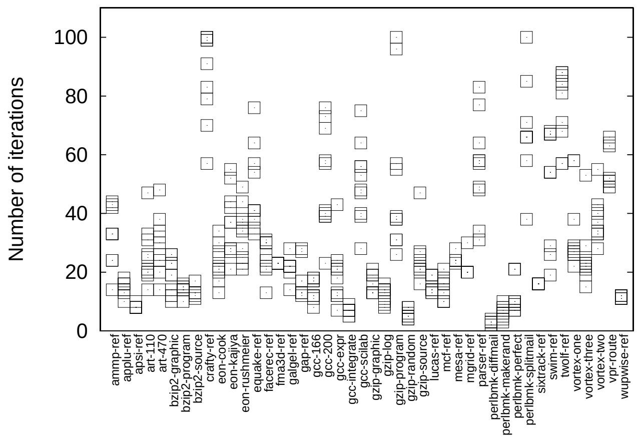


Figure 11: This plot shows the number of iterations required for 10 randomized initializations of each benchmark, with 10 million instruction length intervals, $k = 30$, and 15 dimensions. Note that only three program/inputs had a total of 5 runs that required more than the default limit of 100 iterations, and these all converge within 160 iterations or less.

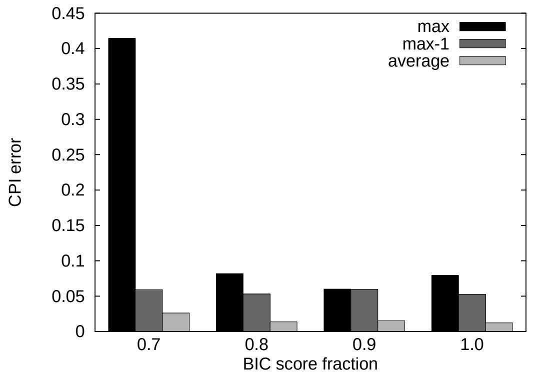
7.2 Searching for a Small *k* with a Good Clustering

We suggest setting the maximum number of clusters K as appropriate for the maximum amount of simulation time a user will tolerate for a single simulation. SimPoint uses three techniques to search over the possible clusterings, which we describe here. The goal is to try to pick a small k so that the number of simulation points is also small, thereby reducing the simulation time required.

7.2.1 SETTING THE BIC PERCENTAGE

As we examine several clusterings and values of k, we need to have a method for choosing the best clustering. The Bayesian Information Criterion (BIC) (Pelleg and Moore, 2000) gives a score of the how well a clustering represents the data it clustered. However, we have observed that the BIC score often increases as the number of clusters increase. Thus choosing the clustering with the highest BIC score can lead to often selecting the clustering with the most clusters. Therefore, we look at the range of BIC scores, and select the score which attains some high percentage of this range. The SimPoint default BIC threshold is 90%. When the BIC rises and then levels off as k increases, this method chooses a clustering with the fewest clusters that is near the maximum BIC value. Choosing a lower BIC threshold would prefer fewer clusters, but at the risk of less accurate simulation.

Figure 12 shows the effect of changing the BIC threshold on both the CPI error (left) and the number of simulation points chosen (right). These experiments are for using binary search (explained in Section 7.2.3) with $K = 30$, 15 dimensions, and 5 random seeds. BIC thresholds of 70%, 80%, 90% and 100% are examined. As the BIC threshold decreases, the average number of simulation points decreases, and similarly the average CPI error increases. At the 70% BIC threshold, `perlbmk-splitmail` has the maximum CPI error in the SPEC suite. This anomaly is an artifact



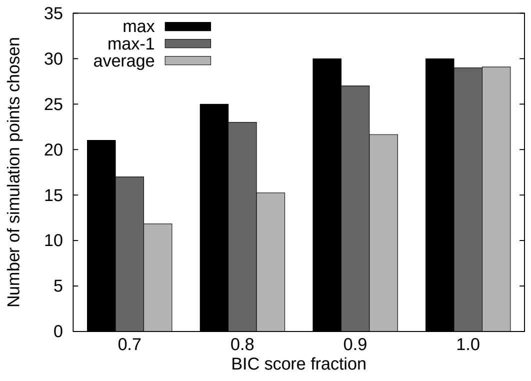


Figure 12: These plots show how the CPI error and number of simulation points chosen are affected by varying the BIC threshold. Bars labeled "max-1" show the second largest value observed.

of the low threshold. Since higher BIC scores point to better clusterings and better error rates, we recommend the BIC threshold to be set at 90%.

7.2.2 Varying the Number of Random Seeds, and *k*-means Initialization

The *k*-means clustering algorithm starts from a randomized initialization, which requires a random seed. Because of this, running *k*-means multiple times can produce very different results depending on the initializations, so *k*-means can sometimes converge to a locally-good solution that is poor compared to the best clustering on the same data for that number of clusters. Therefore, conventional wisdom suggests that it is good to run *k*-means several times using a different randomized starting point each time, and take the best clustering observed, based on the *k*-means variance or the BIC. SimPoint does this, using different random seeds to initialize *k*-means each time. Based on our experience, we have found that using 5 random seeds works well.

SimPoint allows users to provide their own *k*-means initialization, or it will choose an initialization based on one of two methods: sampling and furthest-first (Gonzalez, 1985; Hochbaum and Shmoys, 1985). The sampling method chooses *k* random locations for the initial cluster centers from the input data without replacement. The furthest-first method chooses one input point at random, and then repeatedly chooses a point that is furthest away from all the already-chosen points, until *k* points are chosen. This has the tendency to spread the initially chosen points out along the convex hull of the input space, and subsequently chosen points in the interior.

Figure 13 shows the effect on CPI error of using two different *k*-means initialization methods (furthest-first and sampling) along with different numbers of initial *k*-means seeds. These experiments are for using binary search with $K = 30$, 15 dimensions, and a BIC threshold of 90%. When multiple seeds are used, SimPoint runs *k*-means multiple times with different starting conditions and takes the best result.

Based on these results we see that sampling outperforms furthest-first *k*-means initialization. This can be attributed to the data we are clustering, which can have a large number of outlying points, which furthest-first initialization pays special attention to. The furthest-first method is likely

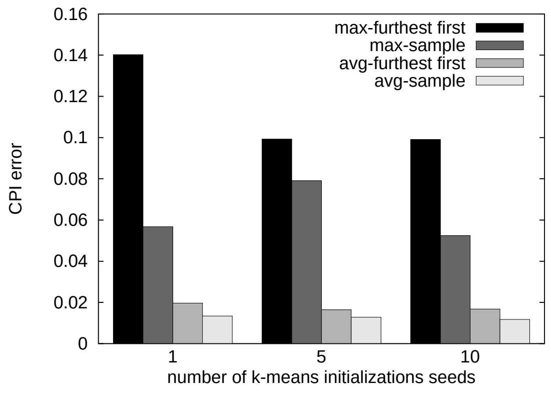


Figure 13: This plot shows the average and maximum CPI errors for both sampling and furthest-first *k*-means initializations, and using 1, 5, or 10 different random seeds. These results are over the SPEC 2000 benchmark suite for 10-million instruction vectors, 15 dimensions, and *k* = 30.

to pick those anomaly points as initial centers since they are the furthest points apart. It is also beneficial to try multiple seed initializations in order to avoid a locally minimal solution. The results in Figure 13 shows that 5 seed initializations should be sufficient in finding good clusterings.

7.2.3 BINARY SEARCH FOR PICKING *k*

SimPoint 3.0 makes it much faster to find the best clustering and simulation points for a program trace over earlier versions. Since the BIC score generally increases as *k* increases, SimPoint 3.0 uses this knowledge to perform a binary search for the best *k*. For example, if the maximum *k* desired is 100, with earlier versions of SimPoint one might search in increments of 5: $k = 5, 10, 15, \ldots, 90, 100$, requiring 20 clusterings. With the binary search method, we can ignore large parts of the set of possible *k* values and examine only about 7 clusterings.

The binary search method first clusters 3 times: at $k = 1$, $k = K$, and $k = (K+1)/2$. It then proceeds to divide the search space and cluster again based on the BIC scores observed for each clustering and the user-specified BIC threshold. Thus the binary search method requires the user only to specify the maximum number of clusters K, and performs at most $\log_2(K)$ clusterings.

Figure 14 shows the comparison between the new binary search method for choosing the best clustering, and the old method, which searched over all *k* values in the same range. The top graph shows the CPI error for each program, and the bottom graph shows the number of simulation points (clusters) chosen. These experiments are for using binary search with $K = 30$, 15 dimensions, 5 random seeds, and a BIC threshold of 90%. Exhaustive search performs slightly better than binary search, since it searches all *k* values. Using the binary search, it possible that it will not find a clustering with as few clusters as found by the exhaustive search. This is shown in the bottom graph of Figure 14, where the exhaustive search picked 19 simulation points on average, and binary search chose 22 simulation points on average. In terms of CPI error rates, the average is about the same across the SPEC programs between exhaustive and binary search. Recall that the binary search

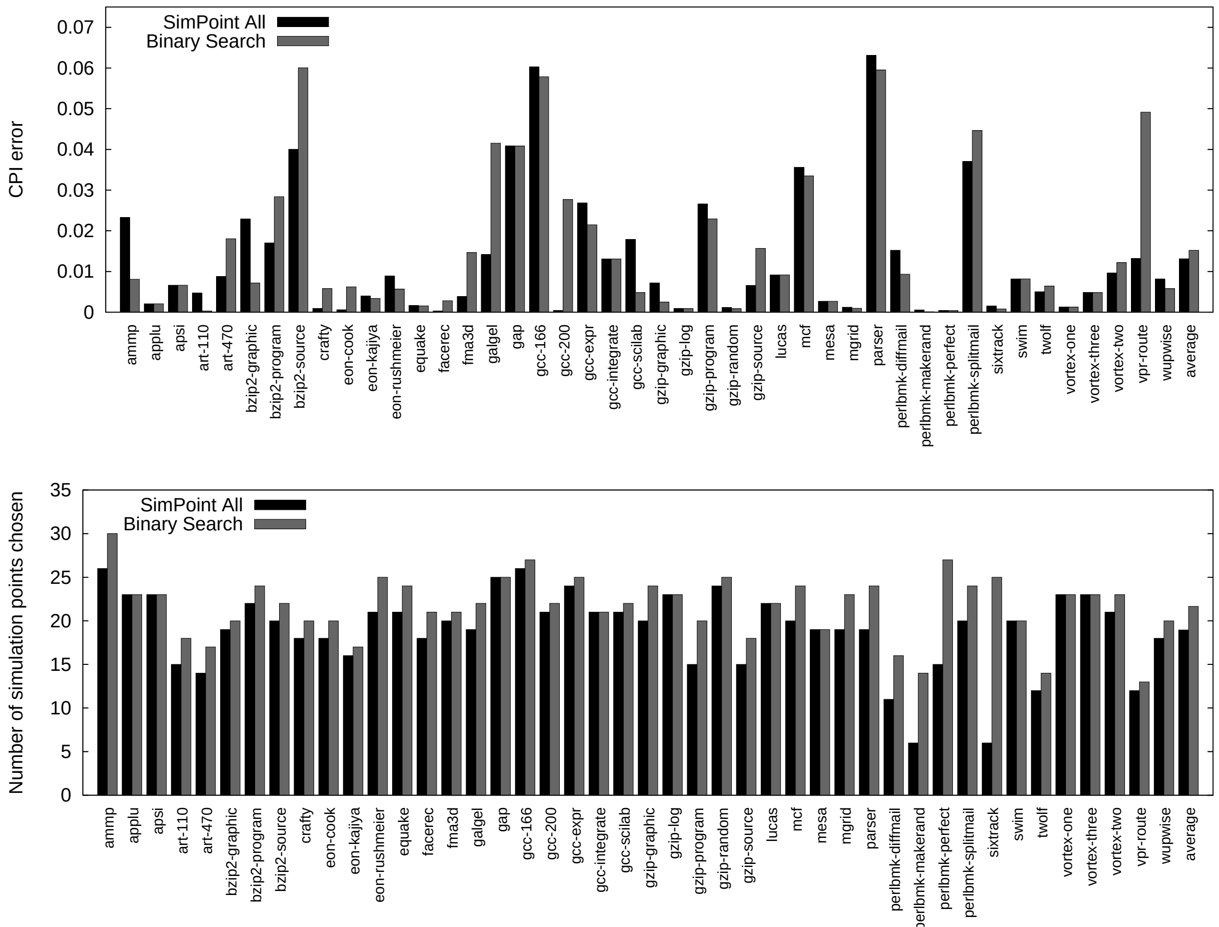


Figure 14: These plots show the CPI error and number of simulation points chosen for two different ways of searching for the best clustering. The first method, which was used in SimPoint 2.0, searches over all k between 1 and 30, and chooses the smallest clustering that achieves the BIC threshold of 90%. The second method is the binary search for $K = 30$, which examines at most 5 clusterings.

method operates many times faster than the brute force search method (see Table 4 for some timing results).

As we can see from the graphs in Figure 14, SimPoint is able to achieve a 1.5% CPI error rate averaged across all SPEC 2000 benchmarks, with a maximum error of around 6%. These results require an average simulation time of about 220 million instructions per program (for the binary search method). These error rates are sufficiently low to make design decisions, and the simulation time is small enough to do large-scale design space explorations.

8. Related Machine Learning Work on Phase Analysis

SimPoint is the first research to apply machine learning techniques (*k*-means, dimension reduction, BIC) to the problem of program phase analysis and workload performance prediction. Recently two other clustering techniques have been examined for SimPoint, which are multinomial clustering (Sanghai et al., 2005) and regression trees (Annavaram et al., 2004). Neither of these perform better than SimPoint with *k*-means clustering.

Sanghai et al. (2005) proposed utilizing mixtures of multinomials trained by EM to cluster program intervals. Unlike a *k*-means cluster, the multinomial is a probability model that explicitly models each dimension. Multinomials are used frequently in machine learning for modeling and clustering text documents, which are high-dimensional and sparse, much like the data we see in program analysis using basic block vectors. Sanghai et al. used a mixture of multinomial models to cluster the program data, and formulated a version of the BIC that applies to multinomial models. They also considered dimension reduction via a different construction of random linear projection. Their random linear projection is based on a sparse matrix where each value may be 0 or 1 (rather than real-valued). This is similar to what Achlioptas (2001) proposed for "database-friendly" projections. Following on their proposed model, we have done a full comparison of multinomial mixtures with *k*-means (Hamerly et al., 2006), and we found that *k*-means performs better for program phase analysis, but that multinomials have some benefits. We summarize that work in Section 9.

Annavaram et al. (2004) employed a regression tree clustering algorithm to predict performance for database applications and SPEC2000. Code signatures were generated through periodic sampling with a tool called VTune that samples the hardware counters. In addition to code signatures, the CPI for each interval of execution was sampled. This is a necessary parameter in the regression tree algorithm. The code signatures are divided into two groups based on the split that would minimize the variance in the CPI for the corresponding execution intervals. Subsequently, each new group is split again based on the same criteria and this is repeated recursively until no more splits can be made. To reduce complexity, up to 50 splits were applied on the data (Annavaram et al., 2004). To determine the number of clusters to be used from the data, a cross-validation step is applied with reserved CPI data that was not used in the splitting process.

The regression tree method may be effective in reducing the variance of CPI within clusters, but the need for CPI in computing clusters is a drawback. It is computationally expensive to compute the CPI for the entire execution of a program via simulation. In addition, the use of CPI data from one architecture configuration to form clusters would bind that clustering to that particular configuration. A different architecture configuration which may produce different CPI values would not necessarily fit under the former clustering formation; thus the method is not architecture independent. The *k*-Means approach employed in SimPoint uses only the code signatures to form clusters, which results in an architecture independent representation that is applicable across many configurations as shown in Section 6.

9. Current Directions

In this section we describe some of our current and future directions for phase analysis.

9.1 Matching Simulation Points to Code Boundaries

With the original SimPoint approach, representatives selected for simulation are identified by dynamic instruction count using fixed length intervals. For example, SimPoint may tell the user to start detailed simulation when 5,000,000 instructions have executed, and stop just before 6,000,000 instructions have executed, using an interval size of 1,000,000 instructions. This ties the simulation points to that specific binary, but the idea of SimPoint should be applicable across different compilations of the same source code. The same phase behavior should occur, though perhaps with different code patterns. If we can identify these behaviors and map them back to the source code level, then we could use the same phase analysis for a program compiled for different compiler optimizations or even architectures with different instruction sets. This will allow us to examine the exact same set of simulation points across different compilations of the same source code.

To address this, we propose breaking the program's execution up at procedure call and loop boundaries instead of breaking up the program's execution using fixed length intervals. Programs exhibit patterns of repetitive behavior, and these patterns are largely due to procedure call and looping behavior. Our software phase marker approach (Lau et al., 2006) detects recurring call chains and looping patterns and identifies the source code instructions to which they correspond. We then mark specific procedure calls and loop branches, so that when they occur during execution, they will indicate the end of one code signature (interval boundary) and the start of another. Therefore, instead of using fixed-length intervals with some fixed number of instructions, intervals are defined by procedure and loop boundaries. This results in *Variable Length Intervals* (VLIs) of execution.

To support VLIs, we had to modify the SimPoint software to allow sub-sampling (since we may be dealing with a huge number of intervals), and clustering with variable-length intervals (Lau et al., 2005a), where the weights of each interval are taken into consideration during the *k*-means clustering. An interesting machine-learning result of clustering variable-length intervals is how we modified the likelihood calculated for the BIC to allow it to consider the length of each interval. Because we view longer intervals as more important than shorter ones, the likelihood should reflect this. Therefore, we reformulate the likelihood we present in this paper to be appropriate for variable-length intervals. When the interval length is uniform, the modified BIC gives the same answer as the BIC presented in this paper.

The accuracy and simulation time results for software phase markers with VLIs are similar to fixed-length-interval SimPoint. Therefore the main advantage of the phase marker approach is portability of the phase analysis across compilations and architectures. In prior work (Lau et al., 2005a), we also showed that there is a clear hierarchy of phase behaviors, from fine-grained to coarse-grained depending upon the interval sizes used, and there is still future research to be done to determine how to pick the correct granularity for the target use of the phase analysis.

9.2 Multinomial Clustering

Recently, Sanghai et al. (2005) proposed using a mixture of multinomial models as a clustering model for phase analysis, as described in Section 8. Their research was a preliminary study; we have performed a more complete set of experiments comparing multinomial clustering with EM to the *k*-means algorithm, as applied to phase analysis (Hamerly et al., 2006).

We found that multinomial clustering does not improve upon *k*-means clustering in terms of performance prediction, despite the fact that basic block vectors seem to be a natural fit to multinomials. We also showed a comparison between different projection methods in conjunction with multinomial clustering, and alternative methods of choosing the sample to simulate from each cluster. Further, we verified Sanghai et al.'s claim that the number of dimensions required to get good results using multinomial clustering may be much higher than the 15 dimensions we use with *k*-means. Following their work, we used up to 100 projected dimensions to find clustering results that work well for phase analysis with this approach.

We also found that EM clustering is much slower than *k*-means. The hard assignment of *k*-means enables optimizations like partial distance search described in Section 7.1. But for EM clustering, its soft assignment requires that we cannot stop short on examining any dimensions, so it cannot benefit from such optimizations. This together with the increase in number of dimensions required by multinomials makes multinomial EM clustering much slower than *k*-means. Even if we use the same number of dimensions to randomly project to, we still find that EM clustering of multinomials is roughly 10 times slower than *k*-means.

We did find that there are some benefits to using multinomials. One benefit is that multinomial clustering tends to choose fewer clusters on average (according to a BIC score formulated for multinomial mixtures), resulting in lower simulation times. Another benefit is that the EM algorithm uses soft assignment, unlike the hard assignment of *k*-means. This allows us to derive a metric of cluster "purity". The idea is that if many vectors have high membership in multiple clusters, then the clustering is more impure than if each vector (interval) belongs mostly to only one of the clusters. This purity score allows us to see if multinomial clustering is a good solution for a particular data set, and gives us a metric for deciding whether to apply multinomial clustering if the purity score is high enough, or *k*-means otherwise. We found that this combined approach provides a solution which picks fewer simulation points compared with using only *k*-means, and gets lower prediction errors than using only multinomial clustering.

10. Summary

Understanding the cycle level behavior of a processor running an application is crucial to modern computer architecture research, and gaining this understanding can be done efficiently by judiciously applying detailed cycle level simulation to only a few simulation points. By targeting only one or a few carefully chosen samples for each of the small number of behaviors found in real programs, the cost of simulation can be reduced to a reasonable level while achieving very accurate performance estimates.

The main idea behind SimPoint is the realization that programs typically only exhibit a few unique behaviors which are interleaved with one another through time. By finding these behaviors and then determining the relative importance of each one, we can maintain both a high level picture of the program's execution and at the same time quantify the cycle level interaction between the application and the architecture. The key to being able to find these phases in a efficient and robust manner is the development of a metric that can detect the underlying shifts in a program's execution that result in the changes in observed behavior. In this paper we have discussed one such method of quantifying executed code similarity, and use it to find program phases through the application of unsupervised learning techniques.

The methods described in this paper are distributed as part of SimPoint (Perelman et al., 2003; Sherwood et al., 2002). SimPoint automates the process of picking simulation points using an off-line phase classification algorithm based on *k*-means clustering, which significantly reduces the amount of simulation time required. Selecting and simulating only a handful of *intelligently* picked sections of the full program provides an accurate picture of the complete execution of a program, which gives a highly accurate estimate of performance. The SimPoint software can be downloaded at:

`http://www.cse.ucsd.edu/users/calder/simpoint/`

For the industry-standard SPEC programs, SimPoint has less than a 6% error rate (2% on average) for the results in this paper, and is 1,500 times faster on average than performing simulation for the complete program's execution. Because of this time savings and accuracy, our approach is currently used by architecture researchers and industry companies (e.g. Patil et al. (2004) at Intel) to guide their architecture design exploration.

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