A benchmark suite and performance analysis of user-space provenance collectors

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1 BACKGROUND

Computational provenance, "the computational input artifacts and computational processes that influenced a certain computational output artifact" [20], has many potential applications, including the following from Pimentel et al. [46] and Sar and Cao [50]:

1. **Reproducibility**. A description of the inputs and processes used to generate a specific output can aid manual and automatic reproduction of that output[1]. Lack of reproducibility in computational experiments undermines the long-term credibility of science and hinders the day-to-day work of researchers. Empirical studies [17, 23, 57, 62] show that reproducibility is rarely achieved in practice, probably due to its difficulty under the short time budget that scientists have available to spend on reproducibility. If reproducibility was easier to attain, perhaps because of automatic provenance tracking, it may improve the reproducibility rate of computational research.
   - **Manual reproducibility**. Provenance data improves manual reproducibility, because users have a record of the inputs, outputs, and processes used to create a computational artifact.
   - **Automatic reproducibility**. Provenance data also has the potential to enable automatic reproducibility, if the process trace is detailed enough to be "re-executed". This idea is also called "software record/replay". However, not all provenance collectors make this their goal.
2. **Caching subsequent re-executions**. Computational science inquiries often involve changing some code and re-executing the workflows (e.g., testing different clustering algorithms). In these cases, the user has to keep track of what parts of the code they changed, and which process have to be re-executed. However, an automated system could read the computational provenance graphs produced by previous executions, look at what parts of the code changed, and safely decide what processes need to be re-executed. The dependency graph would be automatically deduced, leaving less chance for a dependency-misspecification, unlike Make and CMake, which require the user to manually specify a dependency graph.
3. **Comprehension**. Provenance helps the user understand and document workflows. An automated tool that consumes provenance can answer queries like "What version of the data did I use for this figure?" and "Does this workflow include FERPA-protected data?".
4. **Data cataloging**. Provenance data can help catalog, label, and recall experimental results based on the input parameters. For example, a user might have run dozens of different versions of their workflow, and they may want to ask an automated system, "show me the results I previously computed based on that data with this algorithm?".
5. **Space compression**. If the provenance of a particular artifact is known, the artifact may be able to be deleted to save space, and regenerated when needed. Historically, as computing systems has improved, a later regeneration takes less time than the original.

There are three high-level methods by which one can capture computational provenance: 1) by modifying an application to report

[1] "Reproduction", in the ACM sense, where a **different team** uses the **same artifacts** to generate the output artifact [6].

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provenance data, 2) by leveraging a workflow engine or programming language to report provenance data, and 3) by leveraging an operating system to emit provenance data to report provenance data [20].

- **Application-level** provenance is the most semantically rich, since it knows the use of each input at the application-level (see Section 1), but the least general, since each application would have to be modified individually.
- **Workflow-level** or **language-level** provenance is a middle ground in semantic richness and generality; it only knows the use of inputs in a dataflow sense (see Section 1), but all applications using the provenance-modified workflow engine or programming language would emit provenance data without themselves being modified to emit provenance data.
- **System-level** is the most general, since all applications on the system would emit provenance data, but it is the least semantically rich, since observed dependencies may overapproximate the true dependencies (see Section 1 and Section 1). System-level provenance collectors may be implemented in **kernel-space** or in **user-space**. Since kernel-space provenance collectors modify internals of the Linux kernel, keeping them up-to-date as the kernel changes is a significant maintenance burden. High-security national labs may be wary of including a patched kernel. On the other hand, user-space collectors compromise performance in exchange for requiring less maintenance and less privilege.

One may imagine an abstract tradeoff curve between "enabling provenance applications such as reproducibility" as the horizontal axis increasing rightwards and "cost of implementation" that provenance data on the vertical axis increasing upwards). A typical status quo, not collecting any provenance data and not using workflows, is at the bottom left: no added cost and does nothing to enable provenance applications. System-level, workflow/language-level, and application-level are on a curve, increasing cost and enabling more provenance applications.

The implementation cost in adopting system-level provenance in a project which currently has no provenance is low because the user need not change *anything* about their application; they merely need to install some provenance tracer onto their system and run their code, without modifying it, in the tracer. [2] Perceived ease of use is a critical factor in the adoption of new technologies (formalized in the Technology Acceptance Model [18]). Although the user may eventually use more semantically rich provenance, low-initial-cost system-level provenance would get provenance's "foot in the door". While this data is less rich than that of the workflow or application level, it may be enough to enable important applications such as reproducibility, caching, etc. Since system-level provenance collection is a possibly valuable tradeoff between implementation cost and enabling provenance applications, system-level provenance will be the subject of this work.

[2] DSK: what about the performance penalty? Since you talk about performance in contributions, I think you have to introduce it here. SAG: This is referring to the "cost of switching from no-prov to prov", which is low, and I'm only using this argument to explain why I look at system-level over the others. Performance overhead between system-level tools is a concern that I will address later on. DSK: maybe add a word ("implementation"?) before cost to say which cost is meant here?

While there is little added human overhead in using system-level provenance (no user code change), there is a non-trivial implicit overhead in monitoring and recording each computational process. Even a minor overhead per I/O operation would become significant when amplified over the tens of thousands of I/O operations that a program might execute per second.

Prior publications in system-level provenance usually contains some benchmark programs to evaluate the overhead imposed by the system-level provenance tool. However, the set of chosen benchmark programs are not consistent from one publication to another, and overhead can be extermely sensitive to the exact choice of benchmark, so these results are totally incomparable between publications. Most publications only benchmark their new system against native/no-provenance, so prior work cannot easily establish which system-level provenance tool is the fastest.

2 CONTRIBUTIONS

This work aims to summarize state of the art, establish goalposts for future research in the area, and identify which provenance tools are practically usable. [3]

This work contributes:

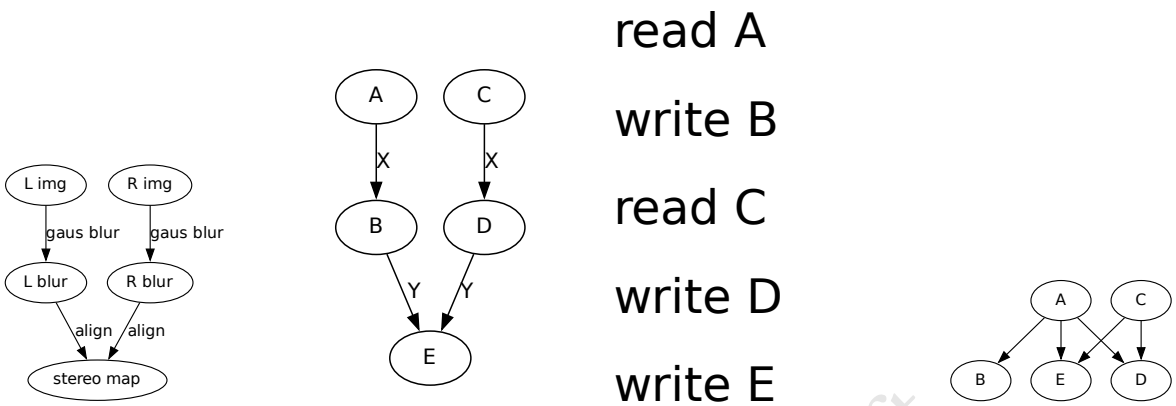
- **A rapid review**: There are scores of academic publications on system-level provenance (see Table 2). We collate as many provenance tools as possible [4] and classify them by *capture method* (e.g., does the provenance collector require you to load a kernel module or run your code in a VM?).
- **A benchmark suite**: Prior work does not use a consistent set of benchmarks; often publications use an overlapping set of benchmarks from prior work. We collate benchmarks used in prior work, add some unrepresented areas, and find a statistically valid subset of the benchmark.
- **A quantitative performance comparison**: Prior publications often only compares the performance their provenance tool to the baseline, no-provenance performance, not to other provenance tools. It is difficult to compare provenance tools, given data of different benchmarks on different machines. We run a consistent set of benchmarks on a single machine over all provenance tools.
- **A predictive performance model**: The performance overhead of a single provenance collector varies from <1% to 23% [42] based on the application, so a single number for overhead is not sufficient. We develop a statistical model for predicting the overhead of $X application in $Y provenance collector based on $Y provenance collector's performance on our benchmark suite and $X application's performance characteristics (e.g., number of I/O syscalls).

3 METHODS

3.1 Rapid Review

We began a rapid review to identify the research state-of-the-art tools for automatic system-level provenance.

[3] DSK: usable globally or perhaps in particular situations?
[4] DSK: as possible is problematic, probably need to rephrase



(a) Application-level provenance has the most semantic information. **(b) Workflow-level provenance has an intermediate amount of semantic information.** **(c) System-level log of I/O operations.** **(d) System-level provenance, inferred from the log in Section 1, has the least amount of semantic information**

Figure 1: Several provenance graphs collected at different levels for the same application.

Rapid Reviews are a lighter-weight alternative to systematic literature reviews with a focus on timely feedback for decision-making. Schünemann and Moja [51] show that Rapid Reviews can yield substantially similar results to a systematic literature review, albeit with less detail. Although developed in medicine, Cartaxo et al. show that Rapid Reviews are useful for informing software engineering design decisions [13, 14].

We conducted a rapid review with the following parameters:

- **Objective**: Identify system-level provenance collection tools.
- **Search terms**: "system-level" AND "provenance"
- **Search engine**: Google Scholar
- **Number of results**: 50
  - This threshold is the point of diminishing returns, as no new tools came up in the 40th – 50th results.
- **Criteria**: A relevant publication would center on one or more operating system-level tools that capture file provenance. A tool requiring that the user use a specific application or platform would be irrelevant.

We record the following features for each system-level provenance tool:

- **Capture method**: What method does the tool use to capture provenance?
  - **User-level tracing**: A provenance tool may use "debugging" or "tracing" features provided by the kernel, e.g., `ptrace(2)` [4], to trace another program's I/O operations.
  - **Built-in auditing service**: A provenance tool may use auditing service built in to the kernel, e.g., Linux Auditing Framework [39], enhanced Berkeley Packet Filter (eBPF) [2], kprobes [31], and ETW [5] for Windows.
  - **Filesystem instrumentation**: A provenance tool may set up a file system, so it can log I/O operations, e.g., using Filesystem in User SpacE (FUSE) interface [3], or Virtual File System (VFS) interface [22].
  - **Dynamic library instrumentation**: A provenance tool may replace a library used to execute I/O operations (e.g., glibc) with one that logs the calls before executing them.
  - **Binary instrumentation**: A provenance tool may use binary instrumentation (dynamic or static) to identify I/O operations in another program.
  - **Compile-time instrumentation**: A provenance tool may be a compiler pass that modifies the program to emit provenance data, especially intra-program control flow.
  - **Kernel instrumentation**: A provenance tool may be a modified kernel either by directly modifying and recompiling the kernel's source tree.
  - **Kernel module**: Rather than directly modify the kernel's source, the provenance tool may simply require that the user load a custom kernel module.
  - **VM instrumentation**: A provenance tool may execute the program in a virtual machine, where it can observe the program's I/O operations.

3.2 Benchmark Selection

Using the tools selected above, we identified all benchmarks that have been used in prior work. We excluded benchmarks for which we could not even find the original program (e.g., TextTransfer), benchmarks that were not available for Linux (e.g., Internet Explorer), benchmarks with a graphical component (e.g., Notepad++), or benchmarks with an interactive component (e.g., GNU Midnight Commander).

We implemented the benchmarks as packages for the Nix package manager[5], so they are runnable on many different platforms.

[5] See https://nixos.org/guides/how-nix-works

Table 1: Our experimental machine description.

Name	Value
CPU	11th Gen Intel(R) Core(TM) i7-1165G7 @ 2.80GHz
RAM	16 GiB of SODIMM DDR4 Synchronous 2400 MHz
Kernel	Linux 6.1.64

Nix has official installers for Linux, Mac OS X, and Windows Subsystem for Linux on i686, x86_64, and aarch64 architectures, but FreeBSD and OpenBSD both package Nix themselves, and it can likely be built from source on even more platforms.

We also added new benchmarks:

- **Data science**: None of the benchmarks resembled a typical data science program, so we added the most popular Notebooks from Kaggle.com, a data science competition website.
- **Compilations**: Prior work uses compilation of Apache or of Linux. We added compilation of several other packages (any package in Spack) to our benchmark. Compiling packages is a good use-case for a provenance tracer, because a user might trial-and-error multiple compile commands and not remember the exact sequence of "correct" commands; the provenance tracker would be able to recall the commands which did not get overwritten, so the user can know what commands "actually worked". [6]

3.3 Performance Experiment

To get consistent measurements, we select as many benchmarks and provenance tracers as we reasonably can, and run a complete matrix (every tracer on every benchmark). Table 1 describes our experimental machine. We use BenchExec [11] to precisely measure the CPU time, wall time, memory utilization, and other attributes of the process (including child processes) in a Linux CGroup without networking, isolated from other processes on the system.

3.4 Benchmark Subsetting

We implemented and ran many different benchmarks, which may be costly for future researchers seeking to evaluate new provenance collector. Given the less-costly results of a small number of benchmarks, one may be able to predict the performance of the rest of the benchmarks. [ˆDSK: grammar in prev sentence needs work.]

In order to find the best subset (most predictive value), we will try several methods and several different k (subset sizes) to identify the most important benchmarks, keeping the ones that perform best. We will feed the algorithms the quantitative features of each benchmark. We stick to features that are invariant between running a program ten times and running it once. This gives long benchmarks and short benchmarks which exercise the same functionality similar feature vectors. In particular, we use

- The log overhead ratio of running the benchmark in each provenance collectors.
- The ratio of CPU time to wall time.
- The number of syscalls in each category per wall time second, where the categories consist of socket-related syscalls, syscalls that read file metadata, syscalls that write file metadata, syscalls that access the directory structure, syscalls that access file contents, exec-related syscalls, clone-related syscalls, exit-related syscalls, dup-related syscalls, pipe-related syscalls, close syscalls, pipe-related syscalls, and chdir syscalls.

We use the following algorithms:

- **Principal component analysis (PCA) and K-means**. This is the traditional benchmark subsetting procedure evaluated by Yi et al. [60].
  1. We form a matrix of all benchmarks by "observed features" of that benchmark.
  2. We apply PCA to that matrix. PCA is a mathematical procedure that combines a large number of "observed features" into smaller number "virtual features", linearly, while maximizing the amount of variance in the resulting "virtual space" (in a sense, spreading out the benchmarks as much as possible from each other).
  3. We apply K-means to the benchmarks in their reduced PCA-space. K-means is a fast clustering algorithm. Once the benchmarks are grouped into clusters, we identify one benchmark from each of the k clusters to consist the benchmark subset.
- **Interpolative decomposition (ID)**.
  1. We form a matrix where each benchmark is a column, each provenance collector is a row, and the elements contain the log of the overhead ratio from the provenance collector to native.
  2. We apply ID to the matrix. ID seeks to estimate a $m \times n$ matrix by retaining k of its columns and using a linear regression to estimate the remaining $n - k$ from those selected k columns, sweeping on k. Cheng et al. [15] give a $O(k(m + n - k))$ algorithm for computing an optimal ID while keeping a reasonable[7] L2 norm of the difference between the estimated and actual columns. Cheng's procedure is implemented in `scipy.linalg.interpolative`[8].
  3. We select the k benchmarks corresponding to columns chosen by ID; these are the "best" k columns which minimize the error when predicting the $n - k$ columns under a specific metric.
- **Random search**. Random search proceeds like ID, but it selects k benchmarks randomly. Like ID, it computes a linear predictor for the $m - k$ benchmarks based on the k benchmarks. Then it evaluates the "goodness of fit" of that predictor, and repeats a fixed number of iterations, retaining the "best" k benchmark subset.

Cross-validation proceeds in the following manner, given m provenance collectors, n benchmarks, and f features:

1. Separate 1 provenance collector for testing from the $m - 1$ provenance collectors used for training.

[6] DSK: this reminds me of VisTrails from Utah

[7] The best possible error for any rank-k factorization of a matrix is given by the $(k+1)^{\text{th}}$ singular value. Since ID constrains the space of permissible factors, the L2 loss will be at least that. Cheng et al.'s ID method guarantees an error within a $\sqrt{1 + k(min(m, n) - k)}$ factor of the $(k+1)^{\text{th}}$ singular value. Read asymptotically, the bound asserts as the singular value decreases, so too does the L2 loss.

[8] See https://docs.scipy.org/doc/scipy/reference/linalg.interpolative.html

2. Use the $(m-1) \times n$ training systems and $f \times n$ in one of the above algorithms to select the best $k < n$ benchmarks and compute predictors for the $n - k$ benchmarks.
3. Feed in the output of the $1 \times k$ testing provenance collector on the selected k benchmarks into the algorithm, and let the algorithm estimate the $n - k$ unselected benchmarks.
4. Score the difference between the algorithm's prediction of the test system on the $n - k$ unselected benchmarks and its actual performance.
5. Repeat to 1 until all systems have been used for testing.

Note that during cross-validation, testing data (used in step 4) must not be allowed to "leak" into the training phase (step 2). For example, it would be invalid to do feature selection on all $m \times n$ data. Cross-validation is supposed to simulate the situation where one is testing on *truly novel* data.

We evaluate these methods based on cross-validated root mean square-error (RMSE). Mean *square* error (MSE) is preferable to mean *absolute* error (MAE) because it punishes outliers more. Imagine a benchmark suite that minimizes MAE and another that minimizes MSE. The MAE-minizing suite one might be very accurate for most provenance collectors, but egregiously wrong for a few; a MSE-minizing suite may be "more wrong" on average, but the worst-case wouldn't be as bad as the MAE one. As such, an MSE subset would be more practically useful for future publictions to benchmark their new provenance collectors.

We score the model on its ability to predict the logarithm of the ratio between a program running in provenance-generating and native systems. We use a ratio rather than the absolute difference because the runtimes of various benchmark spans multiple orders of magnitude. We predict the logarithm of the ratio, rather than the ratio directly because the ratio is multiplicative. Any real number is permissible; 0 indicates "nothing changed", 1 indicates a speedup by a certain factor, and -1 indicates a slowdown *by the same factor.*

While cross-validation does punish model-complexity and overfitting to some extent, we will still take the number of parameters into account when deciding the "best" model in the interest of epistemic modesty. Preferring fewer parameters makes the model more generalizable on out-of-domain data, since even our full cross-validation data is necessarily incomplete.

3.5 Performance Model

A related problem to subsetting is inferring a performance model. There are two motivations for inferring a performance model:

- A sysadmin may wish to provide a computational provenance capturing system to their institution, but getting approval to run new software on their system may be expensive (e.g., on highly secure systems, the sysadmin may need to acquire a security audit of the code before it can be approved for use). They may want to prospectively estimate the overhead of provenance collectors without having to install all the provenance collectors on their system, so they can select the optimal collector for their use-case.
- Inferring a provenance model may improve our understanding of the bottlenecks in provenance collectors.

A performance model should input features of a prospective workload and output the approximate overhead under different systems. A priori, provenance collectors put a "tax" on certain syscalls (e.g., file I/O operations, process forks, process execs), because the system has to intercept and record these Therefore, we expect a low-dimensional linear model (perhaps number of I/O operations per second times a weight plus number of forks per second times another weight) would predict overhead optimally. To estimate this, we use the following models:

- **Ordinary least-squares (OLS) linear regression**. We estimate the runtime of each benchmark on each provenance collector as a linear regression of the features of each benchmark, learning weights for each feature in each provenance collector using ordinary least-squares. This would create a model like $\text{weight}_1 \cdot \text{feature}_1 + \text{weight}_2 \cdot \text{feature}_2 + \cdots$ However, we can reduced its number of parameters, and thereby increase its out-of-domain generalizability, by the next two methods.
- **Low-rank linear regression.** To further reduce the number of parameters, we apply singular value decomposition (SVD) to create a lossily-compressed representation of the learned weights. TODO: describe this model
- **OLS on a subset of features.** This method proceeds like the OLS regression, except it only uses a subset of the features, ignoring the rest. This is like doing a LASSO regression, but with multiple linear predictors sharing the same set of features (LASSO is usually described as solving for just one linear predictor). Unfortunately, we do not know an efficient algorithm like ID for selecting this subset. We tried two algorithms: greedy, which picks one additional feature that decreases loss the most until it has k features, and random, which selects a random k-sized subset.

We use as features:

- The number of $x-syscalls made per walltime second, where $x could be socket-related, file-related, reading-file-metadata, chmod, exec, clone, etc.
- The number of syscalls per walltime second
- The amount of CPU time used per walltime second
- A constant fixed-cost per-execution

Similarly to benchmark minimization, we use cross-validated RMSE errors in log of overhead ratio and the number of features in each model to select the best. [^DSK: grammar in prev sentence needs work.]

4 RESULTS

4.1 Selected Provenance Collectors

Table 2 shows the provenance collectors we collected and their qualitative features. The last column in the table categorizes the "state" of that provenance collector in this work into one of the following:

- **Not for Linux.** Our systems are Linux-based and Linux is used by many computational scientists. Therefore, we did not try to reproduce systems which were not Linux based.
- **VMs too slow.** Some provenance collectors require running the code in a virtual machine. We know a priori that these

methods are prohibitively slow, with Panorama reporting 20x average overhead [61]. The provenance systems we are interested in have overheads in the 1.01x – 3x range. [ˆDSK: maybe say instead that we don't use prov systems that have VM overheads over 3x?]

- **Requires recompilation.** Some provenance collectors require the user to recompile their entire application and library stack. This is prohibitively onerous and negates the otherwise low cost of switching to system-level provenance we are pursuing.
- **Requires special hardware.** Some methods require certain CPUs, e.g., Intel CPUs for a dynamic instrumention tool called Intel PIN. Being limited to certain CPUs violates our goal of promulgating reproducibility to as many people as possible.
- **No source.** We searched the original papers, GitHub, BitBucket, Google, and emailed the first author (CCing the others). If we still could not find the source code for a particular provenance collector, we cannot reproduce it. Note, however, that RecProv is implemented using rr, so we can use rr as a lower-bound for RecProv.
- **Requires custom kernel (Hi-Fi, LPM/ProvMon, CamFlow).** Collectors which modify Linux kernel code are out-of-scope for this work due to their increased maintenance overhead, security risk, and difficulty of system administration. Indeed, many of the systems are too old to be usable: LPM/ProvMon is a patch-set for Linux 2.6.32 (reached end-of-life 2016), Hi-Fi is a patch-set for Linux 3.2 (reached end-of-life in 2018). On the other hand, SingularityCE/Apptainer require Linux ≥ 3.8 for user namespaces.
- **Not reproducible (OPUS).** We tried to get this provenance system to run, with several weeks of effort: we emailed the original authors and other authors who used this system, and we left a GitHub issue describing the expected and actual results [9]. However, we still could not get the system to run properly.
- **Needs more time (DTrace, SPADE, eBPF/bpftrace).** We simply needed more time to implement these provenance collectors.
- **Reproduced/excluded (ltrace).** ltrace is an off-the-shelf tool, available in most Linux package repositories. However, we found it could not handle several of our benchmark workloads. We localized the problem to the following code[10]:

```
/* FIXME: not good -- should use dynamic allocation. 19990703 mortene. */
if (proc->callstack_depth == MAX_CALLDEPTH - 1) {
    fprintf(stderr, "%s: Error: call nesting too deep!\n", __func__);
    abort();
    return;
}
```

- **Reproduced (strace, fsatrace, rr, ReproZip, Sciunit2, ltrace, CDE).** We reproduced this provenance collector on all of the benchmarks[11].

[9] See https://github.com/dtg-FRESCO/opus/issues/1

[10] See https://gitlab.com/cespedes/ltrace/-/blob/8eabf684ba6b11ae7a1a843aca3c0657c6329d73/handle_event.c#L775

[11] TODO: Check to ensure CDE is working as expected.

[12] URSprung depends on IBM Spectrum Scale to get directory change notifications, so it is not for a *generic* Linux system.

Table 2: Provenance collectors mentioned in primary and secondary studies in our search results.

Tool	Method	Status
strace	tracing	Reproduced
fsatrace	tracing	Reproduced
ReproZip [16]	tracing	Reproduced
Sciunit2 [56]	tracing	Reproduced
rr [44]	tracing	Reproduced
CDE [24]	tracing	Reproduced
ltrace	tracing	Reproduced/excluded
SPADE [21]	audit, FS, or compile-time	Needs more time
DTrace [1]	audit	Needs more time
eBPF/bpftrace	audit	Needs more time
OPUS [8]	lib. ins.	Not reproducible
CamFlow [45]	kernel ins.	Requires custom kernel
Hi-Fi [47]	kernel ins.	Requires custom kernel
LPM/ProvMon [10]	kernel ins.	Requires custom kernel
RecProv [28]	tracing	No source
LPROV [59]	kernel mod., lib. ins.	No source
S2Logger [54]	kernel mod.	No source
ProTracer [38]	kernel mod.	No source
FiPS [55]	FS	No source
PANDDE [19]	kernel ins., FS	No source
PASS/Pasta [43]	kernel ins., FS, lib. ins.	No source
PASSv2/Lasagna [42]	kernel ins.	No source
Lineage FS [50]	kernel ins.	No source
RTAG [27]	dyn./static bin. ins.	No source
BEEP [35]	dyn. bin. ins.	Requires HW
libdft [30]	dyn. bin., kernel, lib. ins.	Requires HW
RAIN [26]	dyn. bin. ins.	Requires HW
DataTracker [53]	compile-time ins.	Requires HW
MPI[37]	compile-time ins.	Requires recompilation
LDX [32]	VM ins.	Requires recompilation
Panorama [61]	VM ins.	VMs are too slow
PROV-Tracer [52]	audit	VMs are too slow
ETW [5]	audit	Not for Linux
Sysmon [40]	audit	Not for Linux
TREC [58]	tracing	Not for Linux
URSprung [48]	audit	Not for Linux[12]
Ma et al. [36]	audit	Not for Linux

4.2 Implemented Benchmarks

Of these, Table 3 shows the benchmarks used to evaluate each tool, of which there are quite a few. We prioritized implementing frequently-used benchmarks, easy-to-implement benchmarks, and benchmarks that we believe have value in representing a computational science use-case.

- **HTTP/FTP servers/clients/traffic.** The most common benchmark class from prior work, HTTP servers/traffic, HTTP servers/clients, FTP servers/traffic, and FTP servers/clients are popular because prior work focuses overwhelmingly on provenance for the sake of security (auditing, intrusion detection, or digital forensics). While these benchmarks may not be specifically relevant for computational science workloads, we wanted to include them in our suite to improve our coverage of benchmarks used frequently in prior works. We deprioritized implement additional FTP and HTTP clients and servers beyond the most common ones, because they would likely exhibit similar performance.
- **Compiling packages.** Compiling packages from source is a common operation in computational science, so we implemented as many of these as we could and also implemented some of our own. However, compiling LLVM takes more than twice as long as the longest benchmark, so we

[13] LogGC measures the offline running time and size of garbage collected logs; there is no comparison to native would be applicable.

Table 3: Benchmarks used in various provenance publications.

Publication	Benchmarks	Comparisons
TREC [58]	open/close, compile Apache, compile LaTeX doc	Native
PASS [43]	BLAST	Native ext2
Panorama [61]	curl, scp, gzip, bzip2	Native
PASSv2 [42]	BLAST, compile Linux, Postmark, Mercurial, Kepler	Native ext3, NFS
SPADEv2 [21]	BLAST, compile Apache, Apache	Native
Hi-Fi [47]	lmbench, compile Linux, Postmark	Native
libdft [30]	scp, tar, gzip, bzip2 x extract, compress	PIN
LogGC [34]	RUBiS, Firefox, MC, Pidgin, Pine, Proftpd, Sendmail, sshd, vim, w3m, wget, xpdf, yafc, Audacious, bash, Apache, mysqld	None[13]
LPM/ProvMon [10]	lmbench, compile Linux, Postmark, BLAST	Native
Ma et al. [36]	TextTransfer, Chromium, DrawTool, NetFTP, AdvancedFTP, Apache, IE, Paint, Notepad, Notepad++, simplehttp, Sublime Text	Native
ProTracer [38]	Apache, miniHTTP, ProFTPD, Vim, Firefox, w3m, wget, mplayer, Pine, xpdf, MC, yafc	Auditd, BEEP
LDX [32]	SPEC CPU 2006, Firefox, lynx, nginx, tnftp, sysstat, gif2png, mp3info, prozilla, yopsweb, ngircd, gocr, Apache, pbzip2, pigz, axel, x264	Native
PANDDE [19]	ls, cp, cd, lpr	Native
MPI [37]	Apache, bash, Evince, Firefox, Krusader, wget, most, MC, mplayer, MPV, nano, Pine, ProFTPd, SKOD, TinyHTTPd, Transmission, Vim, w3m, xpdf, Yafc	Audit, LPM-HiFi
CamFlow [45]	lmbench, postmark, unpack kernel, compile Linux, Apache, Memcache, redis, php, pybench	Native
BEEP [35]	Apache, Vim, Firefox, wget, Cherokee, w3m, ProFTPd, yafc, Transmission, Pine, bash, mc, sshd, sendmail	Native
RAIN [26]	SPEC CPU 2006, cp linux, wget, compile libc, Firefox, SPLASH-3	Native
Sciunit [56]	VIC, FIE	Native
LPROV [59]	Apache, simplehttp, proftpd, sshd, firefox, filezilla, lynx, links, w3m, wget, ssh, pine, vim, emacs, xpdf	Native
MCI [33]	Firefox, Apache, Lighttpd, nginx, ProFTPd, CUPS, vim, elinks, alpine, zip, transmission, lftp, yafc, wget, ping, procps	BEEP
RTAG [27]	SPEC CPU 2006, scp, wget, compile llvm, Apache	RAIN
URSPRING [48]	open/close, fork/exec/exit, pipe/dup/close, socket/connect, CleanML, Vanderbilt, Spark, ImageML	Native, SPADE

excluded LLVM specifically from the benchmark suite. We implemented a pattern for compiling packages from Spack that discounts the time taken to download sources, counting only the time taken to unpack, patch, configure, compile, link, and install them. We try compiling Python, Boost, HDF5, glibc, Apache HTTPd, and Perl.[14]

- **Browsers.** Implementing headless for browsers in "batch-mode" without GUI interaction is not impossibly difficult, but non-trivial. Furthermore, we deprioritized this benchmark because few computational science applications resemble the workload of a web browser.
- **Un/archive.** Archive and unarchiving is a common task for retrieving data or source code. We benchmark un/archiving several archives with several compression algorithms. Choosing a compression algorithm may turn an otherwise I/O-bound workload to a CPU-bound workload, which would make the impact of provenance tracing smaller.
- **I/O microbenchmarks (lmbench, postmark, custom).** These could be informative for explicating which I/O operations are most affected. Prior work uses lmbench [41], which focuses on syscalls generally, Postmark [29], which focuses on I/O operations, and custom benchmarks, for example running open/close in a tight loop. We use the specific lmbench cases from prior work, which is mostly the latency benchmarks with a few bandwidth benchmarks. Most provenance systems do not affect the bandwdith; it doesn't matter *how much* this process writes to that file, just *that* this process wrote to that file.
- **BLAST.** BLAST [7] is a search for a fuzzy string in a protein database. Many prior works use this as a file-read heavy benchmark, as do we. This code in particular resembles a computational science workload. However, unlike prior work, we split the benchmark into each of each subtasks; provenance may have a greater overhead on certain subtasks.
- **CPU benchmarks.** SPEC CPU INT 2006 [25] and SPLASH-3 [49] test CPU performance. While we do not expect CPU benchmarks to be particularly enlightening for provenance collectors, which usually only affect I/O performance, it was used in three prior works, so we tried to implement both. However, SPEC CPU INT 2006 is not free (as in beer), so we could only implement SPLASH-3.
- **Sendmail.** Sendmail is a quite old mail server program. Mail servers do not resemble a computational science workload, and it is unclear what workload we would run against the server. Therfore, we deprioritized this benchmark and did not implement it.
- **VCS checkouts.** VCS checkouts are a common computational science operation. Prior work uses Mercurial, but we implemented Mercurial and Git. We simply clone a repository (untimed) and run `$vcs checkout` for random commits in the repository (timed).
- **Data processing/machine-learning Workflows.** VIC, FIE, ImageML, and Spark are real-world examples of scientific workflows. We would like to implement these, but reproducing those workflows is non-trivial; they each require their own computational stack. For FIE, in particular, there is no script that glues all of the operations together; we would have to read the publication [12] which FIE supports to understand the workflow, and write our own script which glues the operations together.
- **Utilities (bash, cp, ls, procps).** We did not see a huge representative value in these benchmarks that would not already be gleaned from lmbench, but due to its simplicity, we implemented it anyway. For `bash`, we do not know what workload prior works are using, but we test the speed of incrementing an integer and changing directories (`cd`).
- The rest of the programs are mostly specific desktop applications used only in one prior work. These would likely not yield any insights not already yielded by the benchmarks we implemented, and for each one we would need to build it from source, find a workload for it, and take the time to run it. They weigh little in the argument that our benchmark suite represents prior work, since they are only used in one prior work.

4.3 Subsetted Benchmarks

We introduce two additional parameters to sweep over:

[14] TODO: Double check what are we compiling? Also update the table below, once that is nailed down.

Table 4: Benchmarks implemented by this work.

Prior works	This work	Benchmark group and examples from prior work
10	yes (5/7 servers)	HTTP server/traffic (Apache httpd, miniHTTP, simplehttp, lighttpd, Nginx, tinyhttpd, cherokee x apachebench)
9	yes (2/4 clients)	HTTP serer/client (simplehttp x curl, wget, prozilla, axel)
8	yes (3/5 orig + 4 others)	Compile user packages (Apache, LLVM, glibc, Linux, LaTeX document)
8	no	Browsers (Firefox, Chromium x Sunspider)
6	yes (1/6) + 2 others	FTP client (lftp, yafc, tnftp, skod, AdvancedFTP, NetFTP)
5	yes	FTP server/traffic (ProFTPd x ftpbench)
5	yes	Un/archive (compress, decompress x tar x nothing, bzip2, pbzip, gzip, pigz)
5	yes	I/O microbenchmarks (Postmark, lmbench, custom)
4	yes	BLAST
3	yes (1/2)	CPU benchmarks (SPEC CPU INT 2006, SPLASH-3)
3	yes	Coreutils and other utils (bash, cp, ls, procps)
2	no	Sendmail
1	yes	VCS checkouts (Mercurial)
1	no	Machine learning workflows (CleanML, Spark)
1	no	Data processing workflows (VIC, FIE)
1	no	RUBiS
1	no	x264
1	no	mysqld
1	no	gocr
1	no	Memcache
1	no	Redis
1	no	php
1	no	pybench
1	no	ImageML
1	no	ping
1	no	mp3info
1	no	ngircd
1	no	CUPS

Table 5: This table shows percent slowdown in various provenance collectors. A value of 1 means the new execution takes 1"Noprov" refers to a system without any provenance collection (native), for which the slowdown is 0 by definition. fsatracea ppears to have a negative slowdown in some cases due to random statistical noise.

collector benchmark types	fsatrace	noprov	reprozip	rr	strace
archive	7	0	164	208	180
blast	-1	0	32	102	6
copy	48	0	7299	322	710
ftp client	-0	0	14	5	4
ftp server	1	0	58	-32	65
gcc	3	0	417	314	321
http client	-16	0	453	200	98
http server	6	0	791	965	516
lmbench	-14	0	31	15	5
notebook	-10	0	116	0	50
pdflatex	-10	0	290	19	79
postmark	9	0	2002	367	928
python	0	0	412	137	184
shell	18	0	4620	698	63
simple	23	0	977	1749	431
splash-3	-1	0	78	64	19
unarchive	6	0	179	190	177
vcs	3	0	453	169	185

- For each method, we may use "performance in each provenance collector" and/or "other quantitative features"; The three non-empty combinations are denoted "perf+other", "perf", or "other" in Figure 2. Training directly on performance features would be optimal if the population were perfectly known. However, since we are training on a small sample of the population, it is possible that all features or just other features may encode knowledge that will help the model find diversity in its benchmarks.

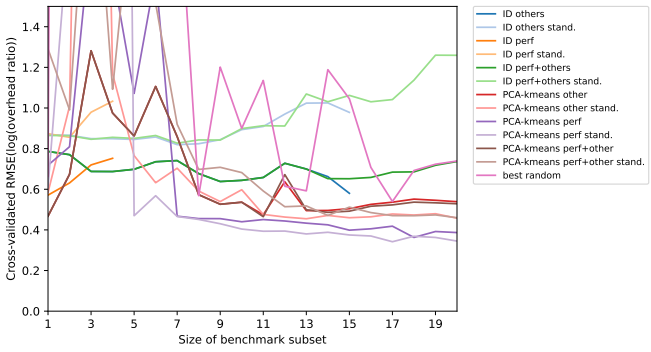


Figure 2: Competition for best benchmark subsetting algorith, sweeping over subset size on the x-axis. The algorithms are scored by how well the selected subset can predict the unselected ones, on the y-axis.

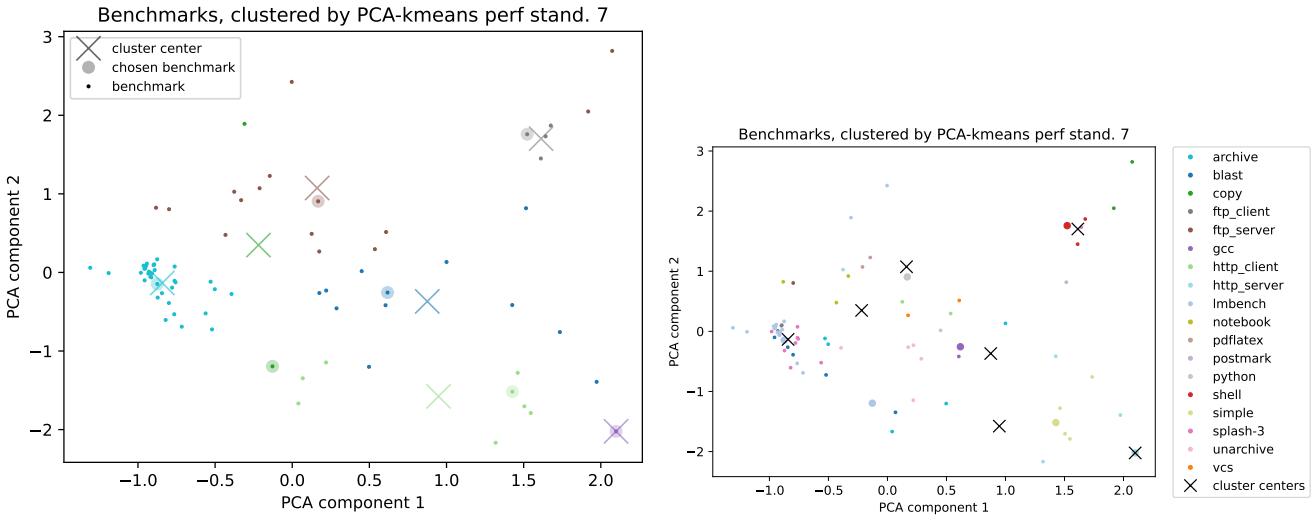
- These features may be standardized with $(x - \bar{x})/\sigma_x$, which is denoted as "stand." in $Fig:subsetting, before use in the underlying algorithm. Standardized discards the "absolute" value of each feature and replaces it with the "relative value"; before standardization, a value of 1 meant a single unit of that quantity, after standardization, a value of 1 means 1 standard deviation greater than the mean of that quantity on the observed data.

We have the following observations:

- We notice that cross-validation seems to be punishing model complexity, because larger k instances do not always preform better. A larger k means each unselected benchmark is predicted by a linear regression of larger number of variables, offering more degrees of freedom.
- For ID, k must be less than the total number of features. Otherwise, one would be factorizing a $m \times n$ matrix into a "taller" $m \times k$ and a $k \times n$ matrix. This is why the "ID perf" and "ID others" lines stop in Figure 2.
- ID seems to not do as well as PCA-kmeans, even though it is more optimal on in-sample data, it seems that PCA-kmeans contains intuition about the underling problem which helps it generalize to the out-of-sample test set.

It seems that "PCA-kmeans perf stand." with $k = 7$ has quite good performance. It achieves an RMSE of about $0.47 = \log 1.6$, so the predictor was within a factor of 1.6 of the actual value most of the time. While larger k may minimally improve performance, it appears to be a point of diminishing return. We examine the generated clusters and benchmark subset in Figure 3.

Section 4.3 shows the a posteriori clusters that kmeans found and the benchmarks it selected for each cluster. It may appear to not select the closest benchmark, but this is because we are viewing a 2D projection of a high-dimensional space, like how three stars may appear next to each other in the sky, but in reality one pair may be much closer than the other, since we cannot perceive the depth to the stars. The dark green cluster has a center near $(0, 0)$ because it has one member near $(0, 2)$ and another near $(0, -1.5)$.



(a) Benchmark subset, where color shows a posteriori kmeans clusters. (b) Benchmark susbet, where color shows a priori benchmark "type".

Figure 3: Benchmarks, clustered by PCA-kmeans into 7 subsets using standardized performance features. These axes show only the 2D of a high-dimensional space.

Section 4.3 shows a priori benchmark "types", similar but more precise than those in Table 4. We would expect the dark green "copy" benchmarks to occupy nearby points, since they are related programs, and indeed they do at (2, 2). However, the benchmark groups globally do not map well to clusters in PCA space; this means that different benchmarks in the same group may have quite different performance characteristics.

4.4 Predictive Model

Figure 4 shows us the competition between predictive performance models. Note that linear regression does not permit sweeping over the number of parameters; it requires a $n_{\text{benchmarks}} n_{\text{features}}$ parameters. Matrix factorization methods use only $(n_{\text{benchmarks}} - k) \times (n_{\text{features}} - k) = n_{\text{benchmarks}} n_{\text{features}} - k(n_{\text{benchmarks}} + n_{\text{features}}) + k^2$ parameters. When k is low, matrix factorization is much fewer parameters than linear regression at the cost of some in-sample accuracy, but when k approaches n_{features}, it is less parameter-efficient than linear regression. Number of parameters is not truly an independent variable that can be directly swept over. Rather k is an independent variable, we sweep over k, and plot the number-of-parameters on the x-axis, since that is more directly interpretable. Models with a large number of parameters are more likely to overfit to spurious correlations on the test sample which generalize poorly on the train sample. Overgeneralization is appropriately punished by cross-validation.

We observe the following:

- When the number of parameters is large, all of the algorithms preform similarly; Even though greedy feature selection is more constrained than low-rank matrix factorization (every solution found by greedy is a candidate used by low-rank, but not vice versa), there are enough degrees of freedom to find similar enough candidates.

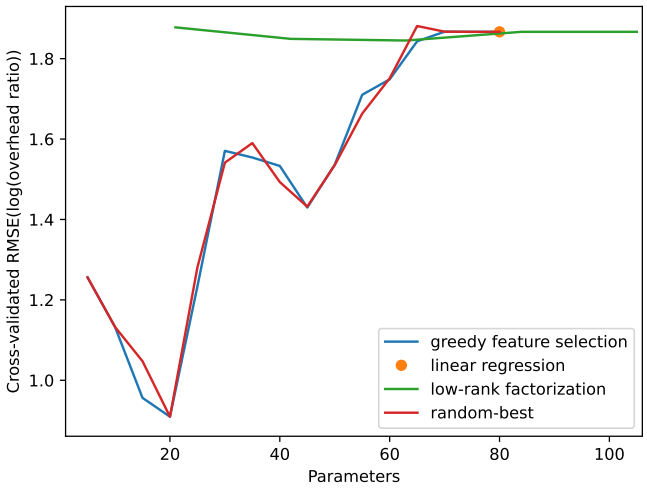


Figure 4: Competition between predictive performance models.

- Linear regression has equivalent goodness-of-fit to matrix factorization with a high k, as expected. When the compression factor is low, the compressed version is just as good as the original.
- Random-best usually does not do better than greedy feature selection. However, greedy is much easier to compute, evaluating n_{features} subsets of size 1, $n_{\text{features}} - 1$ subsets of 2, ... $n_{\text{features}} - k + 1$ subsets of size k; random has to evaluate a large number (1000 in our case) of subsets of size k. Greedy is not necessarily optimal, since a set of features may be individually outscored by other features but may have predictive

Table 6: Benchmark results.

	metadata-reads per walltime second	constant fraction	cputime / walltime	execs-and-forks per walltime second
fsatrace	0.000003	-0.001236	-0.024958	0.000064
noprov	0.000000	0.000000	0.000000	0.000000
reprozip	0.000043	-0.027311	0.266969	0.000438
rr	0.000021	-0.011208	0.404307	0.000878
strace	0.000029	-0.002243	0.229129	0.000312

Table 7

value when taken as a set. Greedy would never pick that set, because it is bound to pick the best additional individual feature at every step, but random-best could. However, our problem domain may lack the complexity to generate these cases.

Greedy feature selection with 20 parameters (predicting the performance on 5 systems using only $k = 4$ of 16 features) seems to preform the best in cross-validation. On 19 out of 20 cross-validation splits, greedy feature selection with $k = 4$ chose the parameters in Table 7.

For example,

$$\log \frac{\text{walltime}_{\text{fsatrace}}}{\text{walltime}_{\text{noprov}}} = 3 \times 10^{-6}\left(\frac{\text{metadata reads}}{\text{walltime}_{\text{noprov}}}\right) - 0.001 \cdot \left(\frac{1}{\text{walltime}_{\text{noprov}}}\right) - 0.02 \cdot \left(\frac{\text{cputime}_{\text{noprov}}}{\text{walltime}_{\text{noprov}}}\right) + 6 \times 10^{-5} \cdot \left(\frac{\text{execs and forks}}{\text{walltime}_{\text{noprov}}}\right)$$

The system calls features can be observed using strace. The CPU time and wall time of noprov can be observed using GNU time. One need not complete an entire execution to observe the these fatures; one merely needs to record the features until they stabilize (perhaps after several iterations of the main loop).

4.5 Threats to Validity

5 FUTURE WORK

In the future, we plan to implement compilation for more packages, in particular xSDK [9] packages.

6 CONCLUSION

We hope this work serves as a part of a bridge from research to practical use of provenance collectors. As such, we address practical concerns of a user wanting to use provenance collector. We identify the reproducible and usable subset of prior work, we evaluate their performance on synthetic and real-world workloads.

A OPEN SOURCE CONTRIBUTIONS

The actual benchmark set and statistical analysis are open-source:

- https://github.com/charmoniumQ/prov-tracer/

This work necessitated modifying Spack, Sciunit, jupyter-contrib-nbextensions, Nixpkgs, ftpbench, and benchexec. Where appropriate, we submitted as pull-requests to the respective upstream projects.

The following are merged PRs developed as a result of this work:

- https://github.com/depaul-dice/sciunit/pull/35
- https://github.com/spack/spack/pull/42159
- https://github.com/spack/spack/pull/42199
- https://github.com/spack/spack/pull/42114
- https://github.com/selectel/ftpbench/pull/5
- https://github.com/selectel/ftpbench/pull/4
- https://github.com/sosy-lab/benchexec/pull/984
- https://github.com/NixOS/nixpkgs/pull/263829
- https://github.com/NixOS/nixpkgs/pull/257396

The following are open PRs developed as a result of this work:

- https://github.com/spack/spack/pull/39902
- https://github.com/spack/spack/pull/42131
- https://github.com/spack/spack/pull/41048
- https://github.com/depaul-dice/sciunit/pull/36
- https://github.com/ipython-contrib/jupyter_contrib_nbextensions/pull/1649
- https://github.com/NixOS/nixpkgs/issues/268542

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