

PyTracer: Automatically Profiling Numerical Instabilities in Python

Yohan Chatelain¹, Nigel Yong Sao Young¹, Gregory Kiar², Tristan Glataud¹

¹Department of Computer Science and Software Engineering, Concordia University, Montreal, Canada

²Center for the Developing Brain, Child Mind Institute, New York, NY, USA

Abstract—Numerical stability is a crucial requirement of reliable scientific computing. However, despite the pervasiveness of Python in data science, analyzing large Python programs remains challenging due to the lack of scalable numerical analysis tools available for this language. To fill this gap, we developed PyTracer, a profiler to quantify numerical instability in Python applications. PyTracer transparently instruments Python code to produce numerical traces and visualize them interactively in a Plotly dashboard. We designed PyTracer to be agnostic to numerical noise model, allowing for tool evaluation through Monte-Carlo Arithmetic, random rounding, random data perturbation, or structured noise for a particular application. We illustrate PyTracer’s capabilities by testing the numerical stability of key functions in both SciPy and Scikit-learn, two dominant Python libraries for mathematical modeling. Through these evaluations, we demonstrate PyTracer as a scalable, automatic, and generic framework for numerical profiling in Python.

Index Terms—Computer arithmetic, Quality analysis and evaluation, Visualization techniques and methodologies, Tracing, Stochastic analysis

1 INTRODUCTION

THE scientific Python ecosystem has become a central component of data analyses in recent years, owing to its rich offering of data manipulation, array programming, numerical analysis, and visualization tools. In particular, libraries such as NumPy [1], SciPy [2], scikit-learn [3] or PyTorch [4] are used in hundreds of publications each year, and serve as a reference set of high-quality open-source core scientific libraries. Researchers have built numerous domain-specific software tools from this ecosystem, leveraging Python’s simplicity and flexibility.

Numerical stability is a crucial requirement of reliable scientific data processing. In unstable analyses, small numerical perturbations introduced by data noise, software and hardware updates, or parallelization have potential to introduce substantial deviations in final results, leading to potentially different scientific conclusions, ultimately threatening the reliability of computational analyses. To prevent this, numerical stability analyses need to be conducted systematically, however, no practical tool currently exists to conduct such analyses for Python programs.

We present PyTracer, a numerical stability profiling and visualization tool for Python programs. PyTracer adopts a dynamic approach that evaluates numerical stability using program execution traces, and is applicable to large programs without manual intervention. The transparent nature of PyTracer is particularly valuable in contrast to theoretical approaches based on condition numbers or backward error analysis [5], which require detailed modeling of the program and its numerical implementation. Similarly, static code analysis techniques [6] hardly scale to large code bases, particularly in dynamically-typed languages such as Python.

PyTracer estimates the variability of floating-point variables by combining program traces obtained with

different numerical perturbations, which requires (a) generating numerically-perturbed executions, (b) tracing floating-point computations along program executions, and (c) visualizing stability evaluations. PyTracer uses the “fuzzy” Python environment instrumented with Monte-Carlo arithmetic to address the requirement (a). PyTracer addresses the remaining requirements with (b) a dynamic instrumentation of Python functions, modules, and classes through meta-programming, (c) an interactive Plotly dashboard to visualize stability measures throughout program executions. PyTracer is available at github.com/big-data-lab-team/pytracer.git under MIT License. ~~PyTracer addresses these requirements with (1) a “fuzzy” Python interpreter instrumented with Monte-Carlo arithmetic, (2) a dynamic instrumentation of Python functions, modules, and classes through meta-programming, (3) an interactive Plotly dashboard to visualize stability measures throughout program executions.~~

This manuscript presents the design of PyTracer and demonstrates its potential in various use cases. Through stability evaluations of the SciPy and scikit-learn libraries, we demonstrate PyTracer as a practical solution to review the numerical stability of extensive code bases.

2 PHILOSOPHY OF PYTRACER

PyTracer follows a three steps approach:

- 1) Automatic instrumentation of Python programs to save the value of inputs and outputs of function in a file.
- 2) Aggregation of the traces generated to produce a statistics summary.

3) Interactive visualization to navigate through the code execution.

The main goal of PyTracer is to help the developer visualizing the numerical stability of Python applications. PyTracer saves time for the user by instrumenting and aggregating values. In the same way that GDB makes the user save time when debugging an application by providing all information in one layout, PyTracer allows the user to visualize the overall numerical quality to quickly detect instabilities. The PyTracer visualization layout improves result analysis in any case since 1) the user does not have to manually instrument its code to dump raw data and creates specific post-processing scripts to visualize it 2) PyTracer allows the user to export the raw data traced to extend the analysis.

The main challenge addresses by PyTracer is the transparent instrumentation of Python applications. Indeed, since Python is interpreted language, one has no complete view of the function that will be executed by a given program. Moreover, since we target Python application used in HPC environments, one has most of the time no access to source codes or with limited write access. Therefore, PyTracer tackles this issue by instrumenting the function dynamically thanks to the Python introspection.

The based-trace approach used by PyTracer permits to limit the overhead at runtime since the statistics computation is reported to the postprocess analysis. However, it limits the aggregation to deterministic executions, although control-flow analysis can help to merge divergent execution paths.

3 PYTRACER DESIGN

PyTracer adopts the three-step workflow shown in Figure 1. First, PyTracer uses *monkey patching* to replace the functions called by the application with a wrapper that saves their arguments and returned values in a trace file. Second, it executes the application multiple times with noise injection, and aggregates the resulting trace files to compute summary statistics about each traced variable. Finally, a Plotly dashboard provides interactive visualizations highlighting unstable code sections.

3.1 Python code instrumentation

PyTracer dynamically instruments Python modules without requiring source code modifications in the application. To do so, it creates a new, instrumented version of each module that preserves its original attributes so that the application can transparently use it. By default, PyTracer instruments all the attributes in a given module except the special ones of the form `__*___` which is common for reserved Python methods. However, some attributes are not writable. In this case, PyTracer `preserves` the original attributes and warns the user. The user can also restrict the list of traced attributes through an inclusion/exclusion mechanism. The main advantage of this instrumentation approach is the lack of required modification in the application source code, in contrast with `decorator-based approaches` [7]. In addition, this technique is scalable and applicable in read-only environments such as Singularity containers or HPC clusters.

3.1.1 Intercepting module import

Python loads modules through an import mechanism triggered by the `import` keyword that involves two objects: finders and loaders. Finders search for packages (or namespaces¹) on the local storage — such as standard packages installed through the pip package manager — or on a distant server. Finders do not load modules. Instead, they return a specification (`spec` object) that includes information on where to find and how to load modules. Loaders create module objects, initialize them, and fill import-related attributes such as `__spec__`. Loaders then execute modules and populate their namespace. Finally, modules are bound to their import name in the `sys.modules` dictionary.

Python supports custom finder classes registered in the `sys.meta_path` list. When Python encounters an `import` statement, it first looks for an existing binding in `sys.modules` and then iterates over the `finder` classes in the `sys.meta_path` list until it finds the module. PyTracer adds a custom finder class at the head of `sys.meta_path` that intercepts the module import and creates the module with a custom loader class.

PyTracer's loader class first loads the original module, then copies it as a new instance of the `ModuleType` class. It then calls the appropriate instrumentation function for each attribute depending on its type (function, class, or instances) and replaces the original module in the `sys.modules` map with the instrumented version. Finally, it updates all existing references to the original module contained in the global symbol table. As a result, the application will transparently call the instrumented module.

3.1.2 Instrumenting module functions

Listings ?? and ?? show PyTracer's function instrumentation mechanism. For each function to instrument, PyTracer's loader class creates a wrapper function, dynamically compiles it with the `compile` builtin function, and substitutes it for the original module function. Although simple, this technique does not apply to callable class instances, i.e., class instances that have a `__call__` attribute and are not of type `FunctionType`. Indeed, applying the wrapper technique would 1) modify the type of the class instance to `FunctionType`, which could cause syntax and semantic errors, and 2) mask class attributes, leading to `AttributeError` exceptions. PyTracer overrides the `__call__` attribute with the wrapper function when possible to overcome this issue. When the `__call__` attribute is not writable, Pytracer does not instrument the class and returns a warning.

3.1.3 Instrumenting classes

PyTracer instruments classes by wrapping their callable attributes as described previously. This instrumentation preserves class types, which avoids type mismatches in the

1. Python distinguishes between regular and namespace packages. A regular package is a directory that contains a `__init__.py` file and potentially subdirectories (sub-packages) that contain themselves a `__init__.py` file and so on recursively. The package hierarchy follows those of the directory. Namespace packages introduced in Python 3.3 (PEP 420) do not contain an `__init__.py` file and allow for flexible directory structures. Hence, parts of the package can be located in zip files, on the network, or in separated directories. There are no functional differences between both types of packages.

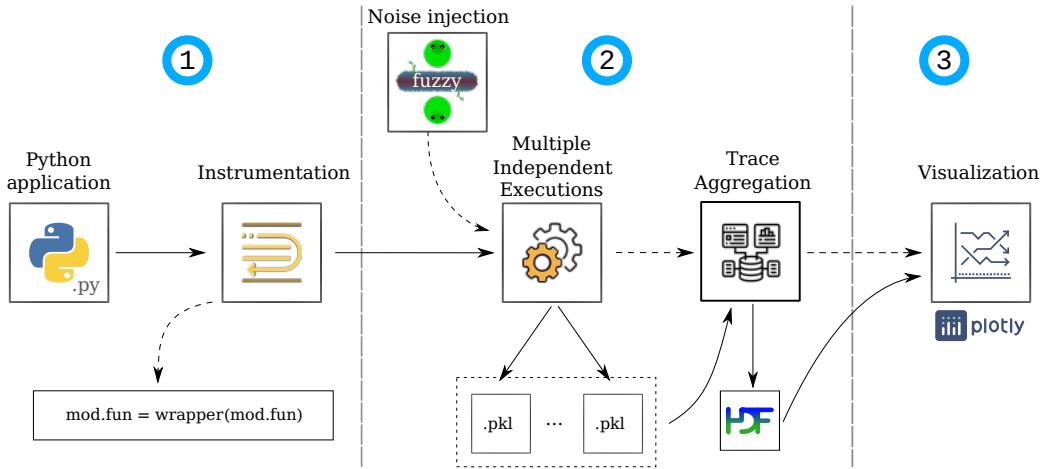


Fig. 1: PyTracer workflow

instrumented application. However, classes that describe particular base types and NumPy’s universal functions (class `ufunc`) contain read-only attributes that cannot be instrumented. By default, PyTracer returns a warning when it encounters such classes.

3.1.4 Instrumenting class instances

PyTracer automatically instruments class instances since it instruments classes. However, it cannot instrument or instantiate classes that have read-only attributes — in particular class `ufunc`, — which is problematic given their pervasiveness in scientific computing. In particular, NumPy’s universal functions include vectorized elementary mathematical and other prevalent functions. Universal functions are implemented in C, which prevents their modification.

To overcome this issue, PyTracer wraps the class instance into a transparent wrap class (`twc`) that overloads 1) function `__getattribute__`, called when an instance attribute is accessed — instrumented to return the attributes from the original class, and 2) function `__call__`, used when an instance behaves like a function through the `()` operator — instrumented with function `generic_wrapper`. The `twc` returns the queried attribute of the instance instead of returning its attributes, allowing transparent access to the instance. Finally, PyTracer overloads the builtin `type` function to preserve the type of the wrapped instance.

3.1.5 Instrumenting iterators

In functional programming, iterators traverse containers lazily, meaning that the next element in the sequence is only computed when the application uses it. This technique allows for the manipulation of virtually infinite sequences with finite memory. However, it implies that no complete mapping of the container returned by an iterator exists in memory since the application computes each element on the fly. Therefore, iterators are not serializable which implies that PyTracer cannot save them to output traces. A workaround would be to convert iterators into explicit containers, however, this would increase the memory footprint significantly. PyTracer, therefore, does not instrument non-built-in iterators.

3.2 Detecting numerical instabilities

PyTracer detects numerical instabilities by computing summary statistics across multiple executions perturbed with numerical noise. While PyTracer’s instrumentation, trace aggregation, and visualization work with various types of numerical noise, we experimented primarily with Monte-Carlo Arithmetic (MCA) as it is an accurate model for floating-point errors [8].

3.2.1 Noise injection

Three main approaches exist to detect numerical instabilities: stochastic arithmetic, uncertainty or sensitivity analysis [23], and random seed analysis [11]. PyTracer is agnostic to the noise model used and therefore works for all methods mentioned. For our use cases, we focus on stochastic arithmetic since it does not make any assumption about the noise model, in contrast to sensitivity analysis.

Stochastic arithmetic leverages randomness to estimate numerical instabilities coming from the use of floating-point representations. The main idea is to treat round-off errors as random variables and characterize them statistically. Monte Carlo Arithmetic (MCA) [9] uses this principle by introducing two improvements: (i) a virtual precision parameter, allowing to simulate reduced working precision, and (ii) different perturbation modes to introduce perturbations on function inputs or output. MCA replaces each floating-point number x with a stochastic counterpart computed as:

$$\text{inexact}(x) = x + \beta^{e_x - t} \xi$$

where β is the number base, e_x is the magnitude of x , t the virtual precision and $\xi \in (-\frac{1}{2}, \frac{1}{2})$ is a random uniform variable. Virtual precision allows for the simulation of reduced working precision. MCA can be applied in three modes but we only used the Random Rounding (RR) in our experiments, Precision Bounding (PB), and full MCA, which apply function `inexact` to the output, the inputs, or both, respectively. While the RR mode is equivalent to stochastic rounding, the PB mode can also identify catastrophic cancellations. Random Rounding simulates roundoff errors.

Stochastic arithmetic quantifies numerical error using the number of significant digits s estimated among the sam-

pled values. A common formula to determine this number from MCA samples is presented in [9]:

$$s = -\log_{\beta} \left| \frac{\sigma}{\mu} \right| \quad (1)$$

where μ and σ are the sample mean and standard deviation of a variable sampled with MCA. This can be seen as the ratio signal over noise. Sohier et al. [10] recently provided a generalization of this formula to include confidence intervals.

We enable MCA in Python programs via Verificarlo [8], a clang-based compiler [11] that replaces floating-point operations by a generic call to a configurable floating-point model. Several floating-point models are available [12], [13], also called backends. PyTracer leverages “fuzzy” [14], a collection of software tools compiled with Verificarlo. In particular, fuzzy provides MCA-instrumented versions of the Python interpreter as well as the BLAS, LAPACK, NumPy, SciPy, and scikit-learn libraries, which enables MCA for a wide range of existing scientific Python programs. Fuzzy is available in Verificarlo’s GitHub organization at github.com/verificarlo/fuzzy.

3.2.2 Trace format

PyTracer stores traces in the pickle format, a binary format to serialize Python objects. The main advantages of the pickle format compared to other serialization approaches such as marshal or JSON are its ability to serialize most Python objects and its native compression. In addition, pickle writes Python objects sequentially, which preserves the temporal ordering required by subsequent trace analyses.

Traces store numerical values at the granularity of function calls. When the application invokes a function, PyTracer saves a call input object containing contextual information (function’s name, module’s function, stacktrace) and the values of the function arguments. When the function returns, PyTracer saves a similar call output object containing the returned value.

3.2.3 Trace aggregation

Once traces are available, PyTracer sequentially parses them and computes the mean, standard deviation, and the number of significant digits (as in Equation 1) of all saved values. PyTracer saves these summary statistics in an HDF5 file, a hierarchical format that facilitates visual browsing since only required information are loaded when requested by the user. This operation critically relies on the ordering of call input and output objects in the traces. Therefore, it assumes that the application is single-threaded and that the control flow does not depend on a random state. Therefore, PyTracer cannot merge traces resulting from a different control flow path and will stop the parsing when encountering one.

To aggregate traces, PyTracer successively unpickles call objects in each trace, checks that the call objects refer to the same function and stacktrace, and terminates the parsing otherwise. PyTracer stores function arguments or returned values in a NumPy array for each matching call object to compute statistics. For compound objects such as tuples, dictionaries, or objects, it recursively parses the fields until finding numeric types or NumPy arrays of numeric types.

3.3 Interactive visualization

The third main component of PyTracer is its interactive trace visualizer built with Plotly Dash [15], a Python framework for web visualization. Plotly Dash abstracts the low-level details of web applications in a highly customizable development interface allowing to offload heavy computations to a server if necessary. Figure 2 presents the general layout of the PyTracer visualizer, divided into five sub-components:

- 1) Timeline view: This view displays the values of each input and output for a given function at a given invocation. By default, PyTracer shows the number of significant digits computed across the traces. The mean and standard deviation across perturbed samples are also available. The visualizer uses an upper triangle for inputs and a lower triangle for outputs. PyTracer internally represents all values as NumPy arrays. In the case of non-scalar values or types that cannot be trivially cast into NumPy arrays, PyTracer splits the value into several variables. Hence, PyTracer will transform a class containing n floating-point parameters into n variables. Each variable is prefixed with the original value and postfixed with the name of the parameter. Finally, non-scalar values (vectors or matrices) are represented by their average and can be inspected with the Zoom view (see below).
- 2) Gantt chart view: This view displays the call graph as a Gantt chart representing the instrumented functions. Each function call is represented with a bar. The time overlaps reflect the caller/callee relation. For example, in the figure, `function1` calls `function2` that itself calls `function4` and `function5`. This view provides insights on the calling context for each function, which may influence numerical stability.
- 3) Source code view: This view displays a local snapshot of the source code file of the variable hovered in the timeline view.
- 4) Zoom view: This view provide details about non-scalar values. For example, a matrix may have instabilities around its diagonal but not in other regions. The visualizer also provides additional metrics such as array shape, infinite norm, or condition number.
- 5) Functions list view: This view allows the user to select the functions plotted in the timeline view.

4 RESULTS

We evaluated PyTracer on two widely-used Python libraries: SciPy [2], the main library for scientific computing in Python, and scikit-learn [3], a reference machine-learning framework that implements a wide range of state-of-the-art algorithms. For each library, we executed the software examples provided in their respective GitHub repositories. We traced each example five times, having activated MCA in the Python interpreter as well as BLAS, LAPACK, NumPy, SciPy, and scikit-learn. Only instrumented the Python interpreter would lead to only perturb pure Python floating-point operations and thus to miss operations in compiled codes (i.e. Cython and shared libraries). We repeated the

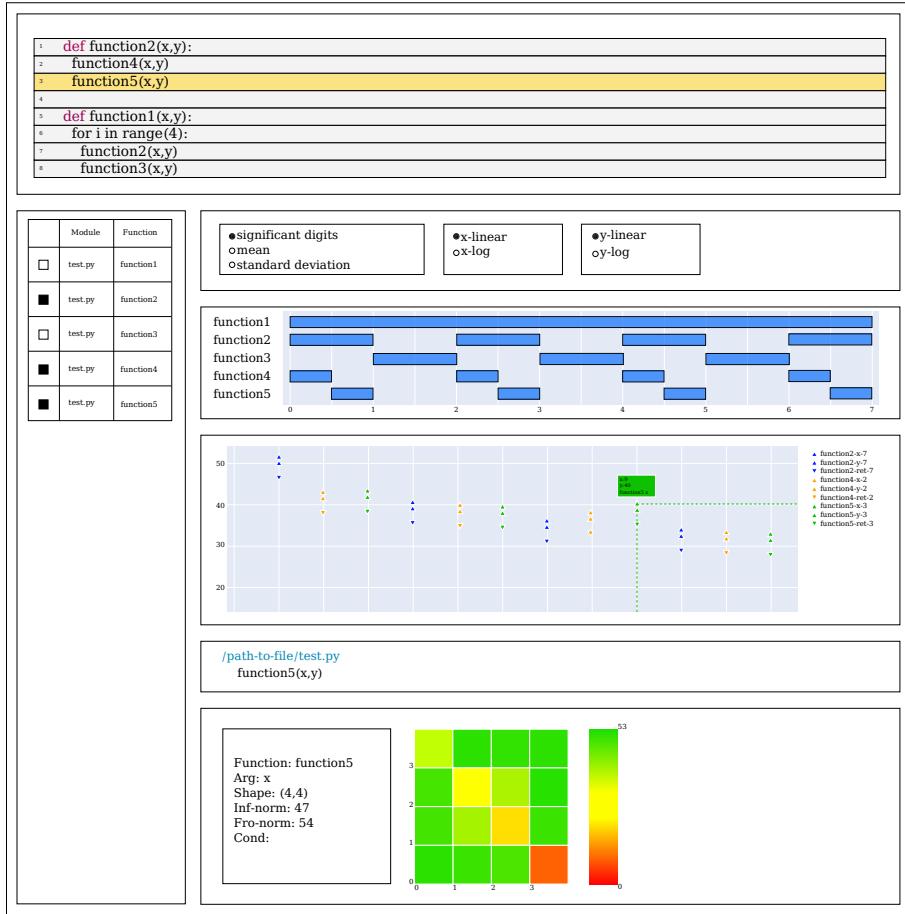


Fig. 2: Pytracer visualization layout.

experiment with two MCA modes, Random Rounding (RR) and Full MCA, resulting in 2 experiments for each example. We used the default virtual precision in Verificarlo, namely 24 bits for single-precision floating-point values and 53 bits for double-precision values, which simulates machine error. We used Python-3.8.5, NumPy-1.19.1, SciPy-1.5.4, and scikit-learn-0.23.2.

Monte Carlo Arithmetic samples the floating-point variability of a given program, and hence the more MCA repetitions we have, the more accurate will be the sampling distribution. In theory, an infinite number of MCA repetitions should give the exact distribution. While in practice low sample size ($3 \approx 30$) can give a good estimate, the issue is to capture "rare events" that could make the computation strongly diverge from the mean. For now, determining the number of MCA samples to use is still an open research question. Recent theoretical works [10] on the significant digits computation allow computing an associated confidence interval depending on the sample size and the underlying distribution of the outputs.

4.1 Pytracer is applicable to scientific computation libraries of reference

Table 1 summarizes PyTracer's outcome on SciPy and scikit-learn examples. Columns *trace* and *parse* report on the tracing and aggregation steps with two possible outcomes: 1) green for success, meaning that the execution ended well

and no issues were raised by the application, and 2) red for numerical error in the application, meaning that the execution raised a Python error before the end. ~~and 3) orange for errors due to the fuzzy noise injection that are not considered numerical errors, meaning that the execution raised a Python error but due to a perturbation that should not have been introduced (i.e. a floating-point value representing an integer).~~ Overall, the tracing and parsing of SciPy and scikit-learn examples in Random Rounding mode was entirely successful for 32/40 examples and showed an average precision loss of 8 bits. The remaining examples failed due to numerical errors in the libraries, which we discuss hereafter. ~~The instrumentation with Full MCA is more invasive and reduced the number of successful executions to 12/40. Among the 28/40 failed executions, one failed due to an actual numerical error (Bayesian Ridge Regression example) and the other ones failed due to perturbations that should not have been introduced.~~

Column *sigbits* in Table 1 summarizes the precision for the main outputs of SciPy and scikit-learn examples. We measured the precision in significant bits on the final primary example output by taking the element-wise mean for non-scalar values and, if the example produces many outputs, the average value among all of them. The numerical quality across all examples varies from 0 to 52, with an average of 44 significant bits. We note that only one example failed due to a numerical error (face_recognition ~~for RR~~

Application			Random Rounding (RR)		
			trace	parse	sigbits
SciPy	FFT	discrete_cosine_transform	✓	✓	52
		fft_1D	✓	✓	41
		fft_2D	✓	✓	52
	Interpolation	interpolation_1D	✓	✓	51
		multivariate_data	✓	✓	51
		bspline	✓	✓	10
		spline_1D	✓	✗	52
		spline_2D	✓	✓	10
	Optimization	broyden_fletcher_goldfarb_shanno	✓	✓	48
		global_optimization	✓	✗	17
		— SHGO ^a			25
		— Dual Annealing			4
		— Differential Evolution			0
		— Basin Hopping			40
		— SHGO Sobol			45
Scikit-learn	Classification	slsqp	✓	✓	45
		least_square_minimization	✓	✓	48
		nelder_mead_simplex	✓	✓	44
		newton_conjugate_gradient	✓	✓	48
		root_findings	✓	✗	52
		root_finding_large	✓	✗	29
		root_finding_large_preconditioned	✓	✗	42
		trust_region_exact	✓	✓	48
		trust_region_truncated_generalized_lanczos	✓	✓	48
		trust_region_newton_conjugate_gradient	✓	✓	52
	Regression	AdaBoost	✓	✓	48
		Bayesian Ridge Regression	✓	✓	25
		— 1 st dataset			25
		— 2 nd dataset			nan
		Online classifier comparison	✓	✓	20
	Dimensionality Reduction	K-Means Clustering	✓	✓	52
		Covariance estimation	✓	✗	48
		Decision Tree Regression	✓	✓	50
		Digits Classification	✓	✓	52
		Face Recognition	✗	✓	-
		L1 Penalty	✓	✓	-
		Lasso and Elastic Net	✓	✓	48
		Separating hyperplane	✓	✓	3
		MNIST classification	✓	✓	43
		Multitask Lasso	✓	✓	50
	Feature Extraction	Orthogonal Matching	✓	✓	52
		PCA decomposition	✓	✓	48
		Robust Linear Regression	✓	✓	50
		— Linear			48
		— RANSAC			50
	Segmentation	Segmentation toy	✓	✓	35
		SVM	✓	✓	43.5
		— Non-weighted			43
		— Weighted			44
	Image Processing	Tomography	✓	✗	-
		SGD weighted samples	✓	✓	44

^a. Simplicial Homology Global Optimization

TABLE 1: PyTracer execution summary on SciPy and Scikit-learn examples. trace: outcome of PyTracer tracing, parse: outcome of PyTracer trace parsing and aggregation, result: precision for main outputs in significant bits. ✓: successful run, ?: error from invalid noise injection, ✗: numerical error or divergent traces. nan stands for (Not-A-Number). Example names are linked to their source code.

and Bayesian Ridge Regression for full MCA).

3.2 Effect of MCA modes

Random Rounding perturbs only the result of a floating-point operation while Full MCA perturbs both the inputs and the result. Therefore, Full MCA may trigger catastrophic cancellations while Random Rounding only introduces round-off errors which generally have a lesser impact. Moreover, Random Rounding preserves exact operations — operations where the result can be exactly represented at the virtual precision — while Full MCA does not.

PyTracer can only aggregate traces obtained from the same control flow path. In particular, program branches triggered by an unstable floating-point comparison lead to different control flows and result in parsing errors. For example, comparing a residual error or the distance between two points to a strict threshold in an iterative scheme generally results in unstable branches. Full MCA even perturbs exact values such as integers represented with floating-point values, leading to many execution failures. For instance, the `fft1` example from SciPy raised an `ValueError: operands could not be broadcast to` error due to an array shape mismatch. A closer inspection showed that one of the arrays involved in the error was created with the NumPy function `linspace` that itself calls function `arange` (Listing ??). Lines 3174–3178 show that the function stores the array size in a floating-point value that will be perturbed by Full MCA, as shown in Table ??, resulting in array sizes that fluctuate between N and $N+1$. It is worth noting that 78% of execution issues encountered in Full MCA mode instrumentation are due to this type of “typing” errors. Those code regions should not be perturbed by MCA since the injected noise does not make sense.

4.2 PyTracer supports the visualization of compound data type

PyTracer supports native floating point formats as well as compound data type, such as complex floating point values, N-dimensional arrays and arbitrary Python classes. For the Python classes, PyTracer recursively parses the class attributes to extract scalar and N-dimensional arrays floating-points values.

Figures 3 and 4 show the visualization of the `fft_1D` inputs and outputs values. Results are complex value encoded on double precision. PyTracer allows visualizing the numerical precision of real (blue points) and imaginary (orange points) parts. The top row in Figures 3 and 4 show the input mean value while the bottom row shows the standard deviation. The points with low magnitude in Figure 3 correspond to inputs near 0 when the input of `sin` or `exp` is close to $k\pi$, $k \in \mathbb{Z}$. Indeed, since MCA introduces a slight noise, the result is not exactly 0. We can see in Figure 3 that the maximal noise introduced by MCA on the inputs is in the order of 10^{-14} , two orders of magnitude higher than the $ulp \simeq 10^{-16}$ for double precision. This slight noise introduced can be interpreted as white noise on the input signal. We can see on the bottom row of Figure 4 that the frequency noise is of the same order of magnitude as the input noise, which is expected. The two peaks at $x=38$

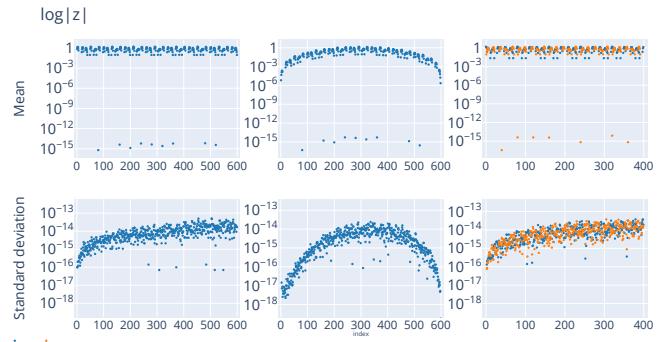


Fig. 3: Absolute value of the mean and standard deviation values for fft 1D inputs within RR mode (log scale). The real part is shown in blue and the imaginary part in orange.

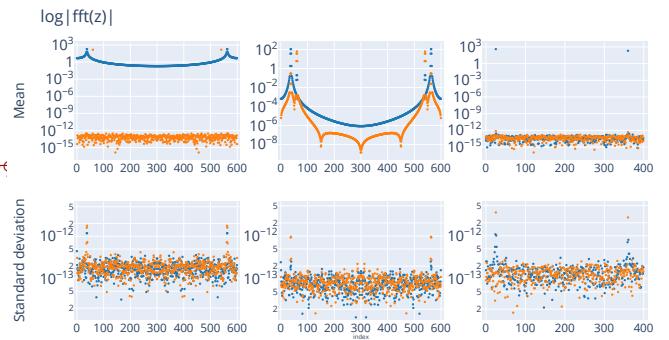


Fig. 4: Absolute value of the mean and standard deviation values for fft 1D outputs within RR mode (log scale).

and $x=562$ corresponds to the actual frequencies of the input signal.

Figure 5 shows the results of the spline evaluation with `bisplev` from the `spline_2D` example. It computes the 2D spline interpolation for function $z = (x + y)e^{-6(x^2 + y^2)}$, with $(x, y) \in [-1, 1] \times [-1, 1]$. The result is a 2D-array that is natively supported by PyTracer. We observe a significant loss of precision in places, which follows an interesting pattern that could be further investigated.

4.3 PyTracer allows visualizing numerical stability at a fine grained level

We illustrate on two examples how PyTracer is effective for analyzing the numerical stability at a fine grained level: Face recognition and Bayesian Ridge Regression. The face recognition example uses eigenfaces (eigenvectors) and Support Vector Machines (SVMs) to classify faces from the Labeled Faces in the Wild dataset. This example uses a Principal Component Analysis (PCA) to extract the eigenfaces and then trains an SVM classifier to predict the name associated with a face. When executing within fuzzy environment, this example crashed with the following Python error raised: “`SVD did not converge`”. This example is the only one to raise an error due to the non-convergence of the Singular Value Decomposition (SVD) performed in the PCA. The PCA uses the Randomized SVD [16] method that first computes a low-rank approximation of the input matrix using a stochastic algorithm and then uses this approximation

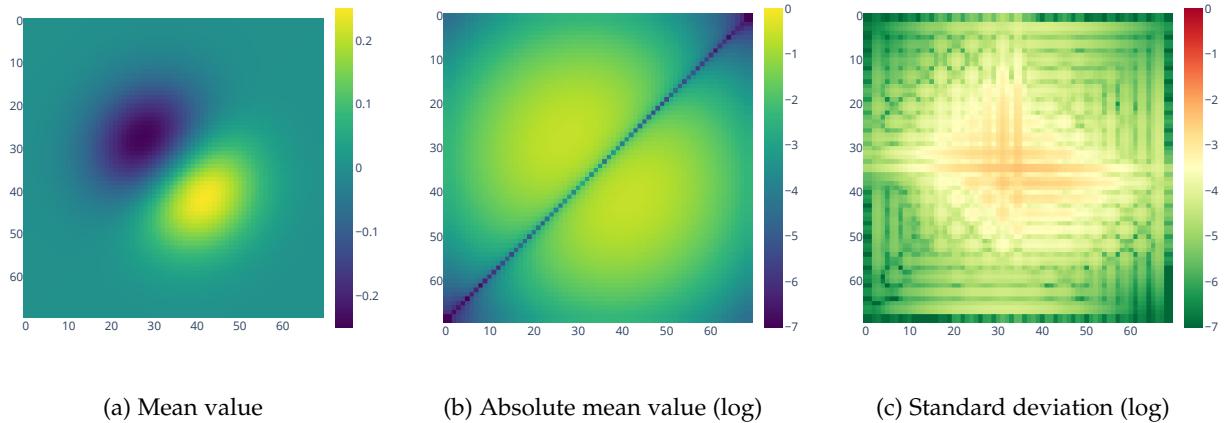


Fig. 5: 2D Spline interpolation results. Figure 5a shows the mean result of the 2D-spline interpolation. Figures 5b and 5c show respectively in the logarithmic scale the absolute mean value and the standard deviation of the 5 samples run within RR mode.

as input for the SVD. When walking through the code with PyTracer, we see that the `randomized_svd` scikit-learn function uses the Divide & Conquer SVD method `gesdd`. The LAPACK library has two main methods for computing the SVD: `gesdd` and `gesvd`. The former uses a Divide & Conquer approach, while the latter uses a QR decomposition. While both methods are expected to have the same accuracy [17], the Divide & Conquer makes the SVD to not converge with MCA.

Replacing `gesdd` for `gesvd` solves the SVD convergence issue. PyTracer allows to quickly visualize the new precision of the result. Figure 6b shows the precision of the eigenvalues computed displayed in decreasing order with `gesvd` in single precision, which varies between 15 and 20 significant bits out of the 24 available in single precision. The classifier metrics (precision, recall, F1-score, and support) are identical to the IEEE execution for all MCA samples. We can note that even with using the `gesvd`, the precision of the singular values (vectors) is not uniform. Indeed, we can see that the precision of the lowest singular values (vectors) decreases until reaching 0 significant bits.

The second example, compares a Bayesian Ridge Regression (BRR) to the Ordinary Least Squares (OLS) estimator on a synthetic dataset and for one-dimensional regression using polynomial feature expansion. Although the example does not raise a runtime error, the regression coefficients computed from the fitting are non-significant. PyTracer traces reveal that the SVD solver used is the root cause for this error. Indeed, the `BayesianRidge` model first computes an SVD before iteratively updating the coefficients until reaching the convergence criterion. However, PyTracer reveals an issue in the singular values computed. We can see on Figure 7a that the last singular values is `NaN` due to numerical error during the SVD although the remaining singular values exhibit high numerical precision (between 44 and 50 bits). Surprisingly, this `NaN` value does not raise issue and is silently propagated. Indeed, the stopping criterion compares that the sum of the absolute differences between coefficients of two successive iterations but coefficients contain `NaN` since they are computed from singular values. Hence, the

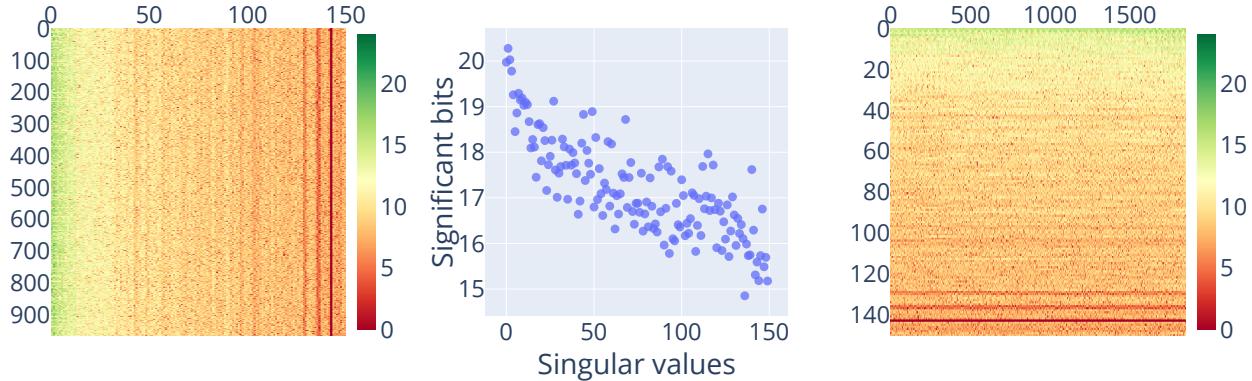
following condition is never met if `iter_ != 0` and `np.sum(np.abs(coef_old_ - coef_)) < self.tol`: since the comparison with a `NaN` is always false.

The OLS uses the Least Square to fit the model. PyTracer shows that the coefficients fitted are `NaN` values. By looking at the callgraph, we can see that the `scipy` calls the `lstsq` method from the `scipy.linalg` package which uses the `gelsd` LAPACK function. Figure 7b shows the singular values returned by the `lstsq` method shows that one singular value has a `NaN` value that corrupted the calculation of the coefficients. By using the `gelss`, PyTracer shows that the `NaN` value disappeared from the singular values (fig. 7d) and thus does not contaminated the computation of the coefficients that exhibit a precision of 42 bits in average. We can see that the full access to all values computed by the application with PyTracer allows the user to quickly identify the issue.

In conclusion, PyTracer and the MCA model were helpful to detect the instability of the `gesdd` method mentioned in several GitHub issues, including the LAPACK repository. Furthermore, it is worth mentioning that a Pull Request has recently been submitted to let the user select the SVD method and avoid this kind of issue. Thus, PyTracer can detect instabilities that affect fundamental scientific computing components such as the LAPACK library. The unify view of all traces allows the user to quickly navigate through the different numerical precision of variables which saves time for the developer compare to the print statement debugging.

4.4 Overhead remains tractable and evolves linearly with the trace size

PyTracer's tracing overhead consists of (1) module instrumentation time (initialization overhead) and (2) data write time during the execution (runtime overhead). The initialization overhead is proportional to the number of functions and classes traced. For example, we measured an average initialization time of 8 seconds during our experiments with NumPy, SciPy, and Scikit-learn. This overhead can be reduced by excluding intensively used functions such as



(a) Left matrix U of the SVD decomposition
(b) Singular values Σ of the SVD decomposition
(c) Right matrix V of the SVD decomposition

Fig. 6: Precision of the `randomized_svd` function in the `face_recognition` example using the `gesvd` SVD method and RR. Figures 6a, 6b, and 6c show respectively the values U , Σ and V . Numerical precision is lower for smaller singular values and this loss of precision translates to singular vectors. It would be interesting to investigate the use of numerical precision for dimensionality reduction.

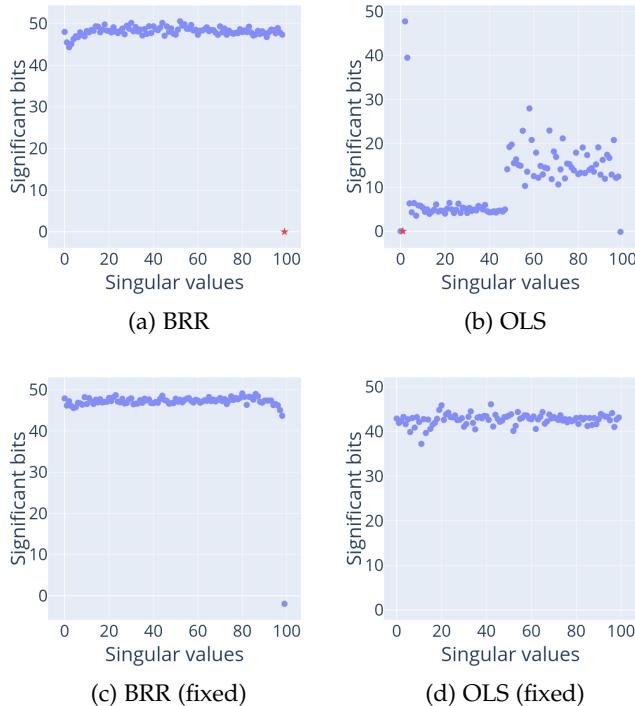


Fig. 7: Numerical precision of the singular values of the SVD from the Bayesian Ridge model fitting (left) and from the Ordinary Least Square model fitting (right) in the Bayesian Ridge Regression example. Red star represents NaN value. Both SVD give NaN coefficients. Switching from Divide & Conquer to QR factorization improve numerical precision. PyTracer helps to quickly visualize improvements.

`numpy.array` from the instrumentation. Figure 8 summarizes PyTracer’s tracing overhead for SciPy and scikit-learn examples. *Slowdown* represents the slowdown of PyTracer without fuzzy measured as the ratio between the actual execution time (without PyTracer) and the execution time using PyTracer. The *Slowdown RR* and *Slowdown MCA* shows the slowdown within the fuzzy environment. Without fuzzy, PyTracer introduces an average slowdown of $17\times$ high for the examples running less than 8 seconds because PyTracer spends most of its time in the initialization step. Since this step is a constant factor of the number of functions instrumented, we also measured the instrumentation cost itself (*Slowdown (Instrumentation)*) calculated by subtracting the initialization time to *Slowdown*. We then obtain an average slowdown of $3.5\times$. Finally, the *fuzzy instrumentation* using MCA operations (through `fuzzy`) instead of the native ones increases the average slowdown to $37\times$ for RR and $43\times$ for Full MCA.

Figure 9 shows the postprocessing time and trace sizes produced by PyTracer. The linear correlation between the log of the size and the log of the time shows a significant correlation (p -value $\leq 10^{-8}$ for RR and p -value $\leq 10^{-3}$ for MCA).

In conclusion, while PyTracer’s overhead is substantial, it remains tractable for real-life examples.

5 DISCUSSION

Through our analysis of SciPy and scikit-learn, we demonstrated PyTracer’s scalability, automaticity, and applicability to a wide range of Python program. The relatively low instrumentation overhead of $3.5\times$ on average enables the analysis of real-scale applications. PyTracer’s instrumentation is fully automatic and does not require manual intervention from the user. Furthermore, PyTracer works on any Python libraries, with any data format supported by pickle and any numerical noise model.

PyTracer is the first tool to enable a systematic numerical analysis of Python codes. Existing tools focus on traditional

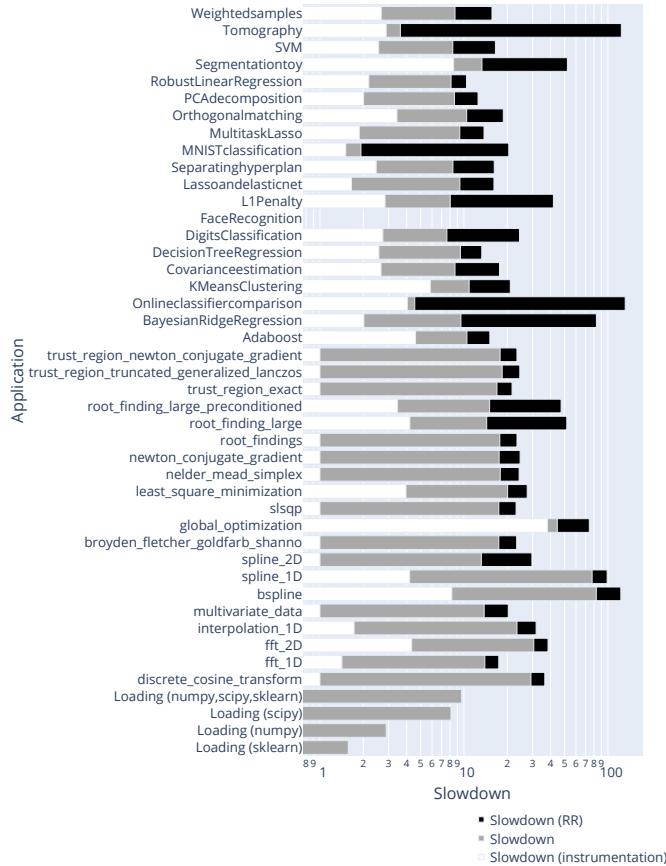


Fig. 8: PyTracer tracing overheads. *Slowdown* represents the slowdown of PyTracer without fuzzy measured as the ratio between the actual execution time (without PyTracer) and the execution time using PyTracer. *Slowdown (Instrumentation)* show the actual instrumentation cost computed by subtracting the initialization step. The *Slowdown (RR)* and *Slowdown (MCA)* are the slowdown of PyTracer using the fuzzy environment with the RR and Full MCA modes. The first four examples measure the initialization steps depending on the modules instrumented.

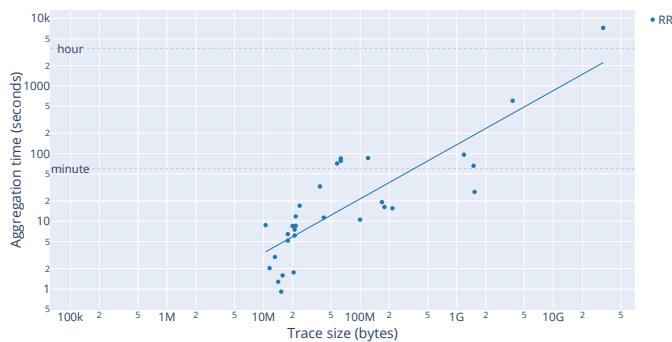


Fig. 9: PyTracer aggregation performance.

languages of the HPC community, such as C, C++, and FORTRAN. However, Python’s high-level abstraction allows for quick application implementations while maintaining high-performance thanks to specialized libraries such as NumPy. Therefore, PyTracer meets the numerical analysis needs of an ever-increasing number of applications.

PyTracer allows users to pinpoint the root causes of numerical instabilities by working at the function level. Numerical stability evaluations are complex since calculations are strongly interdependent. Function-level instrumentation limits the size of the traces since only inputs and outputs of a function are dumped. Moreover, it decreases instrumentation overhead and helps the user identify instabilities quickly. Working at the function level is thus a suitable compromise between analysis conducted at the floating-point operation level and user debug prints. Indeed, fine-grained analyses are costly and hard to interpret as they overwhelm users with information. In contrast, looking at intermediate results through print statements is lightweight but not reliable since developers may not systematically instrument unstable functions. Finally, the SciPy environment wraps many computation kernels written in C, such as BLAS or LAPACK. By working at the function level, PyTracer allows the user to evaluate the numerical precision of such kernels and their impact on the code without getting deep into technical implementation aspects.

Integrating PyTracer at the early stages of the development cycle would improve the overall numerical quality of the developed code. PyTracer’s automaticity facilitates its usage and enables its integration in unit testing. For example, PyTracer could be used in regression tests to ensure that updates do not degrade the numerical quality of a calculation.

PyTracer can also be useful for selecting hyperparameters, as is the case in machine learning. Indeed, it is common for data scientists to explore a range of hyperparameters and select the ones giving the best scores. With PyTracer, the user has a practical way to quantify numerical quality and understand why hyperparameters produce inconsistent results instead of tweaking hyperparameters to make solvers converge. For instance, the Face Recognition example (Figure 6) shows how numerical precision could inform the selection of the number of components in dimensionality reduction.

The visualization provides a global view of the code and interactions between computations. In addition, the Plotly dashboard helps navigate through the code easily, without the need for ad-hoc scripts to visualize data. Finally, the dashboard can be extended to support other data formats to visualize. At this stage, PyTracer currently supports n-dimensional NumPy arrays as well as native Python data.

As we showed in Section ??, using Full MCA mode leads to runtime errors that have a considerable impact on the proper functioning of the execution, which is unfortunate since these errors do not reflect actual numerical errors but are related to perturbations that should not occur. Conversely, RR mode is far more conservative since it preserves exact operations and is easier to use even though it does not simulate all perturbations. Therefore, from our experiments, we recommend the use of RR over Full MCA. More research is required to address the issues encountered with Full MCA.

Finally, the wide range of results precision obtained from our experiments demonstrate that looking at the numerical variability is essential and that such analyses would benefit from being conducted systematically. We showed that well-known scientific libraries are prone to numerical error even though they have been well tested for decades. The omnipresence of these libraries in scientific codes should thus impel users to integrate numerical analysis in their development workflow in addition to testing their implementation.

6 RELATED WORK

Several tools have been developed to assess numerical quality, and can be divided into static and dynamic approaches. Static approaches typically analyze source code, while dynamic approaches trace floating-point computations throughout executions. A detailed review of these approaches is presented in [18]. Numerous tools exists to trace floating-point computations for C, C++, or FORTRAN programs due to the prevalence of these languages in High-Performance Computing (HPC). The main tracing techniques are *source-to-source*, *compiler-based transformations*, and *dynamic binary instrumentation*.

The source-to-source technique requires a rewriting of the application to modify floating-point types and provides a fine-grained control on the analyzed code. CADNA [19] is a library for C, C++, and Fortran implementing CES-TAC [20] stochastic arithmetic. Shaman [21] is a C++ library that uses a first-order error model to propagate numerical error. MCALib [22] is a C library that implements the Monte Carlo Arithmetic (MCA) [9] using the MPFR [23] library.

ADAPT [24] uses Automatic Differentiation to compute a sensitivity profile for each variable of given program. Finally, the work in [25] proposed a source-to-source framework for executing targeted code in infinite and fixed precision with and without stochastic arithmetic. The main drawback of the source-to-source approach is its lacks of scalability since rewriting large codes can be a tedious task.

The compiler-based approach instruments floating-point expressions at compile time and so allows the user to automatically instrument large codebases. Verificarlo [8] is a compiler that supports different types of arithmetic instrumentations, including MCA. The work in [26] modified the GNU Compiler Collection (GCC) to track local floating-point errors across executions. pLiner [27] is a root-cause analyzer based on the Clang compiler that detects floating-point operations responsible for result variability using a source-to-source transformation at the Abstract Syntax Tree (AST) level to rewrite parts of code with higher precision. PFPSanitizer [28], [29] and NSan [30] are compiler based approaches that use shadow execution to detect numerical issues using higher precision. FLiT [31] is a framework to detect variability induced by compilers and their optimizations. The work in [32] proposes a numerical debugger based on GDB [33] for Discrete Stochastic Arithmetic (DSA) on FPGA as an Eclipse plugging. Similarly, Cadtrace [19] and Shaman propose a GDB-based tool to use the CADNA and Shaman libraries with GDB, respectively. The main limitation of the compiler-based approach is that one must have access to the source code.

Dynamic Binary Instrumentation (DBI) operates directly on executables, without the need for recompilation or manual changes. Therefore, it is applicable to any programming language. CraftHPC [34] uses DBI to detect catastrophic cancellations at runtime. Verrou [35] is a Valgrind [36] based tool that dynamically replaces floating-point operations with their stochastic arithmetic counterparts. FPDebug [37] uses DBI to detect numerical inaccuracies by using shadow computations with higher precision. Herbgring [38] is a Valgrind-based tool to detect numerical instabilities. It uses a shadow memory to detect precision losses by comparison with results obtained at in higher precision. It is combined with symbolic computation to backtrack the root of the error. We can note that all methods based on a high-precision oracle suppose that computing with a large number of bits is sufficient to obtain an accurate result, which is not always true (see for example, the famous Muller's sequence [39]). Although versatile, the DBI loses high-level information useful to understand the source-code logic.

Being agnostic to the programming language is a serious advantage of the DBI method compared to source-to-source and compiler-bases methods. However, working at the binary level makes it difficult to access high-level information needed to debug and understand the source-code logic. Conversely, the source-to-source approach provides a fine-grained control on the analyzed code, but it lacks scalability, as rewriting large codes can be a tedious task. Finally, the compiler-based approach takes advantage of the best of both by being automatic and having access to high-level information. However, like source-to-source, the compiler-based method is not suitable for analyzing closed-source libraries.

To the best of our knowledge, PyTracer is the first tool dedicated to the numerical analysis of Python code. Existing tools for tracing Python code focus on performance profiling for time (cProfile) or memory consumption (memprofile). Anteater [40] is a Python tracer tool to debug Python applications. It performs source transformations at the AST level but only deals with native numeric Python types. Moreover, the user needs to manually tag each variable to trace. Finally, according to the authors, Anteater does not scale to large traces. cProfile, memprofile, and Anteater use Python decorators as the primary instrumentation technique, a Python mechanism to instrument a function by adding a line over a function declaration. While this method is appropriate when targeting specific functions, it is not feasible for large codebases where potentially unstable code sections are unknown.

7 CONCLUSION

Evaluating the numerical stability of scientific Python programs is a tedious task that requires substantial expertise. Automatic tools to help users understand the behavior of their code are therefore crucial. In this perspective, PyTracer is the first tool to offer a complete framework for analyzing and visualizing the numerical stability of Python codes. It works by automatically instrumenting Python libraries to produce numerical traces visualized through an interactive Plotly Dash server. PyTracer does not require manual code modification, and we tested it with major scientific libraries

such as NumPy, SciPy, and Scikit-learn. Our results show that PyTracer is scalable, with an average instrumentation slowdown of $3.5\times$. Moreover, PyTracer's visualization interface remains responsive even with traces of up to 1TB. In our experiments, PyTracer enabled the systematic evaluation of 40 examples from the SciPy and scikit-learn libraries.

In future work, we plan to extend the post-processing analysis to aggregate traces when the execution flow path diverges by leveraging techniques used in code coverage analysis. Moreover, we would like to extend PyTracer to instrument elementary arithmetic operations which can be helpful to more profound analyses. Finally, although PyTracer supports multiple noise models, we only tested it with Monte Carlo Arithmetic. Therefore, we would like to compare different models against MCA. PyTracer is available at [github://big-data-lab-team/pytracer](https://github.com/big-data-lab-team/pytracer) under MIT License.

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Tristan Glatard is Associate Professor in the Department of Computer Science and Software Engineering at Concordia University in Montreal, and Canada Research Chair (Tier II) on Big Data Infrastructures for Neuroinformatics. Before that, he was research scientist at the French National Centre for Scientific Research and Visiting Scholar at McGill University.

APPENDIX



Yohan Chatelain received his Ph.D. degree from the University of Paris-Saclay (UVSQ), Versailles, France in 2019. He is a postdoctoral researcher in the Big Data Infrastructures for Neuroinformatics lab at the University of Concordia, Montreal, Canada. His research topics include computer arithmetic, high-performance computing, and reproducibility. Yohan aims at democratizing the use of the analysis of stability for scientific computing codes through automatic tools to improve numerical quality.



Nigel Yong Sao Young was born in Mauritius Island. He is a recent Computer Science graduate at Concordia University. He is currently working on his software startup, based in the city of Montreal.



Gregory Kiar is a research scientist at the Child Mind Institute. Throughout his degrees in Biomedical Engineering, Greg has developed techniques to study biosignal data, a turn-key tool that allows researchers to generate maps of brain connectivity from diffusion MRI data, and techniques to assess and improve the stability of research in neuroscience. Greg's research bridges the fields of numerical analysis and brain imaging to evaluate and improve the trustworthiness of techniques used to study the brain.

We tested PyTracer on SciPy examples provided in the tutorial website section. SciPy is organized in several libraries targeting specific computing domains. We focused on `fftpack` (Fast Fourier Transform routines), `interpolate` (interpolation and smoothing splines), and `optimize` (Optimization and root-finding routines).

.1 Interpolation

This package has five examples: `interpolation_1D`, `multivariate_data`, `bspline`, `spline_1D` and `spline_2D`.

`interpolation_1D` interpolates function $f(x) = \cos\left(\frac{-x^2}{9}\right)$ with 11 points $x \in [0, 10]$. For the five interpolation methods tested (linear, cubic, nearest, previous, next), the solution found is precise, up to 51 bits out of the 53 available.

`multivariate_data` interpolates the grid $f(x, y) = x(1-x)\cos(4\pi.x)\sin(4\pi.y^2)^2$ with $(x, y) \in [0, 1] \times [0, 1]$. It samples 1,000 points for each coordinate and uses three interpolation methods: nearest, linear and cubic. Our results show a precision of 51 bits on average for the three methods.

`bspline` compares two edge filters: `bisplev` evaluates a bivariate B-spline and its derivative whereas `convolved2d` convolves two 2-dimensional arrays. Figure 10 shows the significant bits, mean, and standard deviation maps for the two methods as well as the input image (Fig. 10a). The middle row shows `sepfir2d` results and the bottom row shows `convol2d` results. Both methods exhibit similar precision, with 11 significant bits on average. Standard deviations maps on Figures 10d and 10g show that regions with low spatial frequencies correspond to regions with low standard deviation, similar to the FFT results. The SciPy tutorial mentions that `bisplev` is faster than `convol2d`. The comparable numerical precision observed in our experiments reinforce the use of `bisplev` over `convol2d` in this example.

`spline_1D` computes the 1D spline interpolation for $f(x) = \sin(x)$ on points $x = \frac{2\pi k}{8}$, $k \in [0, 10]$. The spline interpolation uses `splrep` to build the spline representation and `splev` to evaluate the spline at any point. It also computes the integral by using `splint` and the root finder `sproot`. Although the traces diverge, we can analyze the partial aggregation for the `splrep`, `splev` and `splint`. The three functions show results with an average precision of 51 bits with RR mode.

`spline_2D` computes the 2D spline interpolation for function $z = (x+y)e^{-6(x^2+y^2)}$, with $(x, y) \in [-1, 1] \times [-1, 1]$ and a sampling of 21 points for each coordinate. `bisplrep` builds the spline representation with the 21×21 points of z over 71 grid sampling points for (x, y) . Figure 5 shows the results of the spline evaluation with `bisplev`. We observe a significant loss of precision in places, which follows an interesting pattern that could be further investigated.

.2 FFT

This package has three examples : `discrete_cosine_transform`, `fft_1D`, and `fft_2D`. All computations are done in double precision. The results for `discrete_cosine_transform`, `fft_1D` and `fft_2D` show precise numerical results with 48 significant bits on average. We

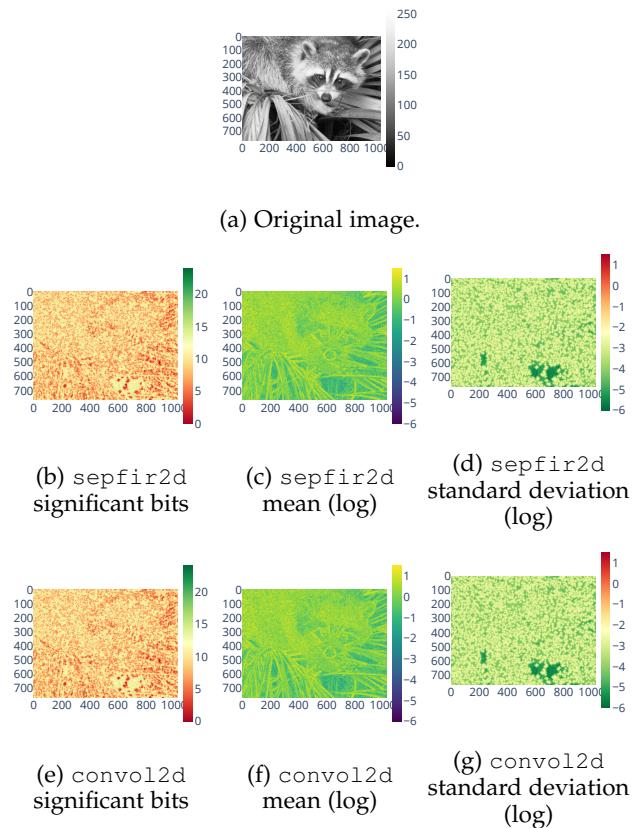


Fig. 10: `bspline` results within RR mode. `sepfir2d` and `convol2d` have a similar precision.

observe that the FFT computation is stable to noisy inputs. Figures 3 (inputs) and 4 (outputs) show the mean and standard deviation of the MCA samples. The three columns correspond to the FFT computations of:

- 1) $z_1 = \sin(50.2\pi.x_i) + \frac{1}{2} \sin(80.2\pi.x_i)$, $x_i = \frac{i}{600}$, $i \in [0, 600]$
- 2) `blackman(400) $\times z_1$`
- 3) $z_2 = e^{50.i2\pi.x_i} + \frac{1}{2} e^{-80.i2\pi.x_i}$, $x_i = \frac{i}{800}$, $i \in [0, 400]$

The top row in Figures 3 and 4 show the input mean value while the bottom row shows the standard deviation. The points with low magnitude in Figure 3 correspond to inputs near 0 when the input of `sin` or `exp` is close to $k\pi$, $k \in \mathbb{Z}$. Indeed, since MCA introduces a slight noise, the result is not exactly 0. We can see in Figure 3 that the maximal noise introduced by MCA on the inputs is in the order of 10^{-14} , two orders of magnitude higher than the $ulp \simeq 10^{-16}$ for double precision. This slight noise introduced can be interpreted as white noise on the input signal. We can see on the bottom row of Figure 4 that the frequency noise is of the same order of magnitude as the input noise, which is expected. The two peaks at $x=38$ and $x=562$ corresponds to the actual frequencies of the input signal.

.3 Optimization

This package has eleven examples. Seven examples involve the same optimization problem solved with and without

constraints using different methods. One example optimizes a chemical problem under constraints. The last three examples solve a different problem each.

.3.1 Unconstrained minimization of multivariate scalar functions

Four Quasi-Newton-Raphson methods minimize function f by using Newton's step: $x_{k+1} = x_k - B^{-1}(x_k)\nabla f(x_k)$, where ∇ and B are the gradient and the approximation of the Hessian matrix of f . The Broyden-Fletcher-Goldfarb-Shanno [41] (BFGS) and Newton-Conjugate-Gradient [42] (NCG) are line search methods that approximate H by adding two symmetric rank-one matrices and by using the Conjugate-Gradient method. The Trust-Region Truncated Generalized Lanczos / Conjugate Gradient [43] (TR-Krylov), Trust-Region Newton-Conjugate-Gradient (TR-NCG), and Trust-Region Nearly Exact [42] (TR-Exact) are trust-region methods approximating H by solving the trust-region subproblem restricted to a truncated Krylov subspace and by solving nonlinear equations for each quadratic subproblem. In addition, the Nelder-Mead [44] simplex-based method iteratively transforms a simplex until its vertices are getting closer to a local minima of the function. All methods are applied to the Rosenbrock function.

3.1.1 Constrained minimization of multivariate scalar functions: Two optimizers solve an optimization problem by taking into account constraints. The Sequential Least Squares Programming uses the SLSQP [45] method to optimize the Rosenbrock function. The Least-squares minimization uses the Trust Region Reflective algorithm [46] to solve a fitting problem from an enzymatic reaction.

The SLSQP and unconstrained minimization methods minimize the **Rosenbrock** function of N variables that reaches its minimum (0) when $x_i = 1, \forall i \leq N - 1$: $f(x) = \sum_{i=1}^{N-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$. Figure 11 shows the number of significant bits of the solution for the different methods used. The (p) notation for the NCG, Trust-Krylov, and Trust-NCG methods in the legend refers to the variant where the Hessian matrix is replaced by a function computing the matrix-vector product of the Hessian and an arbitrary vector, to save memory and time. All the methods have a good precision ranging from 43 to 53 significant bits. The Nelder-Mead method is the least precise one with $\simeq 43$ significant bits on average, while the Trust-Region-Newton-CG is the most precise one with $\simeq 53$ significant bits, the highest precision achievable in double precision. The remaining methods have a similar precision.

The SLSQP also minimizes the Rosenbrock function with the following constraint: $x_0 + 2x_1 \leq 1$ $x_0^2 + x_1 \leq 1$ $x_0^2 - x_1 \leq 1$ $2x_0 + x_1 = 1$ $0 \leq x_0 \leq 1$ $-0.5 \leq x_1 \leq 2$. The problem has a unique solution $[x_0, x_1] = [0.4149, 0.1701]$. Results obtained with RR show a precision of 47 and 44 significant bits for the first and the second solution.

The least-square minimization example solves a fitting problem from an enzymatic reaction [47] with 11 residuals defined as:

$$\begin{aligned} f_i(x) &= \frac{x_0(u_i^2 + u_i x_1)}{u_i^2 + u_i x_2 + x_3} - y_i, \quad i = 0, \dots, 10 \\ 0 &\leq x_j \leq 100, \quad j = 0, \dots, 3 \end{aligned}$$

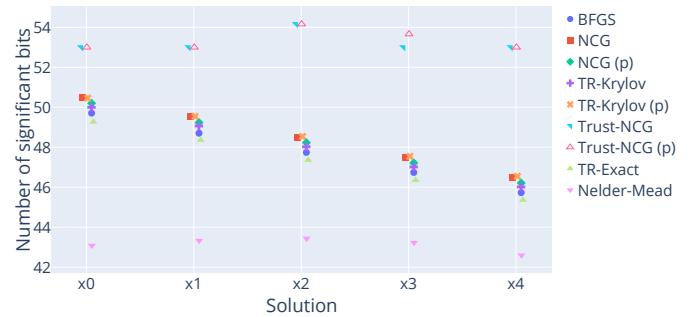


Fig. 11: Comparison of results precision for different optimization solvers within RR mode.

where y_i are measurement values, u_i are values of the independent variable, and x_i the unknown. Results within RR show a precision of 51, 46, 47, and 48 significant bits for each component of the solution respectively.

.3.2 Root finding

The root_* examples use three algorithms to find the root of non-linear equations. root_finding uses the hybrid Powell method to solve a single-variable transcendental equation and the Levenberg-Marquardt method for a set of non-linear equations. root_finding_large and root_finding_large_preconditioned examples use the Krylov method to approximate the inverse Jacobian with and without the help of a preconditioner. They solve an integrodifferential equation on a square $(x, y) \in [0, 1] \times [0, 1]$, $P(x, 1) = 1$, and $P = 0$ elsewhere on the boundary. The function P is discretized with a Cartesian grid $P_{n,n} = P(nh, nh)$, with $n = 75$, and its derivatives are approximated by $\partial_x^2 P(x, y) \simeq (P(x + h, y) - 2P(x, y) + P(x - h, y))/h^2$.

All the examples diverge even within RR, which is not surprising since root-finding methods can easily take a few extra steps to find the root depending on the starting point. Nevertheless, for the root_finding_large example, 3 traces among the 5 samples can be merged for both RR and MCA modes. Figure 12 shows the mean and standard deviation of the result for these 3 samples. We can see that a similar solution was found for RR and Full MCA. Full MCA leads to a lower precision than RR although both standard deviation maps remain in the same order of magnitude. Finally, it is interesting to note the impact of preconditioning on the result numerical quality: as Table 1 shows, the precision doubles between root_finding_large and root_finding_large_preconditioned.

.4 Scikit learn

Scikit-learn offers a well-supplied and documented list of examples that facilitates its use with Pytracer. Among the several available examples, we choose the following representative set listed in Table 1. The following paragraphs focus on the most interesting stability results observed across all experiments.

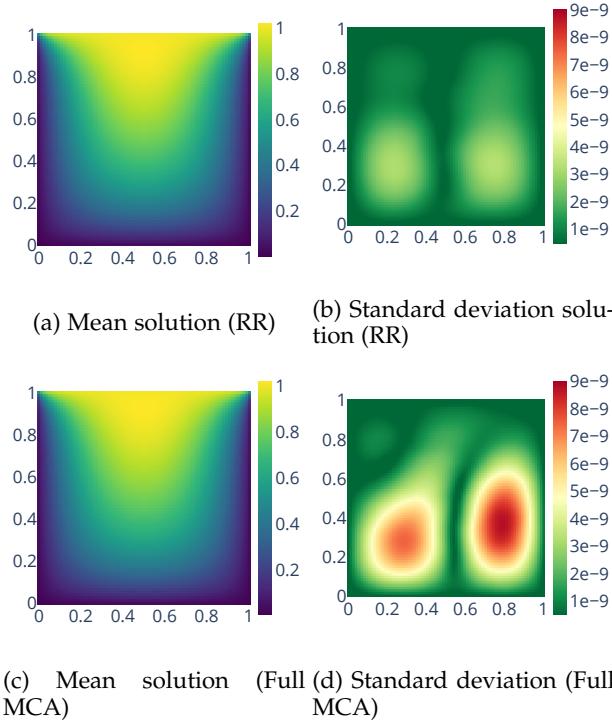


Fig. 12: Solution of `root_finding_large` example. The standard deviation has two maximum for both RR and Full MCA modes. The standard deviation remains lower than the stopping criterion threshold fixed at 6.10^{-6} .

4.1 Separating hyperplane

This example uses a linear Support Vector Machine (SVM) classifier trained using the Stochastic Gradient Descent (SGD) method to find the maximum separating hyperplane between sets of 2D points. The example trains the SVM with 50 random points separated in 2 clusters with hyperparameter $\alpha = 0.01$ and using the hinge loss function. Once the model is trained, the example generates a $[-1, 5] \times [-1, 5]$ Cartesian grid discretized with 100 points and predicts the class label for each point with integer coordinates. Figure 13a shows the number of significant bits obtained with RR for each point of the grid. We can see that yellow regions close to the separating hyperplane are highly unstable with a number of significant bits below 0, meaning that the classifier is unsure about the predicted class.

4.2 SVM

This example uses a plain Support Vector Classification [48] (SVC) to find the best hyperplane separating an unbalanced dataset with two classes of 1000 and 100 points. This example tests two SVC configurations using a linear kernel with and without a class weight parameter. The SVC predicts the class label for each coordinate over a $[-5, 5] \times [-5, 5]$ grid discretized with 900 points. Figures 13b and 13c show the result within RR of the classification with and without taking into account the unbalancing. We can see that the number of significant bits is lower on the separating line and that taking into account class imbalance allows for a better separation.

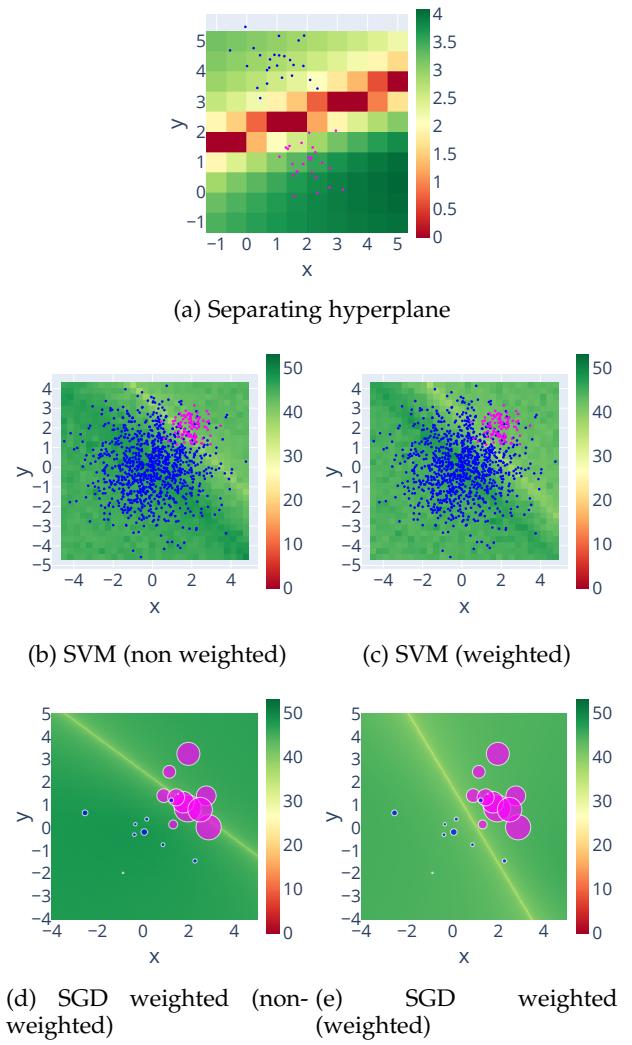


Fig. 13: Three examples of separating hyperplane prediction. All the figures show the number of significant bits of the prediction in RR mode. The separating hyperplane corresponds to a lower-precision region in each figure. Using a large discretization step amplifies this instability.

4.3 SGD weighted samples

This example uses an SGD to separate weighted points. It divides the training set into two classes of 10 points with a bigger weight for the second class. The SGD is trained with hyperparameters $\alpha = 0.01$ and a maximum number of iterations to 100. The prediction is made on a $[-4, 5] \times [-4, 5]$ grid discretized with 250,000 points. Figures 13d and 13e show the number of significant bits of prediction within RR along with dataset points in blue and **violet** purple. We can see that the separating plane corresponds to a region of lower precision, similar to the previous examples.