Timing and Benchmarking Scientific Python

EuroSciPy 2023

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What we're going to cover

Why this talk?

Why does time matter?

Thinking of measurement as an experiment

Taking a single measurement

Running a single Benchmark

What's out there?

Benchmark Design

Our benchmark

Comparing Benchmarks

Why this talk?

Look at timing and benchmarking in the SciPy ecosystem

- · Look at timing and benchmarking in the SciPy ecosystem
- Analyse the methodology of different articles & papers in the scientific Python ecosystem

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- Analyse the methodology of different articles & papers in the scientific Python ecosystem
- Discuss what is done well and where improvements could be made
- · Apply the points learnt to SciPy's benchmarking suite

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- $\boldsymbol{\cdot}$ Cover topics you should consider when timing

What this talk is not

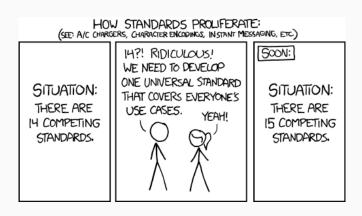


Figure 1: standards

Why does time matter?

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- · How sure are you that it is faster?

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$ python -m timeit "sum(n*n for n in range(10000000))" 1 loop, best of 5: 343 msec per loop
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Which run gives the true time?

Variance makes time measurement hard

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- · Computers can reproduce answers bit for bit
- Computers cannot reproduce runtime

• Who likes waiting?

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- · Who likes waiting?
- There are many performance metrics...
- · ...many of which depend on time
- · Accurate time measurement is crucial for accurate metrics

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experiment

Thinking of measurement as an

Statistically rigorous?

There are three kinds of lies: lies, damned lies, and statistics.

Unknown

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 - **Relevant** The experiment being run should be relevant to what is being studied.
 - **Replicable** Repetition of the experiment under similar conditions strengthens the validity of the results.
- **Documented** Clearly document all aspects of the experiment, including the study design, methods, results, and limitations.

What to measure?

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Clock cycles

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- Clock cycles
- Time

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Reproducible Benchmarks: Documentation

Reproducible Benchmarks: Automation

Taking a single measurement

Analysis of experiments

You can't fix by analysis what you bungled by design.

Light, Singer, and Willett [1990]

Observer Effect

Observer Effect Hardware Effects

Observer Effect Hardware Effects Garbage Collection

Observer Effect Hardware Effects Garbage Collection Warmups & Steady State

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- · Instrumentation normally adds overhead
- "You thought the code was slow to start with, so you made it slower to see how slow it was" - Adelstein-Lelbach [2015]

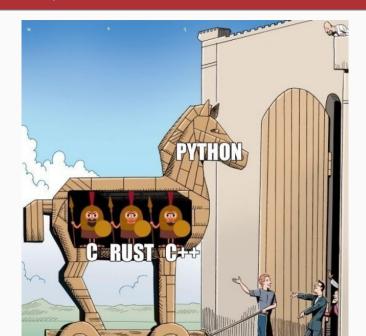
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- Mainly noticeable in low level languages

Why care in Python?

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- The gc module provides an interface to the garbage collector

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```
>>> import gc
>>> gc.collect()
>>> gc.disable()
```

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- · Overhead can vary greatly, especially when using JIT compilers
- \cdot Many benchmarking suites ignore the first n values of a run
- · Warmup vs steady state is still a work in progress

Running a single Benchmark

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- May not always reflect real-world usage scenarios accurately

What's out there?

 Inbuilt Python module to measure execution time of small code snippets

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- · Returns the average of the minimum time of each run

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- · Detect if a benchmark result seems unstable

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- https://asv.readthedocs.io/en/stable/

Benchmark Design

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- · Also, which average do you use?

Average vs Minimum Time

- Minimum time allows us to get a "frictionless model" of performance, this is used by timeit
- Average time allows us to mathematically increase the accuracy of the measure by taking more samples, this is used by pyperformance
- · Also, which average do you use?
- · There is not yet a consensus on which measure should be used

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- The distribution of results might not always follow a normal distribution
- In this case we must adopt different statistical tools

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- Statistical tests can be employed to formally assess the normality assumption, such as the Shapiro-Wilk test

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- see Lemire [2023]

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- The shortest raw value takes less than 1 millisecond

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- It is important to understand how it effects the benchmark result
- pyperformance chooses to include outliers, as it wants to reflect real world usage
- Outliers due to perturbing events may or may not be included in your analysis

Our benchmark

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- https://github.com/python/pyperformance

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- · Model the orbits of Jovian planets, using a simple integrator
- There does not exist an analytical solution
- · Microbenchmark on floating point operations

Eyeballing the distribution

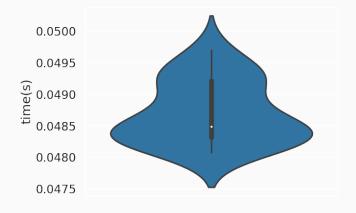


Figure 3: violinplot of n-body runtimes (s)

The summary statistics

count	20
mean	48.706
std	0.495
min	48.071
50%	48.489
max	49.701

Table 1: Summary statistics for the n-body benchmark (ms)

What about our simple error check?

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• Minimum of the runs is 48.071 ms

What about our simple error check?

- · Minimum of the runs is 48.071 ms
- · Mean of the runs is 48.706 ms
- ✓ Very close together

✓ The standard deviation is 1% of the mean

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Comparing Benchmarks

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- Want to compare how a change in the OS affects our runtime performance
- · Ran the benchmark on Linux and Windows
- · Was careful to present a fair and unbiased approach
- Let's compare the results!

Looking at the statistics

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· Linux ran with a mean time of 49 ms

Looking at the statistics

- · Linux ran with a mean time of 49 ms
- · Windows ran with a mean time of 70 ms

For the n-body problem it's obvious...

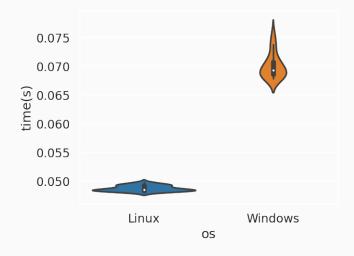


Figure 4: Runtime of the *n-body* benchmark

How comfortable are you saying this speedup is significant?

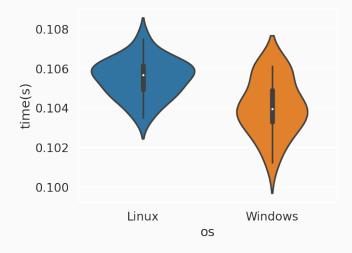


Figure 5: Runtime of the sympy_sum benchmark

· Sample size and data quality

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- · Distributions capture variability

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- · Distributions capture variability
- · Skewness and asymmetry

References i

References

- B. Adelstein-Lelbach. Benchmarking c++ code, 2015. URL https://youtu.be/zWxSzcpeS8Q?t=534.
- distributed?, 2023. URL https://lemire.me/blog/2023/04/06/

are-your-memory-bound-benchmarking-timings-normally-di

R. J. Light, J. D. Singer, and J. B. Willett. *By Design: Planning Research on Higher Education*. Harvard University Press, 1990.

D. Lemire. Are your memory-bound benchmarking timings normally

References ii

T. Mytkowicz, A. Diwan, M. Hauswirth, and P. F. Sweeney. Producing wrong data without doing anything obviously wrong! SIGARCH Comput. Archit. News, 37(1):265–276, mar 2009. ISSN 0163-5964. doi: 10.1145/2528521.1508275. URL https://doi.org/10.1145/2528521.1508275.