Timing and Benchmarking Scientific Python

EuroSciPy 2023

Kai Striega 2023-08-16, 13:30 - 14:00

Software Developer & SciPy Maintainer

How to get the slides

How to get the slides

· Available on GitHub

How to get the slides

- · Available on GitHub
- https://github.com/Kai-Striega/EuroSciPy-2023/ blob/main/EuroSciPy_Speech.pdf

Disclaimer

- · I am not a statistician
- · Many of these techniques are rules of thumb that I work with

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
- Comparing groups of Benchmarks
- Conclusion

Why this talk?

Look at timing and benchmarking in the SciPy ecosystem

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- 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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- Many did not even state their methodology

What this talk is

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 $\boldsymbol{\cdot}$ Advocate for a statistically rigorous approach to timing

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- · Advocate for a statistically rigorous approach to timing
- $\boldsymbol{\cdot}$ Cover topics you should consider when timing

What this talk is not

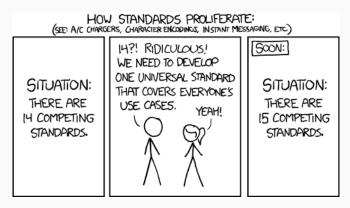


Figure 1: standards

Why does time matter?

You have two solutions S and S'

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- · You are told that:
 - · S runs in 100s
 - S' runs in 95s

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- · You are told that:
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 - *S'* runs in 95s
- · Which is faster?
- · How sure are you that it is faster?

```
$ python -m timeit "sum(n*n for n in range(10000000))" 1 loop, best of 5: 343 msec per loop
```

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$ python -m timeit "sum(n*n for n in range(10000000))" 1 loop, best of 5: 343 msec per loop $ python -m timeit "sum(n*n for n in range(10000000))" 1 loop, best of 5: 310 msec per loop
```

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1 loop, best of 5: 310 msec per loop
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1 loop, best of 5: 312 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

Variance makes time measurement hard

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

Time is an important metric

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• Who likes waiting?

Time is an important metric

- · Who likes waiting?
- \cdot There are many performance metrics...

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- There are many performance metrics...
- \cdot ...many of which depend on time

Time is an important metric

- · 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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Statistically rigorous?

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

Unknown

experiment

Thinking of measurement as an

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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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- Reproducibility Well-documented benchmarking procedures enable others to replicate your experiments, ensuring that results can be verified and compared consistently
- Maintenance Over time, software may undergo changes, and maintaining up-to-date documentation helps future developers understand and modify the benchmarking suite without confusion

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 - Scalability As the benchmarking suite grows with new experiments and datasets, automation helps manage the complexity and handle large-scale experiments efficiently
- Continuous Integration Automation can be integrated into the software's development workflow, running benchmarks automatically with each code change, ensuring that performance regressions are caught early

Taking a single measurement

Analysis of experiments

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

Light, Singer, and Willett [1990]

What effects a single measurement (not exhaustive!)

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Observer Effect

What effects a single measurement (not exhaustive!)

Observer Effect Hardware Effects

Observer Effect

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Observer Effect

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Observer Effect

- · All forms of instrumentation may change the result
- · 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]

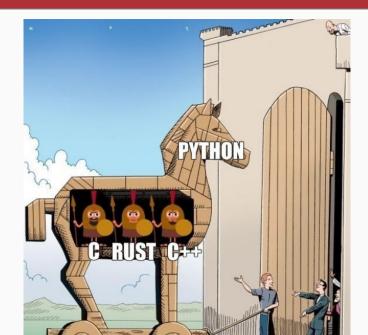
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- Mainly noticeable in low level languages

Why care in Python?

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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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- · Performs multiple runs and repeats of the statement
- · Returns the average of the minimum time of each run

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- · Automatically calibrate a benchmark for a time budget
- · Detect if a benchmark result seems unstable

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

Benchmark Design

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- 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

Can we assume a normal distribution?

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- Normality is assumed in many benchmarking suites
- The distribution of results might not always follow a normal distribution
- In this case we must adopt different statistical tools

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- · Visually "eyeballing" the test
- · Visualising with a QQ-plot
- 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 minimum or the maximum is 50% smaller or greater than the mean
- The shortest raw value takes less than 1 millisecond

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- It is important to understand how it affects 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

 N-body benchmark from the Computer Language Benchmarks Game

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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

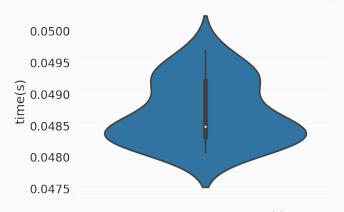


Figure 3: violinplot of n-body runtimes (s)

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

- ✓ The standard deviation is 1% of the mean
- ✓ The minimum and the maximum are very close to the mean

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- ✓ The shortest raw value took 48 milliseconds

Comparing Benchmarks

 Want to compare how a change in the OS affects our runtime performance

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- · Ran the benchmark on Linux and Windows

- 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

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...

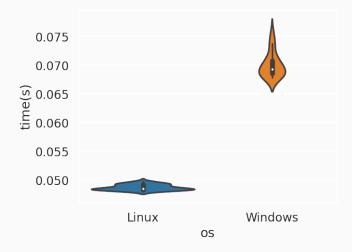


Figure 4: Runtime of the *n-body* benchmark

How comfortable are you saying this speedup is significant?

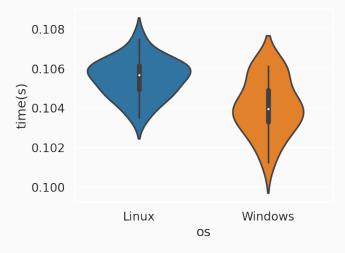


Figure 5: Runtime of the sympy_sum benchmark

Sample size and data quality

- Sample size and data quality
- · Distributions capture variability

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- · Distributions capture variability
- Skewness and asymmetry

Comparing groups of Benchmarks

What are we *trying* to do?

What are we trying to do?

Trying to answer a question:

What are we trying to do?

Trying to answer a question: How does our change effect the system?



A single benchmark does not tell us much about the system

· A single benchmark only illuminates one facet of the system

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- · Want to understand how the system as a whole changes

A single benchmark does not tell us much about the system

- · A single benchmark only illuminates one facet of the system
- · Want to understand how the system as a whole changes
- Need to compare multiple relevant benchmarks for each part of the system

· Total of 95 benchmarks

- Total of 95 benchmarks
- · On some of them Linux is faster, on some Windows is faster

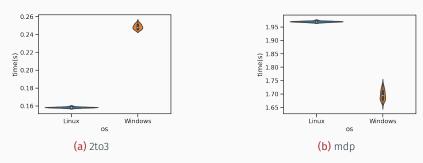


Figure 6: Example difference in benchmark outcomes

Count the number of times Linux or Windows is significantly faster

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- · Compare how likely this difference is to occur due to chance

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- · Compare how likely this difference is to occur due to chance
- · If significant, consider the one with the higher count as faster

Is Linux or Windows faster?

· Linux is faster 78 times

- · Linux is faster 78 times
- · Windows is faster 15 times

- · Linux is faster 78 times
- · Windows is faster 15 times
- The difference is statistically insignificant twice

- · Linux is faster 78 times
- · Windows is faster 15 times
- The difference is statistically insignificant twice
- · According to our rule of thumb, Linux is faster

Conclusion

• Timing is hard because of variance in your measurements

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- · Document & Automate

- Timing is hard because of variance in your measurements
- · Different methods, each with their own trade-offs, exist
- Make sure your choices are relevant to your work
- · Document & Automate
- Analyse distributions, not summary statistics

Let's stay in touch!

- I love to talk about Python & Performance
- · GitHub: https://github.com/Kai-Striega
- · LinkedIn: https://www.linkedin.com/in/kai-striega/



Figure 7: QR code to my LinkedIn profile

References i

References

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

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