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

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- 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?

What this talk was supposed to be

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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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- Dearth of papers looking at the performance of Scientific Python

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- Many lack adequate analysis of their results

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- Dearth of papers looking at the performance of Scientific Python
- Many lack adequate analysis of their results
- Many did not even state their methodology

What this talk is

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- Advocate for a statistically rigorous approach to timing

What this talk is

- Advocate for a statistically rigorous approach to timing
- Cover topics **you** should consider when timing

What this talk is not

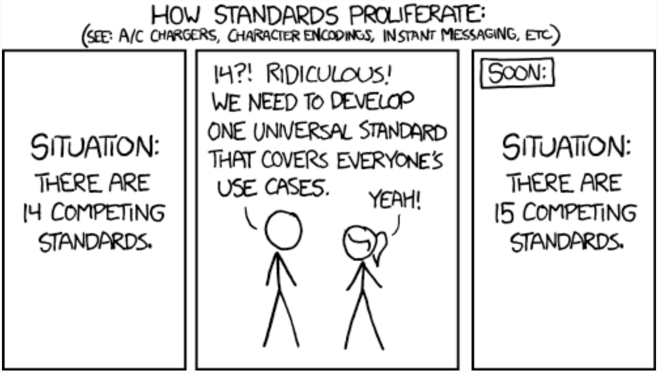

Figure 1: standards

Why does time matter?

A common problem...

A common problem...

- You have two solutions S and S'

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- You have two solutions S and S'
- 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?

Computers can reproduce answers, not performance

```
$ python -m timeit "sum(n*n for n in range(10000000))"
1 loop, best of 5: 343 msec per loop
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1 loop, best of 5: 312 msec per loop
```

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?
- There are many performance metrics...

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- …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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- Different studies use different, often ad-hoc, methodologies
- Many lack statistical treatment of their results
- Many do not even state their methodologies

Statistically rigorous?

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

Thinking of measurement as an experiment

What makes a good experiment?

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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?

What to measure?

- Clock cycles

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- Time

How to make benchmarks reproducible?

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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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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

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Hardware Effects

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- All forms of instrumentation may change the result

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- Instrumentation normally adds overhead

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- 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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- Mytkowicz et al. [2009] showed that link order and environment variable size can significantly affect measurement
- Mainly noticeable in low level languages

Why care in Python?

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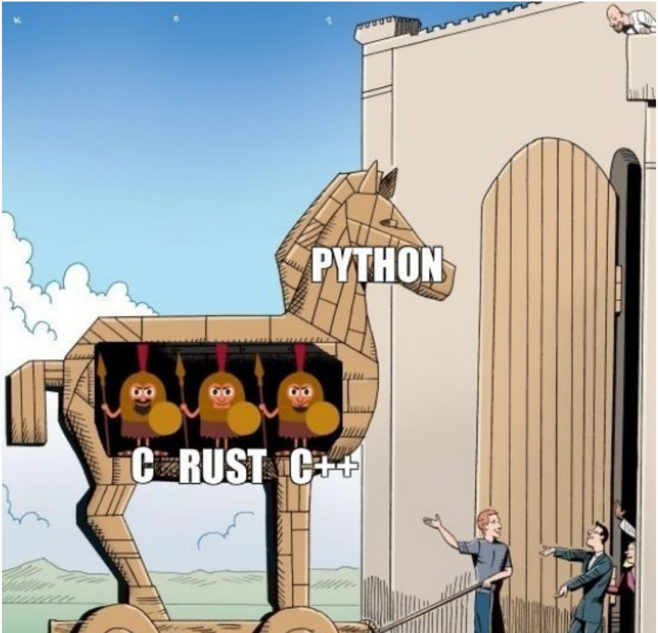

Garbage Collection

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- Garbage collection can freeze your program at any point

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- The *gc* module provides an interface to the garbage collector

Garbage Collection

Consider performing garbage collection then disabling the garbage collector before taking a measurement:

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

Warmups & Steady State

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- Overhead can vary greatly, especially when using JIT compilers
- 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

What is a benchmark?

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- Benchmarks are useful tools for performance analysis
- May not always reflect real-world usage scenarios accurately

What’s out there?

timeit

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- Inbuilt Python module to measure execution time of small code snippets

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- Performs multiple runs and repeats of the statement

timeit

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- Returns the average of the minimum time of each run

pyperf

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- Is a toolkit to write, run and analyze benchmarks

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- Is a toolkit to write, run and analyze benchmarks
- Automatically calibrate a benchmark for a time budget

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- Is a toolkit to write, run and analyze benchmarks
- Automatically calibrate a benchmark for a time budget
- Detect if a benchmark result seems unstable

Air Speed Velocity

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- Tool for benchmarking Python packages over their lifetime

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

Benchmark Design

Average vs Minimum Time

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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`***
- Which average do you use?

Can we assume a normal distribution?

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

Testing for a normal distribution

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- Visually ”eyeballing” the test

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Testing for a normal distribution

- It's essential to inspect the distribution of benchmark
- 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

A simple error check

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- If the average is far from the minimum, then your real-world performance could differ drastically from the minimum
- see Lemire [2023]

More error checks

More error checks

- The standard deviation is greater than 10% of the mean

More error checks

- The standard deviation is greater than 10% of the mean
- The minimum or the maximum is 50% smaller or greater than the mean

More error checks

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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

Outliers and Perturbing Events

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- Perturbing events should be investigated carefully
- 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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- Focus is on real-world benchmarks
- Includes the ability to add your own benchmarks
- https://github.com/python/pyperformance

The `n` body benchmark

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- N-body benchmark from the Computer Language Benchmarks Game

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- Model the orbits of Jovian planets, using a simple integrator

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- N-body benchmark from the Computer Language Benchmarks Game
- 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

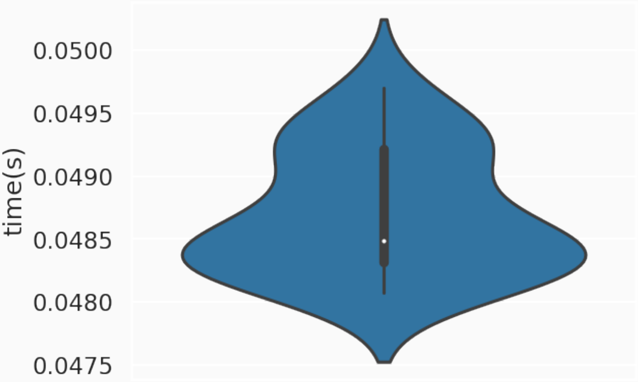

Figure 3: violinplot of n-body runtimes (s)

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?

What about our simple error check?

- 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

Let’s look at our stability checks

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Let’s look at our stability checks

- ✓ The standard deviation is 1% of the mean
- ✓ The minimum and the maximum are very close to the mean
- ✓ The shortest raw value took 48 milliseconds

Comparing Benchmarks

Does Windows or Linux run faster?

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

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- Want to compare how a change in the OS affects our runtime performance
- Ran the benchmark on Linux and Windows

Does Windows or Linux run faster?

- 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...

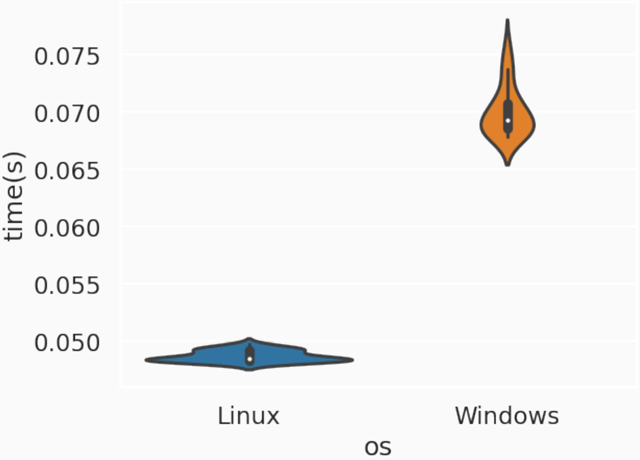

Figure 4: Runtime of the *n-body* benchmark

How comfortable are you saying this speedup is significant?

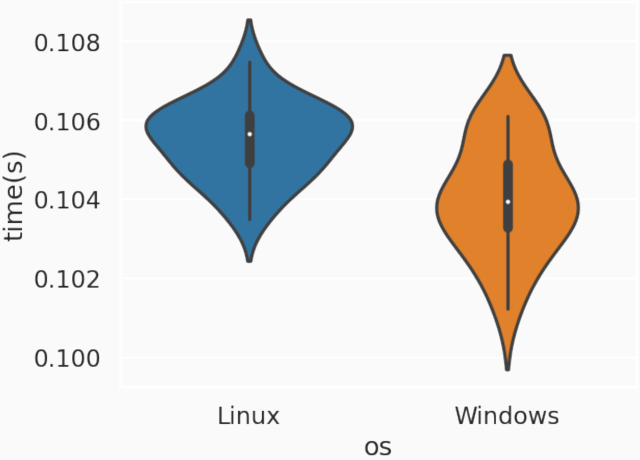

Figure 5: Runtime of the *sympy_sum* benchmark

Compare distributions, not summaries

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- Sample size and data quality

Compare distributions, not summaries

- Sample size and data quality
- Distributions capture variability

Compare distributions, not summaries

- Sample size and data quality
- Distributions capture variability
- Skewness and asymmetry

Comparing groups of Benchmarks

What are we *trying* to do?

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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

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- 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

Back to the pyperformance benchmark

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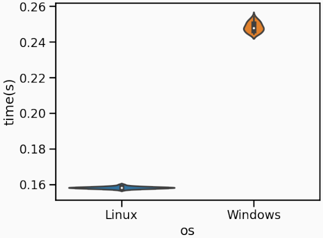
- Total of 95 benchmarks

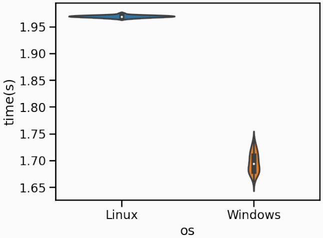
Back to the pyperformance benchmark

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

Back to the pyperformance benchmark



(a) 2to3



(b) mdp

Figure 6: Example difference in benchmark outcomes

A simple test to see which is faster

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- 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

A simple test to see which is faster

- Count the number of times Linux or Windows is significantly faster
- 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?

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- Linux is faster 78 times

Is Linux or Windows faster?

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

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- Windows is faster 15 times
- The difference is statistically insignificant twice

Is Linux or Windows faster?

- 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

What you should take away from this talk

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- Document & Automate

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- 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

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