A Survey of Tools for Writing Faster Programs in Python

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The (dual) simplex method. Used for repeated solves of the relaxations in branch and bound.

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Pop Quiz: Which solvers are fastest for LPs via simplex? Any in the **top 2** counts as a correct answer.

Answer[1]

No, it's not CPLEX or Gurobi.

Since 2018 the top 3 have been:

1. MindOpt (by Alibaba, a Chinese company).
2. COPT (by Cardinal Operations, a Chinese company).
3. Gurobi (the best among U.S. entries).

Newsflash: American dominance in optimization software is **over**.
It is not going to be regained by writing software that doesn't scale.

[1] Source: Mittleman Benchmarks, from Hans Mittleman of ASU Math Dept. Accessed March 4 2022.

Benchmark Details

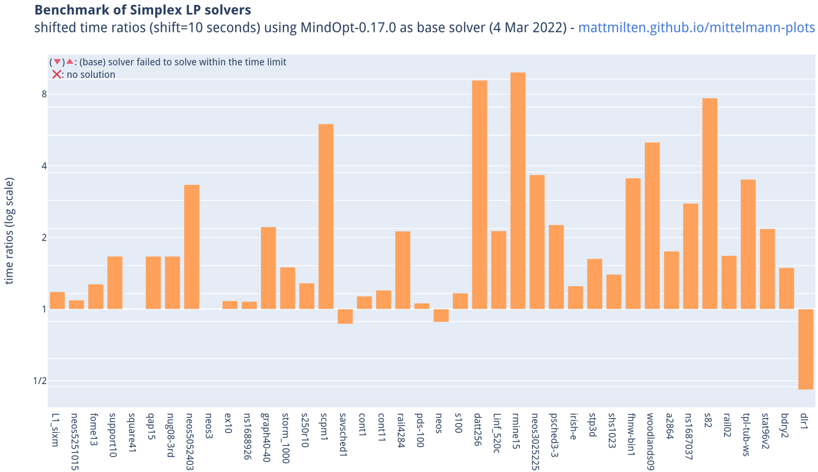

Figure: $\frac{\text{Gurobi-9.5.0 time}}{\text{MindOpt-0.17.0 time}}$ for problems in test suite.

More Motivation

Why should writing fast code should be prioritized?

[2] to project sponsors or publicly, when appropriate

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Second point: Releasing[2] research code increases our impact. It lowers the barrier to other researchers *actually using* our work.

i.e. you can post it on Github.

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Example: How many of us have used an `R` package without reading the white paper on which it was based?

You don't have to be a software engineer to identify low hanging fruit that makes your code run faster. This is important polish for a final product.

[2] to project sponsors or publicly, when appropriate

Python is Great

Python is a wonderful scripting language.

- Python is easy to learn.
- Python is fast to write.
- Python handles many low-level details (i.e. memory management) automatically.
- Python has numerous modules available to extend the language's functionality.
- Python has an enormous user base.
- Python has a business friendly BSD license[3].

[3] this is in contrast to R's GPL license

But Python is Slow

But these advantages come at a cost. Python is **not** fast.[4]

In many applications this is OK. It's often better to prioritize

- rapid prototyping
- readable code
- a developer's time

over writing code which is fast.

"Premature optimization is the root of all evil."

- Donald Knuth, author of *The Art of Computer Programming* and creator of TeX.

[4]Disclaimer: I mean native Python, not when used as a interface to fast code written in other languages, e.g. NumPy

But Python is Slow

The Computer Language Benchmarks Game is a database for comparing language performance.

Here is one numerics-heavy example problem, computing the largest absolute singular value of a matrix.

Timings of two programs on the same task.

Fortran: 0.72 seconds

Python: 112.97 seconds

Python is $\approx$ 156 times slower than Fortran for this task.

But Python is Slow

Python is slow because it is an *interpreted* language, not a *compiled* language.

- Interpreted languages use an *interpreter* to translate source code to CPU instructions *at run time*.
- Compiled languages use a *compiler* to translate source code into CPU instructions *at compile time* (i.e. before run time).

CPU instructions are not human readable but are very fast.

Also, the **Python interpreter does not support parallel execution**.

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Also, the **Python interpreter does not support parallel execution**.

Analogy: You must travel from Monterey to Santa Cruz.

Compiled languages are like programming a route into GPS.

Interpreted languages are like asking for directions at each leg of the journey.

Outline

Getting to compiled code is *the key* to making it fast.

We will look at three ways to do it.

1. **Numba**: A just-in-time (JIT) compiler for Python. JIT compilers assess the input variables and compile the code during/after its first run.

2. **Cython**: An extension of the Python language. Developer provides additional information to Python syntax. Cython translates this into compiled code.

3. **f2py**: An extension of NumPy for calling Fortran functions from Python. Sounds daunting but isn't. Fortran is *very* easy to learn and quickly write fast code.

A Running Example

Swap the location of minimal and maximal elements in an array. Here's a Python implementation.

```python
def swap_min_max(arr):
    max_val = arr[0]
    max_ind = 0
    min_val = arr[0]
    min_ind = 0
    for i in range(1, len(arr)):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[min_ind] = arr[max_ind]
    arr[max_ind] = min_val
```

Note: you may be tempted to compute the min and max separately using built-in Python functions. But doing so loops through the array twice, whereas this only loops through once.

Python Timings

```
In [1]: X = np.array(range(int(1e8))) #100 million numbers

In [2]: %timeit python_version.swap_min_max(X)
20.7 s +/- 3.29 s per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)
```

Numba Version

```
from numba import jit

@jit(nopython=True)
def swap_min_max(arr):
    max_val = arr[0]
    max_ind = 0
    min_val = arr[0]
    min_ind = 0
    for i in range(1, len(arr)):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[min_ind] = max_val
    arr[max_ind] = min_val
```

It really is that easy. In Numba, decorators are used to identify functions that should be JIT compiled.

Numba Timings

First run (longer because it includes compilation):

```
In [1]: X = np.array(range(int(1e8))) #100 million numbers
In [2]: start = time.time(); numba_version.swap_min_max(X);
                 print(time.time() - start)
0.3200979232788086 (seconds)
```

Additional runs:

```
In [3]: %timeit numba_version.swap_min_max(X)
182 ms +/- 3.95 ms per loop
      (mean +/- std. dev. of 7 runs, 1 loops each)
```

Numba runtime is **113.7x faster** than Python runtime.

Parallel Numba Example

By modifying our decorator, we can also parallelize loops when appropriate.

Our example doesn't permit easy parallelization, because `max_val` and `min_val` can't be updated independently within each loop iteration.

But we can parallelize a big sum.

Parallel Numba Example

```
from numba import jit, prange

@jit(nopython=True, parallel=True)
def parallel_sum(arr):
    total = 0
    for i in prange(0, len(arr)):
        total += arr[i]
    return total

@jit(nopython=True)
def numba_sum(arr):
    total = 0
    for i in range(0, len(arr)):
        total += arr[i]
        return total
```

Eye Candy: Utilize your CPUs

Parallel Numba Timings

```
In [1]: np.random.seed(0)

In [2]: X = np.random.normal(size=int(1e9)) #1 billion numbers

In [3]: %timeit sum(X)
1min +/- 618 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [4]: %timeit numba_sum(X)
1.04 s +/- 36.2 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [5]: %timeit parallel_sum(X)
272 ms +/- 2.14 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)
```

Parallelized Numba is **220x** faster than sum in Python.

Downsides to Numba

The benefits of Numba are obvious: Much faster execution with minimal effort.

But there are some limitations.

- Numba only plays well with NumPy arrays and other elementary data types.
- JIT compiler means slow first-time execution.
- Wider Python ecosystem (SciPy, Pandas, etc) cannot be JIT compiled.

Introducing Cython

Cython is an extension of Python that provides enough additional information for the code to be **compiled**.

Compilation usually occurs when installing package, i.e. via **pip** or **conda**.

Cython code can also be compiled directly in a Jupyter notebook. Code should be **developed** but not **distributed** this way.

Good news: All valid Python code is valid Cython code. But providing additional information via Cython's unique syntax is what gives you speed improvements.

Cython Version (No Change From Python)

```
def swap_min_max_cython(arr, n):
    max_val = arr[0]
    max_ind = 0
    min_val = arr[0]
    min_ind = 0
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

14.5 s runtime compared to 20.7 s in original. **1.43x Faster**.

Cython Version: Typing all the Variables

```
cimport numpy as np

def swap_min_max_cython(np.ndarray[ndim=1, dtype=np.int64_t] arr, int n):
    cdef int max_val = arr[0]
    cdef int max_ind = 0
    cdef int min_val = arr[0]
    cdef int min_ind = 0
    cdef int i
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

150 ms runtime compared to 20.7 s in original. **138.0x Faster**.

Cython Version: Ints (32 bit) vs Longs (64 bit)

```
cimport numpy as np

def swap_min_max_cython(np.ndarray[ndim=1, dtype=np.int64_t] arr, int n):
    cdef long max_val = arr[0]
    cdef int max_ind = 0
    cdef long min_val = arr[0]
    cdef int min_ind = 0
    cdef int i
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

125 ms runtime compared to 20.7 s in original. **165.6x Faster**.

Cython Version: Drop NumPy Dependency

```
#dtype[::1] means a contiguous chunk of memory dtype
def swap_min_max_cython(long[::1] arr, int n):
    cdef long max_val = arr[0]
    cdef int max_ind = 0
    cdef long min_val = arr[0]
    cdef int min_ind = 0
    cdef int i
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

86.3 ms runtime compared to 20.7 s in original. **239.9x Faster**.

Cython Version: Tricks with Indices

```
cimport cython

@cython.boundscheck(False) #disable index checking
@cython.wraparound(False) #forbid negative indices
def swap_min_max_cython(long[::1] arr, int n):
    cdef long max_val = arr[0]
    cdef int max_ind = 0
    cdef long min_val = arr[0]
    cdef int min_ind = 0
    cdef Py_ssize_t i #special type for indexing Python arrays
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

77.3 ms runtime compared to 20.7 s in original. **267.8x Faster**.

Cython Timings

```
In [1]: X = np.array(range(int(1e8))) #100 million numbers

In [2]: %timeit python_version.swap_min_max(X)
20.7 s +/- 3.16 s per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [3]: %timeit swap_min_max_cython(X, len(X))
77.3 ms +/- 487 µs per loop
        (mean +/- std. dev. of 7 runs, 10 loops each)
```

Cython is **267.8x times faster** than Python at 20.7 seconds.

Cython Annotation

What if we miss adding some important Cython syntax?

Using Jupyter magic `%%cython -a` can help us find it.

Hypothetical: We forget to type `max_ind` in our running example.

Cython Annotation: Missed Type

Generated by Cython 0.29.21

Yellow lines hint at Python interaction.

Click on a line that starts with a " + " to see the C code that Cython generated for it.

```
cimport cython
cimport numpy as np

@cython.boundscheck(False)
@cython.wraparound(False)
def swap_min_max_cython(long[::1] arr, int n):
    max_val = arr[0]
    cdef int max_ind = 0
    cdef long min_val = arr[0]
    cdef int min_ind = 0
    cdef Py_ssize_t i
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

Cython Annotation: Fixed

Generated by Cython 0.29.21

Yellow lines hint at Python interaction.

Click on a line that starts with a " + " to see the C code that Cython generated for it.

```
cimport cython
cimport numpy as np

@cython.boundscheck(False)
@cython.wraparound(False)
def swap_min_max_cython(long[::1] arr, int n):
    cdef long max_val = arr[0]
    cdef int max_ind = 0
    cdef long min_val = arr[0]
    cdef int min_ind = 0
    cdef Py_ssize_t i
    for i in range(1, n):
        if arr[i] > max_val:
            max_val = arr[i]
            max_ind = i
        if arr[i] < min_val:
            min_val = arr[i]
            min_ind = i
    arr[max_ind] = min_val
    arr[min_ind] = max_val
```

Cython: Parallelism

Parallelizing code is also extremely easy in Cython.

A serialized sum:

```
cimport cython

@cython.boundscheck(False)
@cython.wraparound(False)
def sum_cython(double[::1] arr, int n):
    cdef double total = 0.0
    cdef Py_ssize_t i
    for i in range(n):
        total += arr[i]
    return total
```

Cython: Parallelism

Parallelizing code is also extremely easy in Cython.

A parallelized version:[5]

```
cimport cython
from cython.parallel import prange, parallel

@cython.boundscheck(False)
@cython.wraparound(False)
def parallel_sum_cython(double[::1] arr, int n):
    cdef double total = 0.0
    cdef Py_ssize_t i
    for i in prange(n, nogil=True):
        total += arr[i]
    return total
```

[5] You must add openmp to Jupyter magic syntax to parallelize in a notebook, i.e. `%%cython --compile-args=-fopenmp --link-args=-fopenmp --force`

Cython Parallel Performance

```
In [1]: np.random.seed(0)

In [2]: X = np.random.normal(size=int(1e9)) #1 billion numbers

In [3]: %timeit sum(X)
1min +/- 618 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [4]: %timeit sum_cython(X, len(X))
998 ms +/- 4.63 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [5]: %timeit parallel_sum_cython(X, len(X))
264 ms +/- 3.37 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)
```

Parallelized Cython is **227x faster** than Python.

Pros and Cons of Cython

Pros of Cython

- Fast. No drawbacks of JIT compiler.
- Portable. Pip and Conda installations will compile Cython.
- Versatile. Easily connect Python to C/C++ libraries.

Cons of Cython

- Often assumes developer understands conventions of C/C++.
- Cython only plays well with NumPy arrays and other elementary data types.
- Wider Python ecosystem (SciPy, Pandas, etc) can be included in Cython code, but you won't see speed gains.[6]

[6] Exception: SciPy provides alternative lapack & blas functions directly for Cython.

Introducing f2py

- `f2py` is an extension of NumPy that allows convenient calling of Fortran code from Python.
- Fortran isn't as widely used as C/C++ today. Perceived as primarily used in legacy code.
- Fortran is **amazing** for simple programs which are heavy on numerics. It is a domain-specific language for numerical computation, like R is a domain-specific language for statistics.
- Fortran can be an great resource for eliminating bottlenecks in Python code.
- It's easy to learn, and easy to write fast code.
- `f2py` makes linking Fortran functions to Python extremely easy.

Return to Running Example

```fortran
! file: fortran_version.f90
subroutine swap_min_max(arr, n)
    implicit none !don't use default variable definitions
    integer n, min_ind, max_ind, i
    integer*8 max_val, min_val
    !f2py integer intent(hide) depend(arr):: n = shape(arr,0)
    integer*8 arr(n) !integer*8 gives 64 bit integer i.e. long
    min_ind = 1 !fortran is 1-indexed instead of 0-indexed like Python
    max_ind = 1
    max_val = arr(1) !fortran uses () instead of [] to index arrays
    min_val = arr(1)
    do i=1,n !indents don't matter in Fortran, but help readability
        if (arr(i) > max_val) then
            max_val = arr(i)
            max_ind = i
        end if
        if (arr(i) < min_val) then
            min_val = arr(i)
            min_ind = i
        end if
    end do
    arr(min_ind) = max_val
    arr(max_ind) = min_val
end
```

Compiling and Running

```
[me@computer]$ f2py -c -m fortran_version fortran_version.f90

[me@computer]$ ipython
In [1]: import numpy as np; import python_version

In [2]: import fortran_version

In [3]: X = np.array(range(int(1e8)))

In [4]: %timeit python_version.swap_min_max(X)
20.7 s +/- 3.16 s per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [5]: %timeit fortran_version.swap_min_max(X)
95.5 ms +/- 391 µs per loop
        (mean +/- std. dev. of 7 runs, 10 loops each)
```

Fortran with `f2py` is **216.8x** faster than Python.

Parallel Computation with Fortran/f2py

Again, let's parallelize a large sum. Serial version:

```
! file parallel_sum.f90
subroutine fortran_sum(arr, n, total)
    implicit none
    integer n, i
    !f2py integer intent(hide) depend(arr):: n = shape(arr, 0)
    real*8, intent(in):: arr(n) !fortran intents are parsed by f2py
    real*8, intent(out):: total
    total = 0d0
    do i=1,n
        total = total + arr(i)
    end do
end
```

Parallel Computation with Fortran/f2py

Again, let's parallelize a large sum. Parallel version:

```
! file parallel_sum.f90
subroutine fortran_sum(arr, n, total)
    implicit none !don't use default variable definitions
    integer n, i
    !f2py integer intent(hide) depend(arr):: n = shape(arr, 0)
    real*8, intent(in):: arr(n) !fortran intents are parsed by f2py
    real*8, intent(out):: total
    total = 0d0
    !$omp parallel do reduction(+:total)
    do i=1,n
        total = total + arr(i)
    end do
    !$omp end parallel do
end
```

Fortran gives access to **openmp**, a powerful tool for parallelization.

f2py: Parallel Performance

```
[me@computer]$ f2py -c -m parallel_sum parallel_sum.f90

[me@computer]$ ipython
In [1]: import numpy as np; import parallel_sum

In [2]: np.random.seed(0); X = np.random.normal(size=int(1e9))

In [3]: %timeit sum(X)
1min +/- 618 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [4]: %timeit parallel_sum.fortran_sum(X)
1.03 s +/- 35.8 ms per loop
        (mean +/- std. dev. of 7 runs, 1 loop each)

In [5]: %timeit parallel_sum.fortran_sum_parallel(X)
273 ms +/- 9.08 ms per loop
        (mean +/- std. dev. of 7 runs, 10 loops each)
```

Parallel Fortran/f2py is **219.8x** faster than Python.

Pros and Cons of f2py

Pros of f2py

- Easily call fast Fortran from Python. Eliminate bottlenecks.
- Compiling Fortran into a Python module is a single execution of f2py.
- Fortran is easy to learn. Can also be ported to other languages (R, Julia) easily.
- Fortran is a complete language, with its own fast libraries (BLAS, LAPACK, ScaLAPACK, etc.)

Cons of f2py

- Requires learning some details of yet another language.
- Fortran/f2py only play well with NumPy arrays and other elementary data types.
- Wider Python ecosystem (SciPy, Pandas, etc) cannot be utilitzed within Fortran.

Other Tools

Natural question: What about tools for linking Python with C/C++, similar to `f2py`'s use of Fortran?

These tools exist. Most popular is `pybind11`, with `swig` an older alternative. Python packages like `cppimport` automate the complilation step.

My opinion:

- These tools are **not** designed for Python developers looking to eliminate bottlenecks.
- These tools are best used for C/C++ developers looking to provide a Python interface.
- They are complicated, and require a lot of troubleshooting to get them working.
- C/C++ have conventions which are (a) not geared towards code performance (b) difficult if you primarily work in Python.

Conclusion

We've introduced three tools for writing faster Python programs.

1. Numba
   - **Low effort**. Only requires function decorators.
   - Must be **JIT compiled**, so first runs are not fast.
   - Low amount of developer control, because entire process is automated.
2. Cython
   - **Medium effort**. Takes familiar Python syntax and modifies it to produce very fast code.
   - Portable and universal. Used in libraries like SciPy, Scikit-learn, and Statsmodels.
   - Medium amount of developer control. Flexible within **constraints of Cython and C/C++ interaction**.
3. f2py
   - **Higher effort**. Requires some familiarity with Fortran.
   - Can be ported to other languages besides Python more easily.
   - High amount of developer control, because you have all **Fortran syntax and libraries** at your disposal.

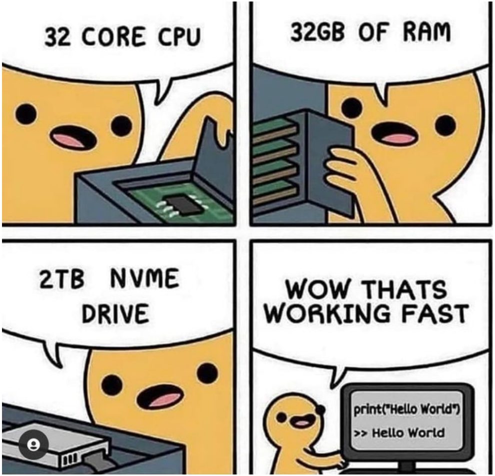
For More Information

1. I'm always available to chat.

2. These slides and the source code for all examples are at my website: faculty.nps.edu/rbassett

3. Documentation (these are links).
   - **Numba**
   - **Cython**
   - **f2py**

Happy Coding!



Cartoon source: @code_memez on twitter