Lab 1

Interfacing With Other Programming Languages Using Cython

Lab Objective: Learn to interface with object files using Cython. This lab should be worked through on a machine that has already been configured to build Cython extensions using gcc or MinGW.

Suppose you are writing a program in Python, but would like to call code written in another language. Perhaps this code has already been debugged and heavily optimized, so you do not want to simply re-implement the algorithm in Python or Cython. In technical terms, you want Python to *interface* (or communicate) with the other language. For example, NumPy's linear algebra functions call functions from LAPACK and BLAS, which are written in Fortran.

One way to have Python interface with C is to write a Cython *wrapper* for the C function. The wrapper is a Cython function that calls the C function. This is relatively easy to do because Cython compiles to C. From Python, you can call the wrapper, which calls the C function (see Figure TODO). In this lab you will learn how to use Cython to wrap a C function.

Wrapping with Cython: An Overview

When you use Cython to wrap a C function, you just write a Cython function that calls the C function. To actually do this, we need to understand a little bit more about how C works.

After you write a program in C, you pass it to a compiler. The compiler turns your C code into machine code, i.e., instructions that your computer can read. The output of the compiler is an *object file*.

In our scenario, we have C code defining a single function that we would like to wrap in Cython. This C code has already been compiled to an object file. The protocol for calling the C code from Cython is similar to calling it from C:

- 1. we need to *include a header file* for the C code in our Cython code, and
- 2. we must *link to the object file* compiled from the C code when we compile the Cython code.

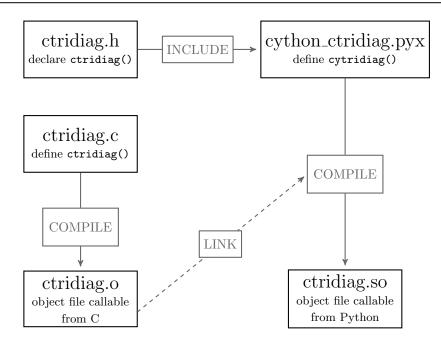


Figure 1.1: This diagram shows the relationships between the files used to write a Cython wrapper for ctridiag(). In fact, the Cython file cython_ctridiag.pyx compiles first to C code and then to the shared object file, but we have omitted this step from the diagram.

A *header* for a file contains the declaration of the function defined in the file. We include the header in the Cython code so that the compiler can check that the function is called with the right number and types of arguments. Then, when we tell the compiler to *link to* the object file, we simply tell it where to find the instructions defining the function declared in the header.

The Cython code will compile to a second object file. This object file defines a module that can be imported into Python. See Figure 1.1.

Wrapping with Cython: An Example

As an example, we will wrap the C function ctridiag() below. This function computes the solution to a tridiagonal system $A\mathbf{v} = \mathbf{x}$. Its parameters are pointers to four 1-D arrays, which satisfy the following:

- Arrays a and c have length n-1 and contain the first subdiagonal and superdiagonal of A, respectively.
- Arrays **b** and **x** have length **n** and represent the main diagonal of A and **x**, respectively.

The array c is used to store temporary values and x is transformed into the solution of the system.

void ctridiag(double *a, double *b, double *c, double *x, int n){

```
// Solve a tridiagonal system inplace.
2
       // Initialize temporary variable and index.
4
       int i;
       double temp;
       // Perform necessary computation in place.
6
       // Initial steps
       c[0] = c[0] / b[0];
8
       x[0] = x[0] / b[0];
       // Iterate down arrays.
10
       for (i=0; i<n-2; i++){</pre>
           temp = 1.0 / (b[i+1] - a[i] * c[i]);
12
           c[i+1] = c[i+1] * temp;
14
           x[i+1] = (x[i+1] - a[i] * x[i]) * temp;
           }
       // Perform last step.
16
       x[n-1] = (x[n-1] - a[n-2] * x[n-2]) / (b[n-1] - a[n-2] * c[n-2]);
       // Perform back substitution to finish constructing the solution.
18
       for (i=n-2; i>-1; i--){
           x[i] = x[i] - c[i] * x[i+1];
20
           }
       }
22
```

ctridiag.c

This terminal command tells the C-compiler gcc to compiles ctridiag.c to an object file ctridiag.o.

\$ gcc -fPIC -c ctridiag.c -o ctridiag.o

The -fPIC option is required because we will later link to this object file when compiling a shared object file. The -c flag prevents the compiler from raising an error even though ctridiag.c does not have a main function.

Write a Header For ctridiag.c

The header file essentially contains a function declaration for ctridiag(). It tells Cython how to use the object file ctridiag.o.

```
1 extern void ctridiag(double* a, double* b, double* c, double* x, int n);
2 // This declaration specifies what arguments should be passed
    // to the function called `ctridiag.'
```

ctridiag.h

Write a Cython Wrapper

Next we write a Cython file containing a function that "wraps" ctridiag(). This file must include the header we wrote in the previous step.

```
1 # Include the ctridiag() function as declared in ctridiag.h
2 # We use a cdef since this function will only be called from Cython
cdef extern from "ctridiag.h":
4 void ctridiag(double* a, double* b, double* c, double* x, int n)
6 # Define a Cython wrapper for ctridiag().
```

```
# Accept four NumPy arrays of doubles
# This will not check for out of bounds memory accesses.
cpdef cytridiag(double[:] a, double[:] b, double[:] c, double[:] x):
cdef int n = x.size
ctridiag(&a[0], &b[0], &c[0], &x[0], n)
```

cython_ctridiag.pyx

Some comments on this code are in order. First, including the header for ctridiag () allows us to call this function even though it was not defined in this file. This is a little like importing NumPy at the start of your Python script.

Second, the arguments of the Cython function cytridiag() are not in bijection with the arguments of ctridiag(). In fact, Cython does not need to know the size of the NumPy arrays it accepts as inputs because these arrays are objects that carry that information with them. We extract this information and pass it to the C function inside the Cython wrapper.

However, it is possible to unintentionally access memory outside of an array by calling this function. For example, suppose the input arrays a, b, c, and x are of sizes 4, 5, 3, and 5. Since x is used to determine the size of the system, the function ctridiag() will expect c to have length 4. At some point, ctridiag() will likely try to read or even write to the 4th entry of c. This address does exist in memory, but it does not contain an entry of c! Therefore, this function must be called by a responsible user who knows the sizes of her arrays. Alternatively, you could check the sizes of the arrays in the Cython wrapper before passing them to the C function.

Finally, the C function expects a parameter double* a, meaning that a is a *pointer* to (i.e., the address of) a double. The function ctridiag() expects this double to be the first entry of the array a. So instead of passing the object a to ctridiag(), we find the first entry of a with a[0], and then take its address with the & operator.

Compile the Cython Wrapper

Now we can compile cython_ctridiag.pyx to build the Python extension. The following setup file uses distutils to compile the Cython file, and may be run on Windows, Linux, or Macintosh-based computers. Notice that in line 28, we link to the existing object file ctridiag.o.

```
# Import needed setup functions.
1
2
   from distutils.core import setup
   from distutils.extension import Extension
  # This is part of Cython's interface for distutils.
4
   from Cython.Distutils import build_ext
   # We still need to include the directory
   # containing the NumPy headers.
   from numpy import get_include
8
   # We still need to run one command via command line.
  from os import system
10
12 # Compile the .o file we will be accessing.
   # This is independent building the Python extension module.
14 shared_obj = "gcc -fPIC -03 -c ctridiag.c -o ctridiag.o"
   print shared_obj
  system(shared_obj)
16
```

```
# Tell Python how to compile the extension.
18
   ext_modules = [Extension(
                             # Module name:
20
                             "cython_ctridiag",
                             # Cython source file:
22
                             ["cython_ctridiag.pyx"],
                             # Other compile arguments
24
                             # This flag doesn't do much this time,
                             # but this is where it would go.
^{26}
                             extra_compile_args=["-fPIC", "-03"],
                             # Extra files to link to:
28
                             extra_link_args=["ctridiag.o"])]
30
   # Build the extension.
   setup(name = 'cython_ctridiag',
32
          cmdclass = {'build_ext': build_ext},
          # Include the directory with the NumPy headers when compiling.
34
         include_dirs = [get_include()],
         ext_modules = ext_modules)
36
```

ctridiag_setup_distutils.py

This setup file can be called from the command line with the following command.

python ctridiag_setup_distutils.py build_ext --inplace

The --inplace flag tells the script to compile the extension in the current directory. The optional section at the end of this lab contains setup files that build the Python extension by hand on various operating systems.

WARNING

If at any point you need to make a change to the source file (in this case ctridiag.c) it is wise to delete all files that are generated in the build process to guarantee you have a clean build.

Test the Python Extension

After running the setup file, you should have a Python module called cython_cytridiag that defines a function cytridiag(). You can import this module into IPython as usual. However, if you modify ctridiag() and then try to recompile the extension, you may get an error if the module is currently in use. Hence, if you are frequently recompiling your extension, it is wise to test it with a script.

The following script tests the module cython_cytridiag.

```
import numpy as np
from cython_ctridiag import cytridiag as ctri
def init_tridiag(n):
    a = np.random.random_integers(-9,9,n).astype("float")
    b = np.random.random_integers(-9,9,n).astype("float")
    c = np.random.random_integers(-9,9,n).astype("float")
8
```

```
A = np.zeros((b.size,b.size))
       np.fill_diagonal(A,b)
10
       np.fill_diagonal(A[1:,:-1],a)
^{12}
       np.fill_diagonal(A[:-1,1:],c)
       return a,b,c,A
14
   if __name__ == "__main__":
16
       n = 10
       a,b,c,A = init_tridiag(n)
       d = np.random.random_integers(-9,9,n).astype("float")
18
       dd = np.copy(d)
20
       ctri(a,b,c,d)
22
       if np.abs(A.dot(d) - dd).max() < 1e-12:
           print "Test Passed"
^{24}
       else:
           print "Test Failed"
26
```

ctridiag_test.py

WARNING

When passing arrays as pointers to C or Fortran functions, be *absolutely sure* that the array being passed is contiguous. This means that the entries of the array are stored in *adjacent* entries in memory. Passing one of these functions a strided array will result in out of bounds memory accesses and could crash your computer. You can check if U is C-contiguous with the flags dictionary associated with any NumPy array. The code U.flags["C_CONTIGUOUS"] returns a boolean.

Problem 1. Following the process described above, compile the shared object file corresponding to ctridiag.c. In your Cython wrapper, add a check to make sure all the inputed arrays are C contiguous. If one of these arrays is not C contiguous, raise a ValueError.

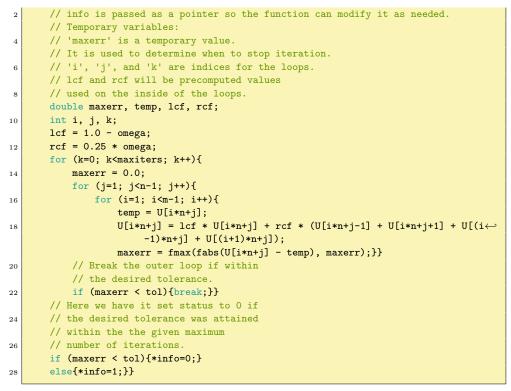
Another Example

The C function cssor() below implements the Successive Over Relaxation algorithm for solving Laplace's equation, which in two dimensions is

$$\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2} = 0$$

In the Successive Over Relaxation algorithm, an input array is iteratively modified until it converges to the solution F(x, y).

void cssor(double* U, int m, int n, double omega, double tol, int maxiters, int* ↔
info){





The function cssor() accepts the following inputs.

- U is a pointer to a C-contiguous 2-D array of double precision numbers.
- *m* is an integer storing the number of rows of *U*.
- *n* is an integer storing the number of columns of *U*.
- ω is a double precision floating point value between 1 and 2. The closer this value is to 2, the faster the algorithm will converge, but if it is too close the algorithm may not converge at all. For this lab just use 1.9.
- *tol* is a floating point number storing a tolerance used to determine when the algorithm should terminate.
- *maxiters* is an integer storing the maximum allowable number of iterations.
- *info* is a pointer to an integer. This function will set info to 0 if the algorithm converged to a solution within the given tolerance. It will set info to 1 if it did not.

Problem 2. Wrap cssor() so it can be called from Python, following these steps:

1. Write a C header for cssor.c.

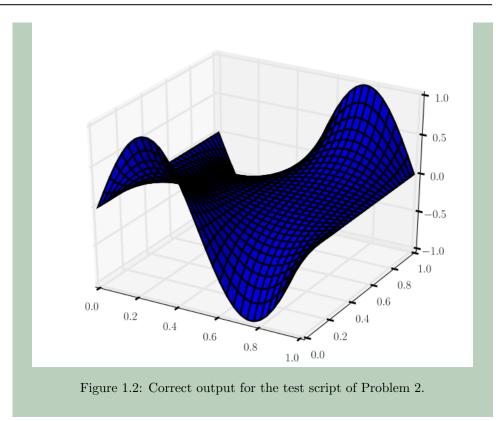
- 2. Write a Cython wrapper cyssor() for the function cssor() as follows:
 - (a) Have cyssor() accept parameters tol and maxiters that default to 10⁻⁸ and 10,000, respectively. What other arguments does cyssor () need to accept?
 - (b) Check that the input u is a C-contiguous array (this means that the array is stored in a certain way in memory). If u is not Ccontiguous, raise a ValueError.

raise ValueError('Input array U is not C-contiguous')

- (c) Raise a ValueError if cssor() fails to converge—i.e., if cssor() sets info to 1.
- 3. Compile cssor.c to an object file and compile your Cython wrapper to a Python extension. Be aware that you may compile cssor.c correctly and still receive warnings from the compiler.
- 4. Write a test script for your Cython function.
 - (a) You can run the function with the following code.

```
import numpy as np
from cython_fssor import cyssor
resolution = 501
U = np.zeros((resolution, resolution))
X = np.linspace(0, 1, resolution)
U[0] = np.sin(2 * np.pi * X)
U[-1] = - U[0]
cyssor(U, 1.9)
```

(b) Have your test script run the code above and plot the modified array \mathbf{v} on the domain $[0, 1] \times [0, 1]$. Note that U is a 501 × 501 array. Your plot should look like Figure 1.2.



Wrapping a C Function from an Existing Library

The example we just discussed one way to wrap a C function if you have the source code. You can also wrap functions that are found inside C libraries.

The following example wraps the sin function found inside math.h that comes standard with the GNU C library. The same principles can be applied to any C library with which you wish to interface.

```
# sin_func.pyx
cdef extern from "math.h":
    double sin(double arg)
cpdef sin_func(arg):
    return sin(arg)
```

Since the sin function is found inside the math.h file of the GNU C library, we do not need the source and header files in the same directory as the Cython Wrapper.

```
# sin_func_setup.py
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext
setup(
    cmdclass={'build_ext':build_ext},
    ext_modules=[Extension("cos_module", ["cos_module.pyx"])]
```

)

The syntax for compiling this wrapper is identical to the previous example.

Problem 3. Create and compile a Cython wrapper for the sqrt function from the math.h header file of the GNU C Library.

Wrapping a C Function using the Python-C-API (Optional)

If you know the C programming language, you can bypass Cython and write your wrapper directly in C. This will provide faster results than using Cython. If you are interested in learning more about how to wrap functions using the Python-C-API, see https://docs.python.org/2/c-api/ or http://www.scipy-lectures.org/advanced/interfacing_with_c/interfacing_with_c.html

Compiling C Extensions For Python (Optional)

If you know more about compilers, you may find it enlightening to manually compile a C extension for Python. Here we show how to manually compile cython_ctridiag.pyx on Windows, Linux, and Macintosh machines.

On Windows, using the compiler MinGW (a version of gcc for windows), the compilation can be performed by running the following setup file.

```
# The system function is used to run commands
1
   # as if they were run in the terminal.
2
   from os import system
   # Get the directory for the NumPy header files.
4
   from numpy import get_include
   # Get the directory for the Python header files.
6
   from distutils.sysconfig import get_python_inc
   # Get the directory for the general Python installation.
8
   from sys import prefix
10
   # Now we construct a string for the flags we need to pass to
   # the compiler in order to give it access to the proper
12
   # header files and to allow it to link to the proper
14 # object files.
   # Use the -I flag to include the directory containing
  # the Python headers for C extensions.
16
   # This header is needed when compiling Cython-made C files.
  # This flag will look something like: -Ic:/Python27/include
18
   ic = " -I" + get_python_inc()
   # Use the -I flag to include the directory for the NumPy
20
   # headers that allow C to interface with NumPy arrays.
  # This is necessary since we want the Cython file to operate
22
   # on NumPy arrays.
^{24}
  npy = " -I" + get_include()
   # This links to a compiled Python library.
  # This flag is only necessary on Windows.
26
   lb = " \"" + prefix + "/libs/libpython27.a\""
```

```
28 # This links to the actual object file itself
   o = " \"ctridiag.o\""
30
   # Make a string of all these flags together.
   # Add another flag that tells the compiler to
32
   # build for 64 bit Windows.
34 flags = "-fPIC" + ic + npy + lb + o + " -D MS_WIN64"
36 # Build the object file from the C source code.
   system("gcc ctridiag.c -fPIC -c -o ctridiag.o")
38 # Compile the Cython file to C code.
   system("cython -a cython_ctridiag.pyx --embed")
40 # Compile the C code generated by Cython to an object file.
   system("gcc -c cython_ctridiag.c" + flags)
42 # Make a Python extension containing the compiled
   # object file from the Cython C code.
44 system("gcc -shared cython_ctridiag.o -o cython_ctridiag.pyd" + flags)
```

ctridiag_setup_windows64.py

The following file works on Linux and Macintosh machines using gcc.

1	# The system function is used to run commands
2	# as if they were run in the terminal.
	from os import system
4	# Get the directory for the NumPy header files.
	from numpy import get_include
6	# Get the directory for the Python header files.
	<pre>from distutils.sysconfig import get_python_inc</pre>
8	
	# Now we construct a string for the flags we need to pass to
10	# the compiler in order to give it access to the proper
	# header files and to allow it to link to the proper
12	# object files.
	# Use the -I flag to include the directory containing
14	# the Python headers for C extensions.
	# This header is needed when compiling Cython-made C files.
16	<pre>ic = " -I" + get_python_inc()</pre>
	# Use the -I flag to include the directory for the NumPy
18	# headers that allow C to interface with NumPy arrays.
	<pre># This is necessary since we want the Cython file to operate # on NumPy arrays.</pre>
20	<pre>npy = " -I" + get_include()</pre>
22	# This links to the actual object file itself
22	<pre>o = " ctridiag.o"</pre>
24	
	# Make a string of all these flags together.
26	# Add another flag that tells the compiler to make
	# position independent code.
28	flags = ic + npy + o + " - fPIC"
30	# Build the object file from the C source code.
	<pre>system("gcc ctridiag.c -c -o ctridiag.o -fPIC")</pre>
32	# Compile the Cython file to C code.
	<pre>system("cython -a cython_ctridiag.pyxembed")</pre>
34	# Compile the C code generated by Cython to an object file.
	<pre>system("gcc -c cython_ctridiag.c" + flags)</pre>
36	# Make a Python extension containing the compiled
	# object file from the Cython C code.
38	<pre>system("gcc -shared cython_ctridiag.o -o cython_ctridiag.so" + flags)</pre>

ctridiag_setup_linux.py

Lab 2 Profiling and Optimizing Python Code

Lab Objective: Identify which portions of the code are most time consuming using a profiler. Optimize Python code using Cython and Numba and other tools.

The best code goes through multiple drafts. In a first draft, you should focus on writing code that does what it is supposed to and is easy to read. After writing a first draft, you may find that your code does not run as quickly as you need it to. Then it is time to *optimize* the most time consuming parts of your code so that they run as quickly as possible.

In this lab we will optimize the function qr1() that computes the QR decomposition of a matrix via the modified Gram-Schmidt algorithm (see Lab ??).

What to Optimize

Python provides a *profiler* that can identify where code spends most of its runtime. The output of the profiler will tell you where to begin your optimization efforts.

In IPython¹, you can profile a function with %prun. Here we profile qr1() on a random 300×300 array.

¹If you are not using IPython, you will need to use the cProfile module documented here: https://docs.python.org/2/library/profile.html.

```
In [1]: A = np.random.rand(300, 300)
In [2]: %prun qr1(A)
```

On this computer, we get the following output.

97206 function calls in 1.343 seconds

Ordered by: internal time

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
1	0.998	0.998	1.342	1.342	<pre>profiling_hw.py:4(qr1)</pre>
89700	0.319	0.000	0.319	0.000	<pre>{method 'dot' of 'numpy.ndarray' objects}</pre>
600	0.006	0.000	0.012	0.000	<pre>function_base.py:526(asarray_chkfinite)</pre>
600	0.006	0.000	0.009	0.000	linalg.py:1840(norm)
1200	0.005	0.000	0.005	0.000	<pre>{method 'any' of 'numpy.ndarray' objects}</pre>
600	0.002	0.000	0.002	0.000	<pre>{method 'reduce' of 'numpy.ufunc' objects}</pre>
1200	0.001	0.000	0.001	0.000	{numpy.core.multiarray.array}
1200	0.001	0.000	0.002	0.000	numeric.py:167(asarray)
1	0.001	0.001	0.001	0.001	<pre>{method 'copy' of 'numpy.ndarray' objects}</pre>
600	0.001	0.000	0.022	0.000	misc.py:7(norm)
301	0.001	0.000	0.001	0.000	{range}
1	0.001	0.001	0.001	0.001	{numpy.core.multiarray.zeros}
600	0.001	0.000	0.001	0.000	<pre>{method 'ravel' of 'numpy.ndarray' objects}</pre>
600	0.000	0.000	0.000	0.000	<pre>{method 'conj' of 'numpy.ndarray' objects}</pre>
1	0.000	0.000	1.343	1.343	<string>:1(<module>)</module></string>
1	0.000	0.000	0.000	0.000	<pre>{method 'disable' of '_lsprof.Profiler' objects}</pre>

The first line of the output tells us that executing qr1(A) results in almost 100,000 function calls. Then we see a table listing these functions along with data telling us how much time each takes. Here, ncalls is the number of calls to the function, tottime is the total time spent in the function, and cumtime is the amount of time spent in the functions.

For example, the first line of the table is the function qr1(A) itself. This function was called once, it took 1.342s to run, and 0.344s of that was spent in calls to other functions. Of that 0.344s, there were 0.319s spent on 89,700 calls to np.dot().

With this output, we see that most time is spent in multiplying matrices. Since we cannot write a faster method to do this multiplication, we may want to try to reduce the number of matrix multiplications we perform.

How to Optimize

Once you have identified those parts of your code that take the most time, how do you make them run faster? Here are some of the techniques we will address in this lab:

- Avoid Recomputing Values
- Avoid Nested Loops
- Use Existing Functions Instead of Writing Your Own
- Use Generators When Possible
- Avoid Excessive Function Calls
- Write Pythonic Code

- Use Cython or Numba
- Use a More Efficient Algorithm

You should always use the profiling and timing functions to help you decide when an optimization is actually useful.

Avoid Recomputing Values

In our function qr1(), we can avoid recomputing R[i,i] in the outer loop and R[i,j] in the inner loop. The rewritten function is as follows:

Profiling qr2() on a 300×300 matrix produces the following output.

```
48756 function calls in 1.047 seconds
```

Ordered by: internal time

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)				
1	0.863	0.863	1.047	1.047	<pre>profiling_hw.py:16(qr2)</pre>				
44850	0.171	0.000	0.171	0.000	<pre>{method 'dot' of 'numpy.ndarray' objects}</pre>				
300	0.003	0.000	0.006	0.000	<pre>function_base.py:526(asarray_chkfinite)</pre>				
300	0.003	0.000	0.005	0.000	linalg.py:1840(norm)				
600	0.002	0.000	0.002	0.000	<pre>{method 'any' of 'numpy.ndarray' objects}</pre>				
300	0.001	0.000	0.001	0.000	<pre>{method 'reduce' of 'numpy.ufunc' objects}</pre>				
301	0.001	0.000	0.001	0.000	{range}				
600	0.001	0.000	0.001	0.000	{numpy.core.multiarray.array}				
600	0.001	0.000	0.001	0.000	numeric.py:167(asarray)				
300	0.000	0.000	0.012	0.000	misc.py:7(norm)				
1	0.000	0.000	0.000	0.000	<pre>{method 'copy' of 'numpy.ndarray' objects}</pre>				
300	0.000	0.000	0.000	0.000	<pre>{method 'ravel' of 'numpy.ndarray' objects}</pre>				
1	0.000	0.000	1.047	1.047	<string>:1(<module>)</module></string>				
300	0.000	0.000	0.000	0.000	<pre>{method 'conj' of 'numpy.ndarray' objects}</pre>				
1	0.000	0.000	0.000	0.000	{numpy.core.multiarray.zeros}				
1	0.000	0.000	0.000	0.000	<pre>{method 'disable' of '_lsprof.Profiler' objects}</pre>				

Our optimization reduced almost every kind of function call by half, and reduced the total run time by 0.295s.

Some less obvious ways to eliminate excess computations include moving computations out of loops, not copying large data structures, and simplifying mathematical expressions.

Avoid Nested Loops

For many algorithms, the temporal complexity of an algorithm is determined by the loops. Nested loop quickly increase the temporal complexity. The best way to avoid nested loops is to use NumPy array operations instead of iterating through arrays. If you must use nested loops, focus your optimization efforts on the innermost loop, which gets called the most times.

Use Existing Functions Instead of Writing Your Own

If there is an intuitive operation you would like to perform on an array, chances are that NumPy or another library already has a function that does it. Python and NumPy functions have already been optimized, and are usually many times faster than the equivalent you might write. We saw an example of this in Lab ?? where we compared NumPy array multiplication with our own matrix multiplication implemented in Python.

Use Generators When Possible

When you are iterating through a list, you can often replace the list with a *generator*. Instead of storing the entire list in memory, a generator computes each item as it is needed. For example, the code

>>> for i in range(100):
... print i

stores the numbers 0 to 99 in memory, looks up each one in turn, and prints it. On the other hand, the code

>>> for i in xrange(100):
... print i

uses a generator instead of a list. This code computes the first number in the specified range (which is 0), and prints it. Then it computes the next number (which is 1) and prints that.

It is also possible to write your own generators. See https://docs.python.org/ 2/tutorial/classes.html#generators and https://wiki.python.org/moin/Generators for more information.

In our example, replacing each range with xrange does not speed up qr2() by a noticeable amount.

Avoid Excessive Function Calls

Function calls take time. Moreover, looking up methods associated with objects takes time. Removing "dots" can significantly speed up execution time.

For example, we could rewrite our function to reduce the number of times we need to look up the function la.norm().

```
def qr2(A):
    norm = la.norm
    ncols = A.shape[1]
    Q = A.copy()
    R = np.zeros((ncols, ncols))
    for i in range(ncols):
```

Once again, an analysis with %prun reveals that this optimization does not help significantly in this case.

Write Pythonic Code

Several special features of Python allow you to write fast code easily. First, list comprehensions are much faster than for loops. These are particularly useful when building lists inside a loop. For example, replace

```
>>> mylist = []
>>> for i in xrange(100):
... mylist.append(math.sqrt(i))
```

with

```
>>> mylist = [math.sqrt(i) for i in xrange(100)]
```

When it can be used, the function map() is even faster.

```
>>> mylist = map(math.sqrt, xrange(100))
```

The analog of a list comprehension also exists for generators, dictionaries, and sets. Second, swap values with a single assignment.

>>> a, b = 1, 2
>>> a, b = b, a
>>> print a, b
2 1

Third, many non-Boolean objects in Python have truth values. For example, numbers are False when equal to zero and True otherwise. Similarly, lists and strings are False when they are empty and True otherwise. So when a is a number, instead of

>>> if a != 0:

use

>>> if a:

Problem 1. Using the profiling techniques discussed in this lab, find out which portions of the code below require the most runtime. Then, rewrite the function using some of the optimization techniques we have discussed thus far.

```
def foo(n):
    my_list = []
    for i in xrange(n):
        num = np.random.randint(-9,9)
        my_list.append(num)
    evens = 0
    for j in xrange(n):
        if j%2 == 0:
            evens += my_list[j]
    return mylist, evens
```

Hint: If you are unsure where to begin optimizing, walk through the code line by line to determine what the code is accomplishing. Then, write your own function to perform the same task in a more efficient way.

Use Cython or Numba

Though it is much easier to write simple, readable code in Python, it is also much closer than compiled languages such as C. Compiled languages, in general, are much faster. Cython and Numba are two tools that you can use to optimize your code. Cython code is compiled before execution whereas Numba uses *just-in-time* (JIT) compilation. We will first discuss Cython.

Cython

Cython code is basically Python with extra type declarations. This code is then compiled into C, which—depending on the details—can run much faster than the Python equivalent. In this section we will introduce Cython as a language and discuss how it can be used to speed up Python code.

Compilation in IPython

Cython code can be compiled and imported to IPython (and IPython Notebooks) with the Cython magic function. Load this function with the following command: $_2$

In [1]: %load_ext Cython

Now you can define any Cython function in IPython by prefacing it with %%cython.

```
In [2]: %%cython
   ...: import numpy as np
   ...: from scipy import linalg as la
   ...: def qr(A):
   ...: norm = la.norm
   ...: ncols = A.shape[1]
   ...: Q = A.copy()
```

 $^2 {\rm In}$ older versions of IPython and Cython, you may need to use the command <code>%load_ext</code> <code>cythonmagic</code>.

```
...: R = np.zeros((ncols, ncols))
...: for i in range(ncols):
...: R[i, i] = norm(Q[:, i])
...: Q[:, i] = Q[:, i]/R[i, i]
...: for j in range(i+1, ncols):
...: R[i, j] = Q[:, j].dot(Q[:, i])
...: Q[:,j] = Q[:,j]-R[i, j]*Q[:,i]
...: return Q, R
...:
```

Note the import statements on lines 2 and 3. Even if these modules were already loaded in the current IPython session, these lines would still be necessary. Now the qr() function has been compiled in Cython and can be called from IPython just as any other function.

It is best to use this method of compilation if you are only using your optimized function once or you are in the stages of developing your optimized algorithm. It can be a little frustrating to fix errors in your function if you are using the IPython shell. The IPython Notebook interface is much easier to use for these types of problems.

Compilation from the Command Line

Compiling Cython from the command line is particularly useful if you need an optimized module that you will use over and over again. As we will discuss in this section, once a function is written and compiled in Cython, it can be imported as a module.

Cython code is usually written in a .pyx file, which is then compiled to C. Next the C is compiled to a Python extension written in machine code. Figure ?? shows how Cython code is compiled and called.

These two compilations (first to C and then to a Python extension) are accomplished by the script setup.py discussed earlier in this lab.

```
1 from distutils.core import setup
2 from Cython.Build import cythonize
4 setup(name="cymodule", ext_modules=cythonize('cymodule.pyx'))
```

setup.py

The call to cythonize() compiles cymodule.pyx to C, and the call to setup() converts the C code to a Python extension.

Note

You can learn more about the Python/C balance in your Cython file with the following line.

\$ cython -a cymodule.pyx

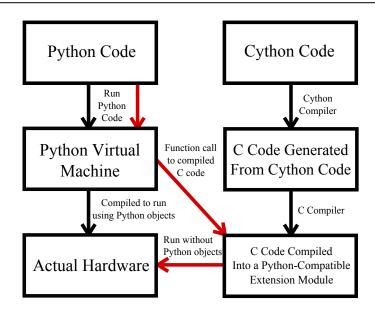


Figure 2.1: A diagram showing how Cython code is compiled and called. The path from calling a Cython function in a Python file to its evaluation is shown in red.

This will generate a html file that you can open with your web browser. It will show the lines that use Python in bright yellow and lines that use C in white.

Speeding up Cython with Type Declarations

So far, our Cythonized qr() function does not run any faster than the Python version.³ The simplest way to take advantage of the C-compilation is to declare data types, as you would in a C program. All Cython data types and their NumPy equivalents are listed in Table ??.

WARNING

Unlike Python integers, which can be arbitrarily large, Cython integers can overflow.

In our example, when we declare the index j to be an int, the inner for loop is pushed into C (instead of Python), speeding up our code immensely. We do this by modifying cymodule.pyx as follows.

```
def qr():
    cdef int j
    ncols = A.shape[1]
    Q = A.copy()
    ...
```

³Sometimes you will see speedup immediately after Cythonizing a Python function.

Cython Type	NumPy Type	Description
float	float32	32 bit floating point number
double	float64	64 bit floating point number
float complex	complex64	64 bit floating point complex number
double complex	complex128	128 bit floating point complex number
char	int8	8 bit signed integer
unsigned char	uint8	8 bit unsigned integer
short	int16	16 bit signed integer
unsigned short	uint16	16 bit unsigned integer
int	int32	32 bit signed integer
unsigned int	uint32	32 bit unsigned integer
long	int 32 or int 64	32 or 64 bit signed integer (depends on
		platform)
unsigned long	uint32 or uint64	32 or 64 bit unsigned integer (depends
		on platform)
long long	int64	64 bit signed integer
unsigned long long	uint64	64 bit unsigned integer

Table 2.1: Numeric types available in Cython.

We could also declare i to be an int, but the effect of doing so is negligible. After modifying cymodule.pyx, we must recompile it by running the script setup.py, and then re-import it into Python. When we profile this function, we see that it is indeed a good deal faster than its Python cousin, and all the speed up is in the function itself (where the for loops are).

 	tottimo	nomen11	aumtima	nomeo11	filename:lineno(function)
licalis		1		1	
1	0.949	0.949	0.961	0.961	{cymodule.qr}

Similarly, you can speed up function calls in Cython by declaring the types of some or all of the arguments.

def myfunction(double arg1, int arg2, arg3):
 ...

Arrays in Cython

You can also declare types for arrays. Doing so produces a *typed memoryview*, or Cython array. As with ordinary variables, typed memoryviews can be initialized when they are declared or later.

```
# Define a NumPy array
A = np.linspace(0,1,6)
# Create typed memoryviews on A and B
cdef double[:] cA = A
cdef int[:,:] cB
```

```
# Initialize cB
cB = np.array([[1,2],[3,4],[5,6]], dtype=np.dtype("i"))
```

Accessing single entries from a memoryview is faster than accessing entries of a NumPy array. Also, passing slices of a memoryview to a Cython function is fast. However, memoryviews do not support mathematical operations. These must be performed on NumPy objects, or by looping through the arrays.

Note

Memoryviews can be passed as arguments to most NumPy functions. NumPy includes functions for all common arithmetic operations. For example, you can add typed memoryviews with c = np.add(a, b). This may or may not be faster than looping through the array.

Putting it All Together

The following Python function computes the dot product of two 1-D arrays.

```
def pydot(A, B):
   tot = 0.
   for i in xrange(A.shape[0]):
      tot += A[i] * B[i]
   return tot
```

A C equivalent can be compiled by running the following code in IPython:

```
%%cython
def cydot(double[:] A, double[:] B):
    cdef double tot=0.
    cdef int i
    for i in xrange(A.shape[0]):
        tot += A[i] * B[i]
    return tot
```

Figure ?? compares the speed of pydot(), cydot(), and the dot() method of a NumPy array.

Problem 2.

1. Write the following function in Python without using the sum() builtin function.

```
def pysum(X):
    """ Return the sum of the elements of X.
    INPUTS:
    X - a 1-D NumPy array
    """
```

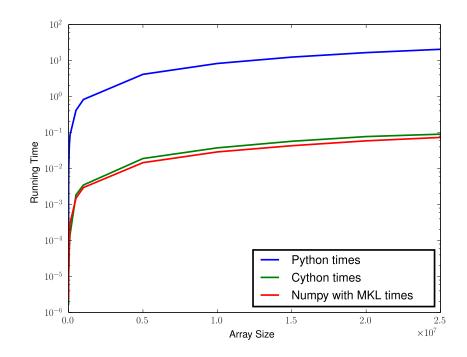


Figure 2.2: The running times of pydot(), cydot(), and the dot() method of a NumPy array on vectors of length "Array Size." The Cython version runs almost as fast as the version built into NumPy.

- Rewrite the same function in Cython using a typed for-loop, and a typed memoryview of x. Call this function cysum(). Assume the input array x is an array of double precision floating point numbers.
- 3. Compare the pysum() function, the cysum(), the Python builtin sum() function, and the np.sum() function. Print the results to the terminal.

Problem 3. In the Affine Transformations Lab (Lab ??) you wrote a function to compute the LU decomposition of a matrix. One possible implementation is found in the following code:

```
def LU(A):
    """Returns the LU decomposition of a square matrix."""
    n = A.shape[0]
    U = np.array(np.copy(A), dtype=float)
    L = np.eye(n)
    for i in xrange(1,n):
        for j in xrange(i):
```

```
L[i,j] = U[i,j]/U[j,j]
U[i,j:] -= L[i,j]*U[j,j:]
return L,U
```

- 1. Cython does not recognize NumPy array slicing. To be able to optimize this function using Cython, all array slicing must be removed. Rewrite the LU decomposition function so it performs every operation elementby-element instead of using NumPy array operations.
- 2. Port your function from Part 1 to Cython. Use typed for-loops and typed memoryviews. You may assume that you are only dealing with real arrays of double precision floating point numbers.
- 3. Compare the speeds of the original code, your solution to Part 1, and your solution to Part 2. Print the results to the terminal.

Numba

As mentioned before, Numba relies on a just-in-time (JIT) compiler. This means that the code is compiled right before it is executed. We will discuss this process a bit later in this section. The API for using Numba is incredibly simple. All one has to do is import Numba and add the <code>@jit</code> function decorator to your function. The following code would be a Numba equivalent to Problem **??**.

```
from numba import jit
@jit
def numba_sum(A):
   total = 0
   for i in xrange(len(A)):
        total += A[i]
   return total
```

Though this code looks very simple, a lot is going on behind the scenes. As we saw with Cython, our code will run faster if datatypes are assigned to all our variables. With Cython, we had to explicitly definite the datatypes of each variable. Rather than requiring us to define the datatypes explicitly, Numba attempts to *infer* the correct datatypes based on the datatypes of the input.

In the code above, for example, say that our array A was full of integers. Though we have not explicitly defined a datatype for the variable total, Numba will infer that the datatype for total should also be an integer.

Once all the datatypes have been inferred and assigned, the code is translated to machine code by the LLVM library. Numba will then cache this compiled version of our code. This means that we can bypass this whole inference and compilation process the next time we run our function.

More Control Within Numba

Though the inference engine within Numba does a good job, it's not always perfect. If you would like to have more control, you may specify datatypes explicitly as demonstrated in the code below.

Also, if you add the keyword argument, nopython=True to the jit decorator, an error will be raised if Numba was unable to convert everything to explicit datatypes.

In this example, we will assume that the input will be doubles. Note that is necessary to import the desired datatype from the Numba module.

```
from numba import double
@jit(nopython=True, locals=dict(A=double[:], total=double))
def numba_sum(A):
    total = 0
    for i in xrange(len(A)):
        total += A[i]
    return total
```

Notice that the jit function decorator is the only thing that changed. Note also that this means that we will not be allowed to pass an array of integers to this function. If we had not specified datatypes, the inference engine would allow us to pass arrays of any numerical datatype. In the case that our function sees a datatype that it has not seen before, the inference and compilation process would have to be repeated. As before, the new version will also be cached.

If your function is running slower than you would expect, you can find out what is going on under the hood by calling the inspect_types() method of the function.

```
# Due to the length of the output, we will leave it out of the lab text.
>>> numba_sum.inspect_types()
```

If you are trying to achieve the fastest runtimes possible, it will be worth trying both Numba and Cython. Since Numba relies on an LLVM compiler and Cython relies on a C compiler, it is possible that these two techniques will produce different results.

Problem 4. The code below defines a Python function which takes a matrix to the *n*th power.

```
def pymatpow(X, power):
    """ Return X^{power}.

Inputs:
    X (array) - A square 2-D NumPy array
    power (int) - The power to which we are taking the matrix X.
Returns:
    prod (array) - X^{power}
"""
prod = X.copy()
temparr = np.empty_like(X[0])
size = X.shape[0]
for n in xrange(1, power):
    for i in xrange(size):
```

```
for j in xrange(size):
    tot = 0.
    for k in xrange(size):
        tot += prod[i,k] * X[k,j]
        temparr[j] = tot
    prod[i] = temparr
return prod
```

- 1. Port pymatpow() to Cython using typed for-loops and typed memoryviews. Call your function cymatpow().
- 2. Create a compiled version of pymatpow() using Numba. Call this function numbamatpow().
- 3. Compare the speed of pymatpow(), cymatpow(), numbamatpow() and the np. dot() function. Remember to time numbamatpow() on the second pass so the compilation process is not part of your timing. Print your results to the terminal.

NumPy takes products of matrices by calling BLAS and LAPACK, which are heavily optimized linear algebra libraries written in C, assembly, and Fortran.

A Caution

NumPy's array methods are often faster than a Cython or Numba equivalent you could code yourself. If you are unsure which method is fastest, time them.

Moreover, a good algorithm written with a slow language (like Python) is faster than a bad algorithm written in a fast language (like C). Hence, focus on writing fast algorithms with good Python code, and only use Cython or Numba when and where it is necessary.

Use a More Efficient Algorithm

The optimizations discussed thus far will speed up your code at most by a constant. They will not change the complexity of your code. In order to reduce the complexity (say from $O(n^2)$ to $O(n \log(n))$), you typically need to change your algorithm. We will address the benefits of using more efficient algorithms in Problem ??.

The correct choice of algorithm is more important than a fast implementation. For example, suppose you wish to solve the following tridiagonal system.

$\lceil b_1 \rceil$	c_1	0	0	• • •		0]	$\begin{bmatrix} x_1 \end{bmatrix}$		$\lceil d_1 \rceil$	
a_1	b_2	c_2	0	•••		0	x_2		d_2	
0	a_2	b_3	c_3	• • •		0	x_3		d_3	
1:	÷	÷	÷	·		÷	:	=	:	
1:	÷	÷	÷	·	·	c_{n-1}	1		:	
0	0	0	0	•••	a_{n-1}	b_n	$\lfloor x_n \rfloor$		$\lfloor d_n \rfloor$	

One way to do this is with the general solve method in SciPy's linalg module. Alternatively, you could use an algorithm optimized for tridiagonal matrices. The code below implements one such algorithm in Python. This is called the Thomas algorithm.

The final result is stored in x, and c is used to store temporary values.

```
def pytridiag(a, b, c, x):
    '''Solve the tridiagonal system Ad = x where A has diagonals a, b, and c.
   INPUTS:
   a, b, c, x - All 1-D NumPy arrays.
   NOTE:
   The final result is stored in `x` and `c` is used to store temporary values.
    1.1
   n = x.size
   temp = 0.
   c[0] /= b[0]
   x[0] /= b[0]
    for i in xrange(n-2):
        temp = 1. / (b[i+1] - a[i] * c[i])
        c[i+1] *= temp
       x[i+1] = (x[i+1] - a[i] * x[i]) * temp
   x[n-1] = (x[n-1] - a[n-2] * x[n-2]) / (b[n-1] - a[n-2] * c[n-2])
    for i in xrange(n-2, -1, -1):
        x[i] = x[i] - c[i] * x[i+1]
```

Problem 5.

- 1. Port the above code to Cython using typed for-loops, typed memoryviews and appropriate compiler directives.
- 2. Compare the speed of your new function with pytridiag() and scipy. linalg.solve(). To compare the first two functions, start with 1000000 × 10000000 sized systems. When testing the SciPy algorithm, start with 1000 × 1000 systems. You may use the code below to generate the arrays, a, b, and c, along with the corresponding tridiagonal matrix A.

```
def init_tridiag(n):
    """Initializes a random nxn tridiagonal matrix A.
Inputs:
    n (int) : size of array
Returns:
    a (1-D array) : (-1)-th diagonal of A
    b (1-D array) : main diagonal of A
    c (1-D array) : (1)-th diagonal of A
    A (2-D array) : nxn tridiagonal matrix defined by a,b,c.
"""
    a = np.random.random_integers(-9,9,n).astype("float")
    b = np.random.random_integers(-9,9,n).astype("float")
    c = np.random.random_integers(-9,9,n).astype("float")
```

```
A = np.zeros((b.size,b.size))
np.fill_diagonal(A,b)
np.fill_diagonal(A[1:,:-1],a)
np.fill_diagonal(A[:-1,1:],c)
return a,b,c,A
```

3. What do you learn about good implementation versus proper choice of algorithm?

Note that an efficient tridiagonal matrix solver is implemented by scipy. sparse.linalg.spsolve().

When to Stop Optimizing

You don't need to apply every possible optimization to your code. When your code runs acceptably fast, stop optimizing. There is no need spending valuable time making optimizations once the speed is sufficient.

Moreover, remember not to prematurely optimize your functions. Make sure the function does exactly what you want it to before worrying about any kind of optimization.

More on Cython (Optional)

This section has a more complete introduction to Cython. For another reference, see http://docs.cython.org/src/tutorial/cython_tutorial.html.

More on Type Declarations

Type declarations make Cython faster than Python because a computer can process numbers faster when it knows ahead of time what type they are. Declaring a variable type in Cython makes the variable a native machine type instead of a Python object.

You can initialize a variable when it is declared or afterwards. It is possible to initialize several variables at once, as demonstrated below.

```
# Declare integer variables i, j, and k.
# Set k equal to 2.
cdef int i, j, k=2
cdef:
    # Declare and initialize m equal to 4 and n equal to 5.
    int m=4, n=5
    # Declare and initialize e equal to 2.71.
    double e = 2.71
    # Declare a double precision complex number a.
    double complex a
```

Compiler Directives

When you access elements of an array, Cython checks that the indices are within bounds. Cython also allows negative indexing the same way Python does. These features slow down code execution. After a program has been carefully debugged, they may be removed via *compiler directives*.

Compiler directives in Cython can be included as comments or function decorators. Directives included in comments will apply to the whole file, while function decorators will only apply to the function immediately following. The comments to turn off bounds checking and negative indices are

```
# cython: boundscheck=False
# cython: wraparound=False
```

To use the function decorators, first import the cython module by including the line cimport cython in your import statements. The decorators are

cimport cython
@cython.boundscheck(False)
@cython.wraparound(False)

Cython has many other compiler directives, including cdivision. When cdivision is set to True, the % operator returns a number with the sign of the first argument (like in C). Also, division by 0 will no longer raise a ZeroDivisionError, which will increase the speed of your program.

More on Functions in Cython

Speed up function calls in Cython by declaring the types of some or all of the arguments.

```
def myfunction(double[:] X, int n, double h, items):
    ...
```

If we pass in a NumPy array for the argument x, Cython will convert it to a typed memoryview before it enters the function. However, if we pass in a NumPy array for *items*, it will remain a NumPy array in the function. Both typed and untyped arguments can be made into keyword arguments.

Cython also allows you to make C functions that are only callable within the C extension you are currently building. They are not ported into the Python namespace. These functions are declared using the same syntax as in Python, except the keyword def is replaced with cdef. The keyword cpdef combines def and cdef by creating two versions of the function: one for Python and one for C.

You can also specify the return type for functions declared using cdef and cpdef, as in the code below.

```
cpdef int myfunction(double[:] X, int n, double h, items):
    ...
```

More Examples

For another example, we will write functions which compute AA^T from A. That is, given A, these functions compute B where B[i,j] = dot(A[i],A[j]).

Here is the Python solution.

```
def pyrowdot(A):
    B = np.empty((A.shape[0], A.shape[0]))
    for i in xrange(A.shape[0]):
        for j in xrange(i):
            B[i,j] = pydot(A[i], A[j])
        B[i,i] = pydot(A[i], A[i])
    for i in xrange(A.shape[0]):
        for j in xrange(i+1, A.shape[0]):
            B[i,j] = B[j,i]
    return B
```

Here is the Cython solution. We changed the function cydot() to a C function since it will only be called by cyrowdot(). Also, the Cython solution uses a typed memoryview of its input.

```
import numpy as np
cimport cython
# cython: boundscheck=False
# cython: wraparound=False
cpdef double cydot(double[:] A, double[:] B):
    cdef double tot=0.
    cdef int i, n=A.shape[0]
    for i in xrange(n):
       tot += A[i] * B[i]
    return tot
def cyrowdot(double[:,:] A):
    cdef double[:,:] B = np.empty((A.shape[0], A.shape[0]))
    cdef int i, j, n=A.shape[0]
    for i in xrange(n):
        for j in xrange(i):
          B[i,j] = cydot(A[i], A[j])
       B[i,i] = cydot(A[i], A[i])
    for i in xrange(n):
       for j in xrange(i+1, n):
           B[i,j] = B[j,i]
    return np.array(B)
```

This can also be done in NumPy by running A.dot(A.T). The timings of pyrowdot (), cyrowdot(), and the NumPy command A.dot(A.T) are shown in Figure ??.

In both of these examples, NumPy's implementation was faster than the version we wrote in Cython.

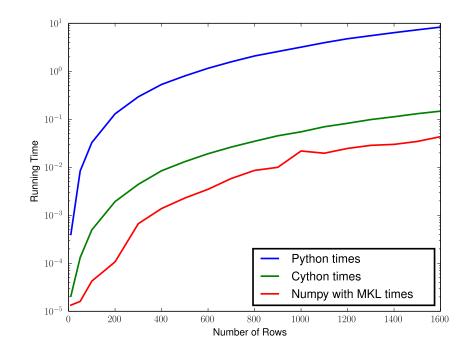


Figure 2.3: The timings of pyrowdot(), cyrowdot(), and the NumPy command A.dot(A.T). The arrays used for testing were $n \times 3$ where n is shown along the horizontal axis.