

GhostiPy: an efficient signal processing and spectral analysis toolbox for large data

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Abstract

Recent technological advances have enabled neural recordings consisting of hundreds to thousands of channels. As the pace of these developments continues to grow rapidly, it is imperative to have fast, flexible tools supporting the analysis of neural data gathered by such large scale modalities. Here we introduce **ghostipy** (**g**eneral **h**ub of **s**pectral **t**echniques **i**n **P**ython), a Python open source software toolbox implementing various signal processing and spectral analyses including optimal digital filters and time-frequency transforms. **ghostipy** prioritizes performance and efficiency by using parallelized, blocked algorithms. As a result, it is able to outperform commercial software in both time and space complexity for high channel count data and can handle out-of-core computation in a user-friendly manner. Overall, our software suite reduces frequently encountered bottlenecks in the experimental pipeline, and we believe this toolset will enhance both the portability and scalability of neural data analysis.

Introduction

Advancements in neural recording technologies have enabled the collection of large data in both space (high density/channel count) and time (continuous recordings). During subsequent analysis, the scale of the data induces certain challenges which may manifest

as the following scenarios: (1) analysis code takes a long time to complete (high time complexity), (2) code is unable to complete due to insufficient memory on the hardware (high spatial complexity). Moreover the scientist may have difficulty finding existing tools that address both (1) and (2) and that implement the desired analyses.

Although a potential remedy is to simply upgrade the hardware, it is not an acceptable solution for scientists desiring portability of analyses. In those situations hardware resources may be limited (e.g. using a laptop at the airport). We thus took an alternate approach by efficiently implementing analyses that would trivially scale for different hardware configurations. Our solution is **ghostipy** (**g**eneral **h**ub of **s**pectral **t**echniques in **P**ython), a free and open source Python toolbox that attempts to optimize both time and space complexity in the context of spectral analyses. Methods include linear filtering, signal envelope extraction, and spectrogram estimation, according to best practices. **ghostipy** is designed for general purpose usage; while well suited for high density continuous neural data, it works with any arbitrary array-like data object.

In this paper we first describe **ghostipy**'s software design principles to increase efficiency. We then elaborate on featured methods along with code samples illustrating user friendliness of the software. Finally we benchmark our software against a comparable implementation, and we discuss strategies for working under an out-of-core (when data cannot fit into system memory) processing context.

Materials and methods

An overview of implemented methods can be found in Table 1. Excluding out-of-core support, it is possible to use multiple different packages to achieve the same functionality. However the mix-and-match approach can reduce user friendliness since application programming interfaces (APIs) differ across packages and dependency management is more difficult. We believe our unified package provides an attractive solution to this challenge.

Software Design Considerations

As previously noted, successful completion of analyses may be hampered by long computation times or lack of system memory. Specifically, algorithmic time and space complexity are major determinants for the efficiency and performance of a software method. In general it is difficult to optimize both simultaneously. For example, time complexity may be reduced by increasing hardware parallelization, at the expense of higher space complexity (memory requirements). While we sought to lower both kinds of complexity compared to existing solutions, we gave space complexity a higher priority. Stated concretely, slow computation time is primarily a nuisance, but failure to complete an analysis due to insufficient memory is catastrophic.

Our design decision to prioritize space complexity was particularly critical because it directly influenced which backend library we chose for the Fast Fourier Transform (FFT), an operation used in the majority of `ghostipy`'s methods. While investigating the different options, we saw that `numpy` currently uses the `pocketfft` backend [26, 20]. When accelerated with Intel's MKL library, it can be slightly faster than FFTW [6]. However, we have found FFTW [9, 10] superior for memory management and better suited for arbitrary length FFTs, including prime and odd numbers. An additional benefit of FFTW was its multithreaded capabilities. We therefore selected FFTW as our FFT backend.

To lower space complexity we used blocked algorithms, including overlap save convolution, which is not offered in any of the standard Python numerical computing libraries such as `numpy` or `scipy` [26, 27]. This approach enabled us to process very large data that could not fit in memory (also known as out-of-core processing). Throughout our code, we also employed other strategies such as in-place operations.

To lower the time complexity, we used efficient lengths of FFTs wherever possible, and we leveraged modern computing hardware by parallelizing our algorithms. For example a wavelet transform can be trivially parallelized since the transform for each scale is not dependent on other scales.

	Python	Overlap save convolu- tion	Multi- taper method	Hilbert Trans- form	Morse CWT	Synchro- squeezed trans- form	Out-of- core
Ghostipy	+	+	+	+	+	+	+
SciPy	+	+	-	+	-	-	-
Chronux	-	-	+	-	-	-	-
Elephant	+	+	-	+	-	-	-
Brain- storm	+	+	+	+	-	-	-
PyWt	+	-	-	-	-	+	-
Field Trip	-	+	+	+	-	-	-
MNE	+	+	+	+	-	-	-
MATLAB	-	+	+	+	+	+	-

Table 1. Features implemented by `ghostipy` compared to existing software [27, 1, 28, 22, 13, 18, 12]

Multitaper Method

Users often wish to perform a spectral decomposition on a signal of interest. This can be accomplished by using the multitaper method [25, 19]. The technique is well-suited to reduce the variance of a spectrum estimate, which is particularly useful when working with noisy neural data. The spectrum estimate is obtained as an average of multiple statistically independent spectrum estimators for a discrete signal $x[n]$ with sampling frequency f_s :

$$\hat{S}_W^{mt}(k) = \frac{1}{L} \sum_{l=1}^L \hat{S}_{l,W}^{mt}(k) \quad (1)$$

$$\hat{S}_{l,W}^{mt}(k) = \frac{1}{f_s} \sum_{n=0}^{N-1} v_{l,W}[n] x[n] e^{-2\pi jkn/N} \quad (2)$$

Given the length of data N and a smoothing half-bandwidth W , the tapers $v_{l,W}[n]$ are computed by solving for vectors that satisfy the energy and orthogonality properties

$$\sum_{n=0}^{N-1} v_{l,W}[n] v_{l,W}[n] = 1 \quad (3)$$

$$\sum_{n=0}^{N-1} v_{l,W}[n] v_{m,W}[n] = 0, \quad l \neq m \quad (4)$$

An example using `ghostipy` is shown in Figure 1.

Continuous Wavelet Transform

Neuroscientists often use a continuous wavelet transform (CWT) to study transient oscillatory activity. The CWT itself is defined in the time domain by

$$W(a, b) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{a}} \psi^* \left(\frac{t-b}{a} \right) x(t) dt \quad (5)$$

where $\psi(\dots)$ is the mother wavelet function. The transform represents a two-dimensional decomposition in the scale (a) and time (b) planes. In the frequency domain, the CWT

```
psds = []
bandwidths = [10, 15, 20, 25]
for bandwidth in bandwidths:
    psd, freqs = gsp.mtm_spectrum(ripple_data,
                                  fs=asa.fs,
                                  n_fft_threads=8,
                                  bandwidth=bandwidth)
psds.append(psd)
```

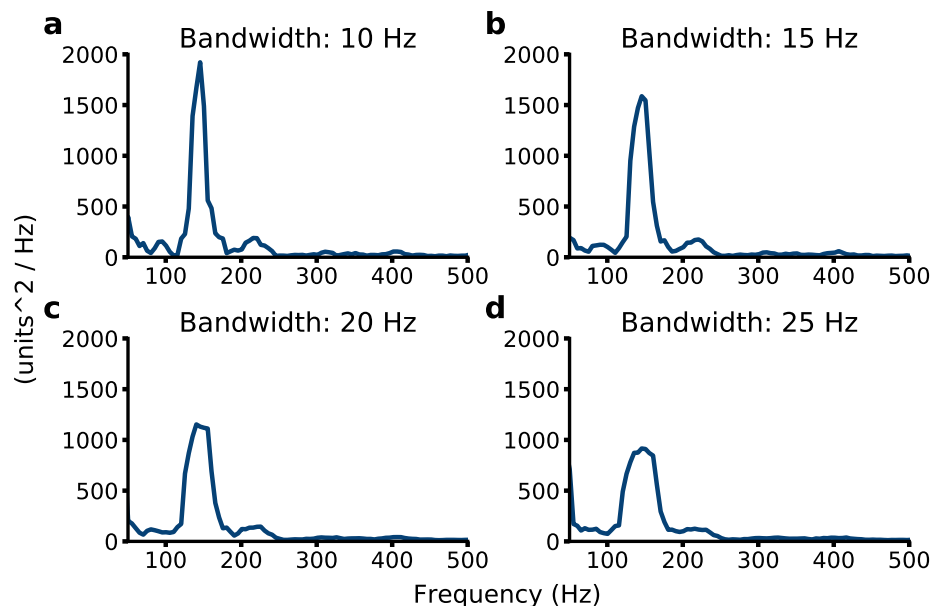


Fig 1. Multitaper spectrum estimates can be readily generated. The example uses a sharp wave ripple event, where energy occurs mainly between 100 and 250 Hz.

is given by the inverse Fourier transform of

$$W(a) = X(\omega)\Psi^*(a\omega) \quad (6)$$

for a given scale (a), where X and Ψ are the Fourier transforms of x and ψ , respectively.

Many mother wavelet functions have been investigated in the literature, but we have focused on the analytic wavelets, as they are found to be superior, particularly for estimating phase [17, 14, 16, 15]. We have implemented the analytic Morse, Morlet, and Bump wavelets, whose respective frequency domain definitions are

$$\Psi(a\omega) = 2 e^{-(a\omega-\omega_0)^2/2} H(\omega), \quad (7)$$

$$\Psi(a\omega) = 2 \left(\frac{e\gamma}{\beta} \right)^{\frac{\beta}{\gamma}} (a\omega)^\beta e^{-(a\omega)^\gamma} H(\omega) \quad (8)$$

$$\Psi(a\omega) = 2 e^{1-\left(1-\left(\frac{\mu-\sigma}{a}\right)^2\right)^{-1}} \mathbb{1}_{(\mu-\sigma)/a, (\mu+\sigma)/a} \quad (9)$$

where $\mathbb{1}_{(\mu-\sigma)/a, (\mu+\sigma)/a}$ is the indicator function for the interval $(\mu - \sigma)/a \leq \omega \leq (\mu + \sigma)/a$ and $H(\omega)$ is the Heaviside step function. In our implementation, we use Equation 6 to compute the CWT.

Note that in practice the timeseries $x(t)$ is sampled, and the CWT is likewise sampled. Then equation 6 becomes a pointwise complex multiplication of discrete Fourier transforms, where the discretized angular frequencies ω_k are determined by

$$\omega_k = \frac{2\pi k}{N\Delta t} \quad (10)$$

where N is the number of data samples and Δt is the sampling interval.

For electrophysiological data, a typical wavelet analysis will require computing Equation 6 for 50-500 scales. This is an obvious candidate for parallelization since the wavelet transform for each scale can be computed independently of the others. We use a backend powered by `dask` to carry out the parallelization [21]. Users can set the number of parallel computations to execute and thereby leverage the multicore capabilities offered by modern computing hardware.

Synchrosqueezing Transform

One disadvantage of the wavelet transform is that its frequency resolution decreases as the temporal resolution increases. Strictly speaking the CWT results in information contained in the (time, scale) plane, but a single frequency is typically assigned to each scale. Regardless, spectral smearing can be observed for at higher frequencies/lower scales. However, [4, 24] showed the synchrosqueezing transform (SST) could mitigate this issue by transferring a CWT's (time, scale) plane information to the (time, frequency) plane.

The synchrosqueezing transform proceeds as the following. For every scale a :

1. Compute the CWT $W(a)$ using equation 6
2. Compute the partial derivative

$$\partial_b W(a) = j\omega X(\omega)\Psi(a\omega) \quad (11)$$

3. Compute the phase transform

$$\omega_f(a) = \frac{1}{2\pi} \Im \left(\frac{\partial_b W(a)}{W(a)} \right) \quad (12)$$

The phase transform contains the real frequencies each point in the CWT matrix should be assigned to. In practice the real frequency space is discretized, so the CWT points are assigned to frequency bins. Note that multiple CWT points at a given time coordinate b may map to the same frequency bin. In this situation, a given frequency bin is a simple additive accumulation of CWT points.

Note the similarity of the SST to the spectral reassignment algorithms in [11, 8]. However an important distinction is that the SST only operates along the scale dimension. In addition to preserving the temporal resolution of the CWT, this makes SST data easy to work with since uniform sampling can be maintained.

Overall, the spectrogram methods implemented by `ghostipy` give an experimenter a more complete picture of the time-varying spectral content of neural data. Figure 2 illustrates using the `scipy` standard spectrogram method along with `ghostipy`'s methods.

```
import scipy.signal as sig
fs = asa.fs
nperseg = 64
noverlap = 16
w = 25

f_spect, t_spect, psd_spect = sig.spectrogram(data, fs=fs,
                                              nperseg=nperseg,
                                              noverlap=noverlap)

psd_mtm, f_mtm, t_mtm = gsp.mtm_spectrogram(data, w, fs=fs,
                                             nperseg=nperseg,
                                             noverlap=noverlap)

coefs_cwt, _, f_cwt, t_cwt, _ = gsp.cwt(data, fs=fs, freq_limits=[1, 500])
coefs_wsst, _, f_wsst, t_wsst, _ = gsp.wsst(data, fs=fs, freq_limits=[1, 500],
                                             voices_per_octave=32)

psd_cwt = np.abs(coefs_cwt)**2 / fs
psd_wsst = np.abs(coefs_wsst)**2 / fs
```

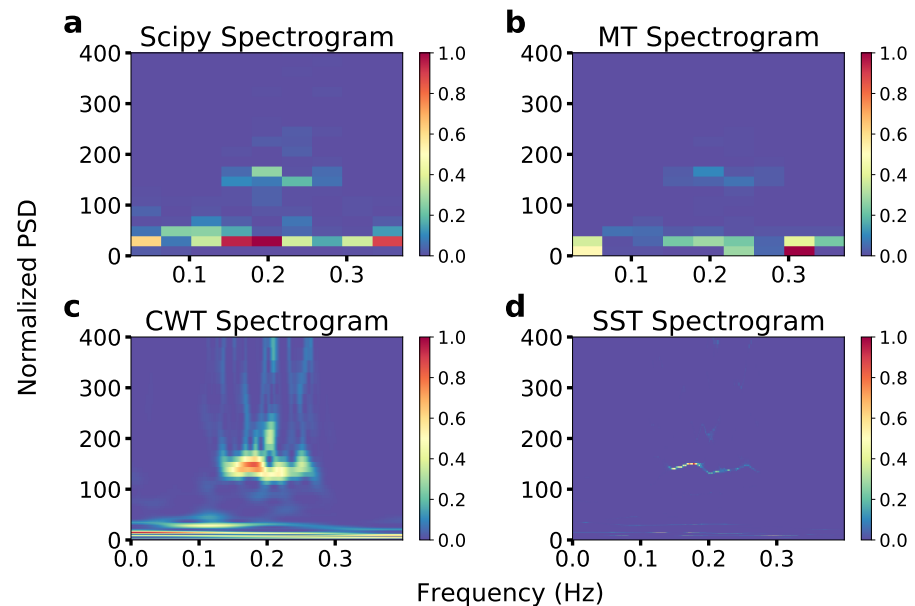


Fig 2. Users can leverage scipy's spectrogram along with ghostipy's methods to determine different time-frequency representations. The synchrosqueezed transform in (d) gives the overall sharpest time and frequency resolution.

FIR Filter Design

In addition to the time-frequency transforms described above, `ghostipy` provides classical signal processing capabilities such as filtering data, using the efficient overlap save convolution. Filtering data is an ubiquitous operation, but before this stage, the filter must itself be designed. While this step may appear somewhat trivial, it can make a significant difference. Consider theta-gamma phase amplitude coupling (PAC), a phenomenon in which the amplitude of the gamma band (approximately 30-120 Hz) oscillation is modulated by the phase of the theta band (approximately 6-10 Hz) oscillation. [7] states that "It is not possible to measure significant amounts of PAC with amplitudes filtered with narrower bandwidths than the frequency of the modulatory rhythm", but one of the early studies documenting theta-gamma coupling used 4 Hz bandwidth filters [3]. How could theta-gamma PAC have been discovered if the filters were nominally 4 Hz in bandwidth? The answer was that the software library used by the seminal paper scaled the transition bandwidth according to the passband center frequency, so the effective bandwidth was larger than the initially requested 4 Hz [7]. Theta-gamma coupling was thus a serendipitous discovery. Clearly it is important to control the transition bands of the filter, not just the passband. Existing packages such as `scipy` and `MNE` offer a variety of FIR filter design methods [27, 12]. However they suffer from certain issues, as documented below:

1. Least squares method: A solution may result in a filter with magnitude response effectively zero throughout. This situation is more common when designing filters with passband relatively low compared to the sampling rate.
2. Remez exchange method: The algorithm may simply fail to converge.
3. Window method: The transition bands cannot be controlled exactly, and optimality can not be defined, as is the case for the least squares (L2 optimal) and Remez exchange (L1 optimal)

Therefore `ghostipy`'s filter design uses the method defined in [2] for the following reasons:

1. It is simple to design. The computational complexity is similar to that of a window method and can be implemented on embedded hardware if desired.

2. Optimality can be defined, as it is optimal in the L2 sense. 149
3. Transition bands can be defined exactly, and the steepness of the passband rolloff 150
can be controlled by the spline power parameter. 151
4. The filter impulse response can be defined analytically. Consequently its 152
computation does not suffer from the failure modes of the least squares or Remez 153
exchange methods, as those must solve systems of linear equations. In other 154
words, the design process is reliable and stable. 155

This method designs a low pass filter according to 156

$$h(n) = \frac{\sin(\omega_0 n)}{\pi n} \left[\frac{\sin(\Delta n/p)}{\Delta n/p} \right]^p \quad (13)$$

$$\omega_0 = \frac{\omega_2 + \omega_1}{2} \quad (14)$$

$$\Delta = \omega_2 - \omega_1 \quad (15)$$

where ω_1 and ω_2 are radian frequencies defining the transition band boundaries. 157

`ghostipy` uses the low pass filter defined in 13 as a prototype to design more 158
complicated filters. As a result, users can request filters with arbitrary magnitude 159
response. Two examples are shown in Figure 3. 160

Results 161

Spectral analysis is ubiquitous in systems neuroscience experiments involving 162
electrophysiology. One of the primary goals of our development was to facilitate clear 163
and simple workflows with high performance. Of special note is that our tool enables 164
wavelet-based spectral analysis using the Morse wavelet [15], a feature that has 165
previously only been conveniently available in commercial tools such as Matlab. In 166
particular, the Morse wavelet is exactly analytic and nicely parameterized to tradeoff 167
frequency and temporal resolution. For very long data, most investigators will not be 168
interested in the sub-Hz frequency components, and performance can be improved by 169
restricting the frequencies/scales that are actually used for the transform. 170

```
tw = 2
p = 2
fs = 30000

numtaps = gsp.estimate_taps(fs, tw)
band_edges = [4, 6, 10, 12]
desired = [0, 1, 1, 0]
theta_filter = gsp.firdesign(numtaps, band_edges, desired,
                             fs=fs, p=p)

numtaps = gsp.estimate_taps(30000, 2)
band_edges = [10, 12, 55, 60, 100, 150, 200, 250, 300, 350]
desired = [1, 0, 0, 1, 1, 0, 0, 1, 1, 0]
arbitrary_filter = gsp.firdesign(numtaps, band_edges, desired,
                                 fs=fs, p=p)
```

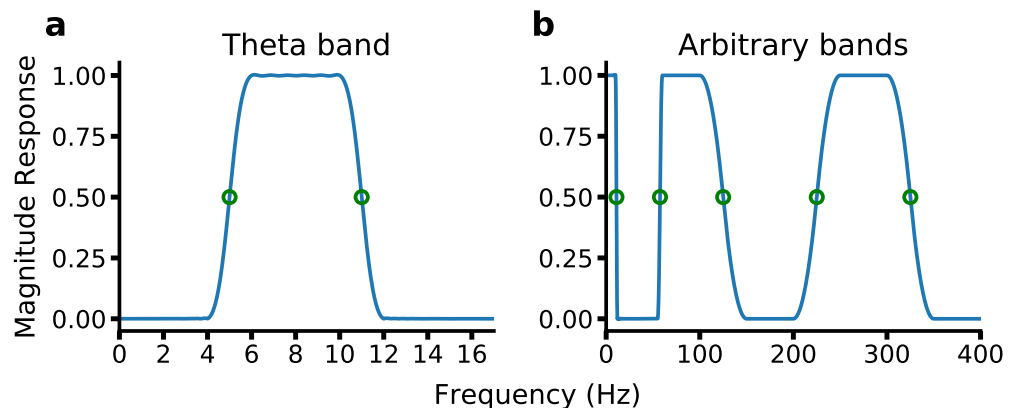


Fig 3. (a) A theta band filter designed for full bandwidth data. The specification of the transition bands allows for easy determination of critical frequencies. The -6 dB points are exactly the midpoints of the transition bands. (b) Filters with arbitrary pass and stop bands may also be designed.

A naive implementation of the Morse wavelet transform calculates untruncated wavelets the same length as the input data. This is often inefficient because it is equivalent to convolving the data with a time-domain wavelet mainly consisting of leading and trailing zeros. In our approach we exploit the fact that wavelets are finite in time and frequency, and we use an overlap-save algorithm to compute the CWT purely in the frequency domain. Note that the latter point is particularly critical: Due to the Gibbs phenomenon, using any time-domain representation of the wavelet may violate numerical analyticity for wavelet center frequencies near the Nyquist frequency. It is therefore necessary to use only the frequency domain representation of the wavelet. While we offer both traditional/naive and blockwise convolution implementations, the latter will give superior performance for longer-duration data. We believe that this is a valuable option for researchers and that this is the first tool which uses blockwise

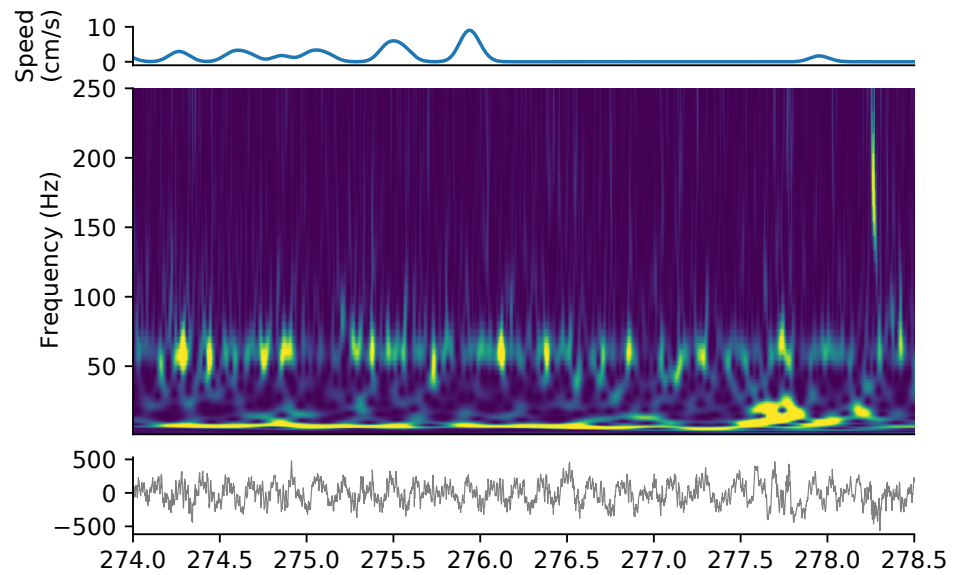


Fig 4. Spectrogram of local field potential recordings from area CA1 of the hippocampus of a rat during exploration (middle), with movement speed (top) and the raw electrophysiological signal (bottom). A number of features of the hippocampal rhythms can be noted in this example, including the pervasive theta oscillation (~ 8 Hz), theta-nested gamma oscillations (~ 60 Hz) during movement, and, towards the end, a sharp wave ripple (~ 200 Hz).

convolution to implement the CWT. 183

An example spectrogram of local field potentials recorded in area CA1 of the rat 184
hippocampus is shown in figure 4. Clearly apparent are the theta oscillation, 185
theta-nested gamma oscillations, and a sharp-wave-ripple, which occurs after the animal 186
has stopped moving. 187

Performance and Complexity 188

The calculation of the CWT is computationally intensive and consequently a good 189
method to benchmark performance. Of the software packages listed in Table 1, only 190
MATLAB offered an equivalent solution. It was thus chosen as the reference to compare 191
our implementation against. Figure 5 shows that our implementation results in faster 192
computation times and better memory usage. 193

It is not entirely clear what accounts for the higher jaggedness in the MATLAB curves 194
from Figure 5. A possible explanation is that the FFT computation is less efficient for 195

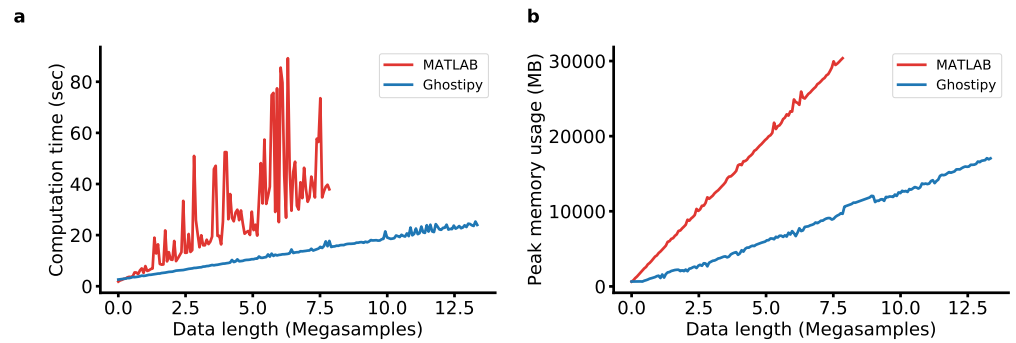


Fig 5. Our implementation of the Morse continuous wavelet transform outperforms MATLAB's in both (a) time and (b) space complexity. Note that MATLAB was unable to complete execution for the full range of the test parameter (data length) due to out-of-memory exceptions. The test machine was an Intel Core i7-4790 (8 hyperthreads) equipped with 32 GB RAM.

an odd-length transform, but the magnitude of the spikes in the curve is surprising 196
given that MATLAB's FFT backend also uses FFTW. Regardless, we have demonstrated 197
that our implementation is able to achieve lower time and space complexity. When 198
using the functionality offered by `ghostipy`, three primary scenarios arise with regards 199
to the sizes of data involved in the processing: 200

1. both the input and output data fit into core memory 201
2. the input fits into core memory but the output does not 202
3. neither the input nor the output fit 203

In all of the previous examples, we have restricted ourselves to case 1. However, with 204
the ever-increasing sizes of data, the other cases will inevitably be encountered. Case 2 205
may arise when attempting to generate spectrograms. As the input is a single channel, 206
memory constraints are rarely an issue. For example, even a 10 hr LFP recording 207
sampled at 1 kHz and saved as 64-bit floating point values will require less than 300 208
MiB of memory. However, the size of a wavelet spectrogram computed from this data 209
will be directly proportional to the number of scales/frequencies. For a typical range of 210
1 to 350 Hz at 10 voices per octave, this amount to a space requirement of 85 times that 211
of the input data. Given that this can well exceed the core memory size of a machine, 212
`ghostipy`'s CWT routine can also accept a pre-allocated output array that is stored on 213
disk (Figure 6). 214

```
shape, dtype = gsp.cwt(data, fs=1250, freq_limits=[1, 350],
                       describe_dims=True)

cwt_data = outfile.create_dataset('cwt_data', shape=shape, dtype=dtype)
out_of_core_params = {}
out_of_core_params['output_array'] = cwt_data

gsp.cwt(data, fs=fs, freq_limits=[1, 350],
        out_of_core_params=out_of_core_params)
```

Fig 6. Example code when the output array is too large for main memory. The CWT method is first executed as a dry run to compute the necessary array sizes.

Case 3 may arise when a user wishes to filter many channels of full bandwidth data. 215
One use case is a 1 hour recording for a 256 channel probe sampled at 30 kHz and stored 216
as a 2-byte signed integer type; already this requires 51 GiB. Our strategy is similar to 217
case 2, where an output array is allocated and stored on disk. As for the input, it is 218
read in chunks, and the size of these can be chosen to lower memory usage, although 219
potentially at a cost to computation time. The code in Figure 7 illustrates an example: 220

```
with h5py.File(input_filepath, 'r') as infile:
    with h5py.File(output_filepath, 'w') as outfile:

        ds = 300
        K = filter_delay
        N = infile['chdata'].shape[1]
        shape, dtype = gsp.filter_data_fir(infile['chdata'],
                                          theta_filter,
                                          axis=1,
                                          ds=ds,
                                          output_index_bounds=[K, K+N],
                                          describe_dims=True)

        outdata = outfile.create_dataset('theta_data',
                                         shape=shape,
                                         dtype=dtype)
        gsp.filter_data_fir(infile['chdata'],
                            theta_filter,
                            axis=1,
                            ds=ds,
                            output_index_bounds=[K, K+N],
                            outarray=outdata)
```

Fig 7. Filtering data from a large array stored on disk and likewise storing the output on disk. Similar to the CWT out-of-core features, the method is called once as a dry run to compute array sizes, which the user can then pass in to store the result. The filtering method also allows to correct for the delay of the filter and to downsample without storing any intermediate results. Although example uses the h5py library, any object that behaves like an array can be used.

Several points can be made about the scheme in Figure 7. Our method allows for downsampling during the convolution, which can reduce the number of stages in a computational scheme. Given full bandwidth data, a traditional strategy to filter to the theta band would look like the following:

1. Apply an anti-aliasing filter.
2. Downsample to obtain LFP.
3. Store the LFP to disk.
4. Apply a theta-band filter.
5. Downsample this output.
6. Save the result.

Using `ghostipy`'s method, it is not necessary to generate the intermediate LFP. To our knowledge, we do not know of other software that allows out-of-core filtering and downsampling in a single function call. The result is a simultaneous reduction in time and space complexity, by storing only the downsampled result and by filtering only once. Filtering to the theta band is now simplified to the following steps:

1. Apply a theta filter to the full bandwidth data.
2. Downsample the result.
3. Save the result to disk.

Conclusion

We have described the key features of `ghostipy` and given examples of its ease of use to perform computations efficiently. Users can thus conduct exploratory spectral analyses quickly across a range of parameters while reducing their concerns for running out of memory, especially since out-of-core computation is supported for many of the methods. Thus we believe `ghostipy` is well-suited to handle the ever-increasing size of experimental data.

In the future we plan to improve `ghostipy` with various enhancements. For example, currently the methods are designed to offer the user a lot of low level control over areas such as multithreading, and to work with raw array types. However, users may desire a higher-level API. For this reason we believe it would be a worthwhile endeavor to incorporate our work into frameworks such as `NWB` [23]; this would also facilitate more widespread adoption. Lastly, there are other analyses we could implement, including the adaptive multitaper method [19] and other time-frequency reassignment techniques similar to the synchrosqueezing transform [5].

Our primary contribution is improving the ease and speed at which data analysis can be conducted, by developing user-friendly software implementing efficient algorithms well-suited for large data sizes. This point is specifically demonstrated by our ability to outperform existing solutions in space and time complexity, and to run computations even in out-of-core memory conditions, which enables machines with 1-10s of GBs of memory to process data on the scale of 10-100s GBs and higher. In these ways, we have increased the accessibility of neural data analysis by enabling it to be run on hardware such as laptops, a scenario that often was not previously possible.

Lastly, the software we developed has a much larger potential impact than the scope described in this paper. Although many of the examples given in this paper were specific to extracellular rodent hippocampal data, the functionality we implemented is intentionally generic and applicable to many fields. As an example, our code can easily be adapted for use in real-time processing, whether running on embedded hardware or on a laptop in a clinical EEG setting. Given the functionality already developed and the full scope of our work, we are optimistic that `ghostipy` can help accelerate modern scientific progress.

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