SIGNATORY: DIFFERENTIABLE COMPUTATIONS OF THE SIGNATURE AND LOGSIGNATURE TRANSFORMS, ON BOTH CPU AND GPU

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Abstract. Signatory is a library for calculating signature and logsigature transforms and related functionality. The focus is on making this functionality available for use in machine learning, and as such includes features such as GPU support and backpropagation. To our knowledge it is the first publically available GPU-capable library for these operations. It also implements several new algorithmic improvements, and provides several new features not available in previous libraries. The library operates as a Python wrapper around C++, and is compatible with the PyTorch ecosystem. It may be installed directly via pip. Source code, documentation, examples, benchmarks and tests may be found at https://github.com/patrick-kidger/signatory. The license is Apache-2.0.

Key words. signature, logsignature, Python, PyTorch, GPU

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1. Introduction. The signature transform, sometimes referred to as the path signature or simply signature, is a transformation on differentiable paths\(^1\) [10]. There is another related transformation, called the logsigature transform [6], that we will also consider. Both may be thought of as loosely analogous to the Fourier transform.

The signature transform is a central object in the theory of rough paths and controlled differential equations. There is also a significant body of work using the signature and logsigature transforms in machine learning, for problems where the data is given as a stream of data [3, 5, 12, 16, 17, 18], with examples ranging from handwriting recognition to sepsis prediction.

In these examples, the signature and logsigature transforms are then used as a feature transformation. In this context it is sufficient to simply preprocess and then save the entire dataset, and simple implementations of the signature and logsigature transforms have been sufficient.

However, recent work has focused on embedding the signature and logsigature transforms within neural networks [1, 6, 13]. In this context, the signature and logsigature transforms are instead evaluated many times throughout a training procedure, and as such efficient implementations are crucial. Additionally, this implementation should be GPU-capable, as that is the typical context in which deep neural networks are trained.

Previous implementations [9, 14] of the signature and logsigature transforms have been CPU-only and single-threaded. Furthermore they do not exploit new algorithms that have been developed for the computation of these transforms. These limitations mean that they quickly become the major source of slowdown when training and evaluating these networks.

It is thus both necessary and timely that we introduce Signatory, a CPU- and GPU-capable library for performing and backpropagating through the signature transform, logsigature transform, and other related functionality. Signatory is dramati-

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\(^1\)It may also be extended to paths of bounded variation, and rough path theory shows how to extend the signature transform to paths of finite p-variation [11].
callly faster than previous libraries (whether run on the CPU or the GPU) thanks to a combination of parallelism and to novel algorithmic improvements. It also provides functionality not available in previous libraries.

The library integrates with the open source PyTorch ecosystem, is compatible with both Python 2 and Python 3, and runs on Mac, Linux and Windows. At time of writing Signatory is at version 1.1.6.

Documentation, examples, benchmarks and tests form a part of the project.

The creation of Signatory was motivated by the desire to support a broader research program on the use of the signature and logsignature transforms within machine learning. We believe it is reasonable to claim that Signatory enables this research program to achieve its goals at a speed and scale that was not previously possible.

The source code is found at https://github.com/patrick-kidger/signatory, the documentation and examples at https://signatory.readthedocs.io, and the project may be installed directly via pip.

The rest of this paper is laid out as follows. Section 2 gives a brief overview of the theory of the signature transform that we will use. Section 3 describes our algorithmic improvements. Section 4 describes the new features within Signatory that are not available in any previous library. Section 5 details the results of benchmarks against existing libraries. Section 6 is the conclusion. Appendix A describes further details of the algorithmic improvements. Appendix B details further benchmarks.

2. Background. We begin by providing a brief overview of the theory related to the signature transform that is applicable to machine learning, and thus relevant to Signatory. We do not assume any familiarity beyond what is presented here. For further details see [14] for an easy-to-read introduction with a focus on computational concerns, see [2] for a more thorough introduction to its use in machine learning, and [1, 6] for how it fits into modern deep learning frameworks.

2.1. The signature transform. For completeness we begin with a simple definition of the tensor product $\otimes$.

**Definition 2.1.** The notation $\mathbb{R}^{d_1} \otimes \mathbb{R}^{d_2}$ refers to the space of all real matrices with shape $d_1 \times d_2$. Similarly $\mathbb{R}^{d_1_1} \otimes \mathbb{R}^{d_2_2} \otimes \ldots \otimes \mathbb{R}^{d_n_n}$ refers to the space of all real tensors with shape $d_1 \times d_2 \times \ldots \times d_n$.

There is a corresponding binary operation $\otimes$, which maps a tensor of shape $(d_1, \ldots, d_n)$ and a tensor of shape $(e_1, \ldots, e_m)$ to a tensor of shape 

$$(d_1, \ldots, d_n, e_1, \ldots, e_m).$$

It is given as follows.

\[ \otimes : (\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_n}) \times (\mathbb{R}^{e_1} \otimes \cdots \otimes \mathbb{R}^{e_m}) \rightarrow \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_n} \otimes \mathbb{R}^{e_1} \otimes \cdots \otimes \mathbb{R}^{e_m}, \]

\[ \otimes : (A_{i_1 \cdots i_n})_{1 \leq i_1 \leq d_1, \ldots, 1 \leq i_n \leq d_n} \times (B_{j_1 \cdots j_m})_{1 \leq j_1 \leq e_1, \ldots, 1 \leq j_m \leq e_m} \mapsto (A_{i_1 \cdots i_n}B_{j_1 \cdots j_m})_{1 \leq i_1 \leq d_1, \ldots, 1 \leq i_n \leq d_n, 1 \leq j_1 \leq e_1, \ldots, 1 \leq j_m \leq e_m} \]

For example when applied to two vectors, it becomes the outer product.
**Definition 2.2.** Let \( N \in \mathbb{N} \). The signature transform to depth \( N \) is defined as

\[
\text{Sig}^N : \{ f \in C([0,1]; \mathbb{R}^d) \mid f \text{ differentiable} \} \rightarrow \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k},
\]

(2.1) \( \text{Sig}^N(f) = \left( \int \cdots \int \prod_{j=1}^k \frac{df_{ij}}{dt}(t_j) dt_1 \cdots dt_k \right)_{1 \leq i_1, \ldots, i_k \leq d, 1 \leq k \leq N} \).

The signature transform is sometimes also referred to as the path signature or simply signature.

The signature transform may naturally be extended to streams of data.

**Definition 2.3.** We define the space of streams of data over a set \( V \) as

\[
S(V) = \{ x = (x_1, \ldots, x_L) \mid L \in \mathbb{N}, x_i \in V \text{ for all } i \}.
\]

An interval of \((x_1, \ldots, x_L) \in S(V)\) is \((x_i, \ldots, x_j) \in S(V)\) for some \( 1 \leq i < j \leq L \).

**Definition 2.4.** Let \( x = (x_1, \ldots, x_L) \in S(\mathbb{R}^d) \) with \( L \geq 2 \). Let

\[
f = (f_1, \ldots, f_d) : [0,1] \rightarrow \mathbb{R}^d
\]

be continuous such that \( f(iL^{-1}) = x_i \) for all \( i \), and linear on the intervals in between.

Let \( N \in \mathbb{N} \). Then define \( \text{Sig}^N(x) = \text{Sig}^N(f) \). In this way we interpret \( \text{Sig}^N \) as a map

\[
\text{Sig}^N : S(\mathbb{R}^d) \rightarrow \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k}.
\]

Note that the choice of \( iL^{-1} \) is unimportant; any \( L \) points in \([0,1]\) would suffice, and in fact the definition is invariant to this choice [1, Definition A.10].

### 2.2. The grouplike structure

The image of the signature transform actually forms a noncommutative group, with operation \( \boxtimes \). Given a stream of data \((x_1, \ldots, x_L) \in S(\mathbb{R}^d)\) and some \( j \in \{1, \ldots, L\} \), then the group structure of signatures is such that

(2.2) \( \text{Sig}^N((x_1, \ldots, x_L)) = \text{Sig}^N((x_1, \ldots, x_j)) \boxtimes \text{Sig}^N((x_j, \ldots, x_L)) \).

This relation is known as Chen’s identity [11, Theorem 2.1.2].

Furthermore the signature of a stream of length two takes a special form, and may be written as

\[
\text{Sig}^N((x_1, x_2)) = \exp(x_2 - x_1)
\]

\(^2\)Note that many texts also include a \( k = 0 \) term, which is defined to equal one. We omit this as it does not carry any information, and is therefore irrelevant to the task of machine learning. Furthermore most texts use the notation of stochastic calculus; we instead sacrifice some unneeded generality for more widely-understood notation.

\(^3\)Most texts use \( \otimes \) to denote the group operation, as it may actually be regarded as a generalisation of the tensor product. That this is the case will not be important to us, however, so we choose to use differing notation to aid interpretation.
for a particular notion of exponential [1, Example A.2]

\[ \exp: \mathbb{R}^d \to \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k}. \]

Together this implies that the signature transform may be computed by evaluating

\[ (2.3) \quad \text{Sig}^N((x_1, \ldots, x_L)) = \exp(x_2 - x_1) \otimes \exp(x_3 - x_2) \otimes \cdots \otimes \exp(x_L - x_{L-1}). \]

2.3. The logsignature, inverted signature, and inverted logsignature transformations. The group inverse we denote \( ^{-1} \). Additionally a notion of logarithm may be defined [6], where

\[ \log: \text{im } (\text{Sig}^N) \to \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k}. \]

This then defines the notions of inverted signature transform, logsignature transform and inverted logsignature transform

\[
\text{InvertSig}^N(x) = \text{Sig}^N(x)^{-1}, \\
\text{LogSig}^N(x) = \log(\text{Sig}^N(x)), \\
\text{InvertLogSig}^N(x) = \log(\text{Sig}^N(x)^{-1})
\]

respectively. We emphasise that the inverted signature or logsignature transforms are not the inverses of the signature or the logsignature transforms.

The logsignature transform may be thought of as extracting the same information as the signature transform, but represents the information in a much more compact way, as \( \text{im } (\log) \) is a proper subspace\(^4\) of \( \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k} \). Its dimension is \( w(d, N) \), where

\[
w(d, N) = \sum_{k=1}^N \frac{1}{k} \sum_{i|k} \mu \left( \frac{k}{i} \right) d^i
\]

is Witt’s formula [7], and \( \mu \) is the Möbius function.

2.4. Signatures in machine learning. In terms of the tensors used by most machine learning frameworks, then the (inverted) signature and logsignature transforms of depth \( N \) may both be thought of as consuming a tensor of shape \((b, L, d)\), corresponding to a batch of \( b \) different streams of data, each of the form \((x_1, \ldots, x_L)\) for \( x_i \in \mathbb{R}^d \). The (inverted) signature transform then produces a tensor of shape \((b, \sum_{k=1}^N d^k)\), whilst the (inverted) logsignature transform produces a tensor of shape \((b, w(d, N))\).

All of these transforms are in fact differentiable with respect to \( x \), and so may be backpropagated through. These transforms may thus be thought of as differentiable operations between tensors, in the way usually performed by machine learning frameworks.

\(^4\log \) is actually a bijection. \( \text{im } (\text{Sig}^N) \) is some curved manifold in \( \prod_{k=1}^N (\mathbb{R}^d)^{\otimes k} \), and \( \log \) is the map that straightens it out into a linear subspace.
2.5. Efficiency of computation. Efficient algorithms for computing the signature and logsignature transforms are nontrivial. It is possible to evaluate the transform without resorting to numerical integration of equation (2.1), primarily by exploiting the grouplike structure as in equation (2.3).

Additionally, the grouplike structure implies that multiple signature transforms on overlapping data may be computed particularly efficiently. Any library aiming to be efficient must offer ways to exploit this structure.

Besides this, we remark that there are other computational tricks that may be exploited. For example, the backward (gradient) pass through the signature transform may be implemented in only $O(1)$ memory in the stream length $L$ due to a reversibility property of the signature [13, Section 4.9.3]; and the forward and backward passes of a particular version of the logsignature transform may be implemented by exploiting a triangularity property [15, Theorem 5.1], [13, Theorem 32]. We will not address these further here.

3. Algorithmic improvements. Several new algorithmic improvements were discovered and implemented as part of the development of Signatory.

3.1. Fused multiply-exponentiate. Recall from equation (2.3) that the signature may be computed by evaluating several exponentials and several $\otimes$. However a novel observation is that

$$\prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k} \times \mathbb{R}^d \rightarrow \prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k},$$

$$A, z \mapsto A \otimes \exp(z)$$

may be computed as a fused operation, with fewer scalar multiplications than the composition of the individual exponential and $\otimes$.

The bulk of a signature computation may be sped up by writing it in terms of this fused operation. This reduces the asymptotic complexity of computing a signature from $O(LNd^N)$ to just $O(Ld^N)$, and in fact the number of scalar multiplications is lower uniformly over $L, d, N$.

This gives dramatic real-world speedups; see the benchmarks of Section 5, which include running Signatory on the CPU without parallelism.

See Appendix A.1 for further mathematical details, as the precise analysis is somewhat tedious.

3.2. Improved precomputation strategies. Given a stream of data $x = (x_1, \ldots, x_L)$, it may be desirable to know $\text{Sig}^N((x_i, \ldots, x_j))$ for many $i, j$ such that $1 \leq i < j \leq L$. However it is a novel observation that this may be computed in just $O(1)$ (in $L$) time and memory by using $O(L)$ precomputation and storage. Previous theoretical work has achieved only $O(\log L)$ inference with $O(L \log L)$ precomputation [8].

Doing so uses a simple but novel algorithmic trick. Precompute $\text{Sig}^N((x_1, \ldots, x_j))$ and $\text{InvertSig}^N((x_1, \ldots, x_j))$ for all $j$, and then at inference time calculate

$$\text{Sig}^N((x_i, \ldots, x_j)) = \text{InvertSig}^N((x_1, \ldots, x_{i-1})) \otimes \text{Sig}^N((x_1, \ldots, x_j)).$$

Done naively this precomputation requires $O(L^2)$ work (as there are $O(L)$ signatures each requiring $O(L)$ work to compute). However this computation may be actually done in only $O(L)$ work, by iteratively computing each signature via

$$\text{Sig}^N((x_1, \ldots, x_j)) = \text{Sig}^N((x_1, \ldots, x_{j-1})) \otimes \text{Sig}^N((x_{j-1}, x_j)).$$

(3.1)
(And a similar relation holds for the inverted signature.) See also Section 4.5.2.

3.3. More efficient logsignature basis. The logsignature transform of a path has multiple possible representations, corresponding to different possible bases of the ambient space, which may in fact be interpreted as a free Lie algebra [15]. The Lyndon basis is a typical choice; for example this is used by iisignature [14]. A novel observation is that there exists a more computationally efficient basis. It is mathematically unusual, as it is not a Hall basis. But in machine learning, the choice of basis is unimportant if the next operation is a learnt linear transformation. For further details see Appendix A.2.

4. New features. The Signatory library provides several significant features not available in any previous library.

4.1. Inverted signatures and logsignatures. Signatory provides the capability to compute inverted signatures and logsignatures, via the optional inverse flag to the signature and logsignature functions.

4.2. Parallelism. Unlike previous implementations, the CPU implementation of Signatory takes advantage of parallelism.

Besides trivially parallelising over the batch dimension, an additional level of parallelism is provided over the stream dimension. Consider equation (2.3); it takes the form of a noncommutative reduce with respect to $\otimes$. Thus it can be parallelised by splitting it up into chunks.

4.3. GPU Support. An important feature is GPU support. This is parallelised in the same way as the CPU implementation described in Section 4.2. This also elides the need for copying the data to and from the GPU, as has previously been necessary when using CPU-only implementations.

4.4. Backpropagation. Crucial for any library used in deep learning is to be able to backpropagate through the provided operations. Signatory provides full support for backpropagation through every provided operation. There has previously only been limited support for backpropagation through a handful of simple operations, via the iisignature library.

4.5. Exploiting the grouplike structure. It is often desirable to compute signatures (or logsignatures, ...) over multiple intervals of the same stream of data. These calculations may jointly be accomplished much more efficiently than by evaluating the signature transform for them all separately. In some cases, if the original data has been discarded and only its signature is now known, exploiting this structure is the only way to perform the computation.

Here we detail several notable cases, and how Signatory supports them. In all cases the aim is to provide a flexible set of tools that may be used together, so that wherever possible unnecessary recomputation may be elided. Their use is also discussed in the documentation, including examples.

4.5.1. Combining adjacent intervals. Recall equation (2.2). If the two signatures on the right hand side of the equation are already known, then the signature of the overall stream of data may be computed using only a single $\otimes$ operation.

This has two particular implications.

First, given the two signatures on the right hand side of equation (2.2), then the signature of the overall stream of data may be computed in only $O(1)$ (in $L$) work, without expensively re-iterating over the original stream of data.
Second, this means that the signature of the overall stream of data may be computed without actually knowing the original data; only the two signatures (on the right hand side of equation (2.2)) are required. This is useful if the original data has been discarded, for example due to memory constraints.

This operation is provided for by the \texttt{signature\_combine} and function and by the \texttt{multi\_signature\_combine} function.

\textbf{4.5.2. Expanding intervals.} Given a stream of data \((x_1, \ldots, x_L) \in S(\mathbb{R}^d)\), we might wish to compute the signature over an expanding interval of the data,

\[
(Sig^N((x_1, x_2)), Sig^N((x_1, x_2, x_3)), \ldots, Sig^N((x_1, \ldots, x_L))).
\]

This may be interpreted as a stream of signatures in \(S\left(\prod_{k=1}^N (\mathbb{R}^d)^{\otimes k}\right)\).

Done na"ively this requires \(O(L^2)\) work: to compute \(O(L)\) signatures, each taking \(O(L)\) work to compute. However as described in equation (3.1), this may in fact be done in only \(O(L)\) work overall, which is the same as is required to compute just the final element \(Sig^N((x_1, \ldots, x_L))\).

This is handled by the optional \texttt{stream} argument to the \texttt{signature} function and to the \texttt{logsignature} function.

This scenario is particularly important for its use in Sections 3.2 and 4.5.4.

\textbf{4.5.3. Keeping the signature up-to-date.} Suppose we have a stream of data \((x_1, \ldots, x_L) \in S(\mathbb{R}^d)\), whose signature \(Sig^N((x_1, \ldots, x_L))\) has already been computed. New data subsequently arrives, some \((x_{L+1}, \ldots, x_{L+M}) \in S(\mathbb{R}^d)\), and we now wish to update our computed signature, either to compute just \(Sig^N((x_1, \ldots, x_{L+M}))\),

or to compute the stream of signatures

\[
(\text{4.1}) \hspace{1cm} (Sig^N((x_1, \ldots, x_{L+1})), \ldots, Sig^N((x_1, \ldots, x_{L+M})))
\]

as in Section 4.5.2.

The simplest approach of direct computation is clearly inefficient, as it requires iterating over \((x_1, \ldots, x_L)\), which as in Section 4.5.1 is unnecessary.

If \(Sig^N((x_L, \ldots, x_{L+M}))\) is itself of interest then we could apply the technique of Section 4.5.1, by computing the signature of \(Sig^N((x_L, \ldots, x_{L+M}))\), and then applying

\[
(\text{4.2}) \hspace{1cm} Sig^N((x_1, \ldots, x_{L+M})) = Sig^N((x_1, \ldots, x_L)) \boxtimes Sig^N((x_L, \ldots, x_{L+M})).
\]

However if \(Sig^N((x_L, \ldots, x_{L+M}))\) is not of interest then this approach may be improved upon, especially in the case of (4.1). This is because Section 4.5.1 only uses the grouplike structure with \(\boxtimes\), but not the fused multiply-exponentiate described in Section 3.1. In this case it is thus advantageous to use the fused multiply-exponentiate (but does not give \(Sig^N((x_L, \ldots, x_{L+M}))\) as an intermediate result).

This scenario is provided for by combining the \texttt{basepoint} and \texttt{initial} arguments to the \texttt{signature} and \texttt{logsignature} functions.

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\(^5\)Note that we start with \(Sig^N((x_1, x_2))\), as two is the shortest a stream of data can be to define a path; see Definition 2.4.
Fig. 5.1: Time taken on benchmark computations to compute the specified operation. In all cases the input was a batch of 32 streams of data, each of length 128. For varying channels, the depth was fixed at 7. For varying depths, the channels was fixed at 4. Every test case was repeated 50 times and the fastest time taken. Note that esig is only shown for certain operations as it is incapable of computing large operations or of computing backward operations. Note the logarithmic scale.

4.5.4. Arbitrary intervals. This case generalises Sections 4.5.1 and 4.5.2; it is the also most time and memory intensive case to solve. Signatory provides this capability via the Path class. It consumes a stream of data, performs some precomputation, and subsequently allows for $O(1)$ inference for the signature or logsignture of any interval of the stream of data.

The method is described in Section 3.2.

In addition, Path handles the case of incoming data (as in Section 4.5.3) via its update method.

5. Benchmark performance. We are aware of two existing software libraries providing similar functionality, esig [9] and iiisignature [14]. The major limitation of both is that they only operate on the CPU, without parallelism.

We ran a series of benchmarks against the latest versions of both of these libraries, namely esig 0.6.31 and iiisignature 0.24. The computer used was equipped with a
Xeon E5-2660 v4 and a Quadro GP100, and was running Ubuntu 18.04 and Python 3.7.

In the case of esig and iisignature we report run time on only the CPU, whilst for Signatory we report times for running on the GPU, CPU with parallelism, and CPU without parallelism.

The benchmarks shown here test the forward and backward operations through the signature transform, for both increasing depth or for increasing numbers of input channels. For further benchmarks on the precise numerical values of the graphs presented here, and for code to reproduce the benchmarks, consult Appendix B.

The results are shown in Figure 5.1. Note the logarithmic scale.

We observe that iisignature is Signatory’s strongest competitor in all cases. We see that Signatory and iisignature are roughly comparable for the very smallest computations, with iisignature typically being on the order of milliseconds faster. As the computation increases in size, then the CPU implementations of Signatory almost immediately overtake iisignature, shortly followed by the GPU implementations. For larger computations, Signatory is orders of magnitude faster, and in particular we observe the expected increase in speed, when moving from single-thread CPU to parallelised CPU to GPU. We note also that it is entirely expected that the GPU should be slower than CPU for smaller problems, when the parallelisation available on a GPU is not useful.

6. Conclusion. We have introduced Signatory, a library for performing functionality related to the signature and logsignature transforms, with a particular focus on applications to machine learning. Notable contributions include its available functionality, its algorithmic innovations, and the efficiency of its implementation.

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Appendix A. Further details of algorithmic improvements.

A.1. Fused multiply-exponentiate. The conventional way to compute a signature is to iterate through the computation described by equation (2.3): for each new increment, take its exponential, and \( \otimes \) it on to what has already been computed; repeat.

Our proposed alternate way is to fuse the exponential and \( \otimes \) into a single operation.

We now count the number of multiplications required to compute

\[
\left( \prod_{k=1}^{N} (R^d)^{\otimes k} \right) \times R^d \rightarrow \prod_{k=1}^{N} (R^d)^{\otimes k},
\]

\[A, z \mapsto A \otimes \exp(z)\]

for each approach.

We will establish that the fused operation uses fewer multiplications for all possible \( d \geq 1 \) and \( N \geq 1 \). We will then demonstrate that it is in fact of a lower asymptotic complexity.

A.1.1. The conventional way. The exponential is defined as

\[
\exp : R^d \rightarrow \prod_{k=1}^{N} (R^d)^{\otimes k},
\]

\[
\exp : x \mapsto \left( x, x^{\otimes 2}, x^{\otimes 3}, \ldots, x^{\otimes N} \right),
\]

see [1, Proposition 15].

Note that every tensor in the exponential is symmetric, and so in principle requires less work to compute than its number of elements would suggest. For the purposes of this analysis, to give the benefit of the doubt to a competing method, we shall assume that this is done (although taking advantage of this in practice is actually quite hard [14, Section 2]). This takes

\[
\sum_{k=2}^{N} \binom{d + (d + k - 1)}{k}
\]

scalar multiplications, using the formula for unordered sampling with replacement [14, Section 2], and assuming that each division by a scalar costs the same as a multiplication (which can be accomplished by precomputing their reciprocals and then multiplying by them).

Next, we need to count the number of multiplications to perform a single \( \otimes \).
Let
\[ A, B \in \prod_{k=1}^{N} (\mathbb{R}^d) \otimes^k. \]

Let \( A = (A_1, \ldots, A_N) \). Let
\[ A_i = (A_{i_1}^{j_1}, \ldots, A_{i_k}^{j_k}), \quad 1 \leq i_1, \ldots, i_k \leq d, \]
and every \( A_{i_1}^{j_1}, \ldots, A_{i_k}^{j_k} \in \mathbb{R} \). Additionally let \( A_0 = 1 \). Similarly for \( B \). Then \( \boxtimes \) is defined by
\begin{align*}
\boxtimes & : \left( \prod_{k=1}^{N} (\mathbb{R}^d) \otimes^k \right) \times \left( \prod_{k=1}^{N} (\mathbb{R}^d) \otimes^k \right) \rightarrow \prod_{k=1}^{N} (\mathbb{R}^d) \otimes^k, \\
(A.1) \quad \boxtimes & : A, B \mapsto \left( \sum_{i=0}^{k} A_i \otimes B_{k-i} \right)_{1 \leq k \leq N},
\end{align*}
where each
\[ A_i \otimes B_{k-i} = \left( A_{i_1}^{j_1}, \ldots, A_{i_k}^{j_k}, B_{k-i_1}^{\hat{j}_1}, \ldots, B_{k-i_k}^{\hat{j}_{k-i}} \right)_{1 \leq i_1, \ldots, i_k \leq d, \hat{j}_1, \ldots, \hat{j}_{k-i} \leq d} \]
is the usual tensor product, the result is thought of as a tensor in \((\mathbb{R}^d) \otimes^k\), and the summation is taken in this space. See \([1, \text{Definition A.13}]\).

As previously mentioned, \( \boxtimes \) is a generalised version of the tensor product \( \otimes \), which is itself a generalisation of the outer product. As such we don’t expect to be able to compute this with any fewer multiplications than a naïve approach would suggest. (Although this is of course not a proof, and to the authors’ knowledge there is no formal analysis of a lower bound on the computational complexity of this generalised tensor product.)

This, then, requires
\begin{align*}
&\sum_{k=1}^{N} \sum_{i=1}^{k-1} \sum_{j_1, \ldots, j_i=1}^{d} \sum_{j_{k-i}=1}^{d} 1 = \sum_{k=1}^{N} \sum_{i=1}^{k-1} d^k \\
&= \sum_{k=1}^{N} (k-1)d^k
\end{align*}
scalar multiplications.

Thus the overall cost of the conventional way involves
\begin{align*}
(A.2) \quad C(d, N) = \sum_{k=2}^{N} \left( d + \binom{d + k - 1}{k} \right) + \sum_{k=1}^{N} (k-1)d^k
\end{align*}
scalar multiplications.
A.1.2. The fused operation. Let $A \in \prod_{k=1}^{N} (\mathbb{R}^{d})^{\otimes k}$ and $z \in \mathbb{R}^{d}$. Then

$$A \boxplus \exp(z) = \left( \sum_{i=0}^{k} A_{i} \otimes \frac{z^{\odot (k-i)}}{(k-i)!} \right)_{1 \leq k \leq N},$$

where the $k$-th term may be computed by a scheme in the style of Horner’s method:

$$\sum_{i=0}^{k} A_{i} \otimes \frac{z^{\odot (k-i)}}{(k-i)!} = \left( \cdots \left( \frac{z}{k} + A_{1} \right) \otimes \frac{z}{k-1} + A_{2} \right) \otimes \frac{z}{k-2} + \cdots \otimes \frac{z}{2} + A_{k-1} \right) \otimes z + A_{k}. \tag{A.3}$$

As before, we assume that the reciprocals $\frac{1}{2}, \ldots, \frac{1}{N}$ have been precomputed, so that each division costs the same as a multiplication.

Then we begin by computing $z/2, \ldots, z/N$, which takes $d(N-1)$ multiplications.

Computing the $k$-th term as in equation (A.3) then involves $d^{2} + d^{3} + \cdots + d^{k}$ multiplications. Working from innermost bracket to outermost, the first $\otimes$ produces a $d \times d$ matrix as the outer product of two size $d$ vectors, and may thus be computed with $d^{2}$ multiplications; the second $\otimes$ produces a $d \times d \times d$ tensor from a $d \times d$ matrix and a size $d$ vector, and may thus be computed with $d^{3}$ multiplications; and so on.

Thus the overall cost of a fused multiply-exponentiate is

$$\mathcal{F}(d, N) = d(N-1) + \sum_{k=1}^{N} \sum_{i=2}^{k} d^{i} \tag{A.4}$$

scalar multiplications.

A.1.3. Comparison. We begin by establishing the uniform bound $\mathcal{F}(d, N) \leq C(d, N)$ for all $d \geq 1$ and $N \geq 1$.

First suppose $d = 1$. Then

$$\mathcal{F}(1, N) = (N-1) + \sum_{k=1}^{N} (k-1) \leq 2(N-1) + \sum_{k=1}^{N} (k-1) = C(1, N).$$

Now suppose $N = 1$. Then

$$\mathcal{F}(d, 1) = 0 = C(d, 1).$$

Now suppose $N = 2$. Then

$$\mathcal{F}(d, 2) = d + d^{2} \leq d + \left( \frac{d+1}{2} \right) + d^{2} = C(d, 2).$$
Now suppose \( d \geq 2 \) and \( N \geq 3 \). Then

\[
F(d, N) = d(N - 1) + \sum_{k=1}^{N} \sum_{i=2}^{k} d^i
= d(N - 1) + \sum_{k=1}^{N} \frac{d^2(d^{k-1} - 1)}{d - 1}
= d(N - 1) - \frac{Nd^2}{d - 1} + \frac{1}{d - 1} \sum_{k=1}^{N} d^{k+1}
= d(N - 1) - \frac{Nd^2}{d - 1} + \frac{1}{d - 1} \cdot \frac{d^2(d^N - 1)}{d - 1}
= \frac{d^{N+2} - d^3 - (N - 1)d^2 + (N - 1)d}{(d - 1)^2}.
\]

(A.5)

And

\[
C(d, N) = \sum_{k=2}^{N} \left( d + \binom{d + k - 1}{k} \right) + \sum_{k=1}^{N} (k - 1)d^k
\geq \sum_{k=1}^{N} (k - 1)d^k
= \frac{(N - 1)d^{N+2} - Nd^{N+1} + d^2}{(d - 1)^2}.
\]

(A.6)

Thus we see that it suffices to show that

\[
d^{N+2} - d^3 - (N - 1)d^2 + (N - 1)d \leq (N - 1)d^{N+2} - Nd^{N+1} + d^2,
\]

for \( d \geq 2 \) and \( N \geq 3 \). That is,

\[
0 \leq d^{N+1}(d(N - 2) - N) + d(d^2 + N(d^2 - 1) + 1).
\]

(A.7)

At this point \( d = 2, N = 3 \) must be handled as a special case, and may be verified by direct evaluation of equation (A.7). So now assume \( d \geq 2, N \geq 3 \), and that \( d = 2, N = 3 \) does not occur jointly. Then we see that equation (A.7) is implied by

\[
0 \leq d(N - 2) - N,
0 \leq d^2 + N(d^2 - 1) + 1.
\]

The second condition is trivially true. The first condition rearranges to \( N/(N-2) \leq d \), which is now true for \( d \geq 2, N \geq 3 \) with \( d = 2, N = 3 \) not jointly true.

This establishes the uniform bound \( F(d, N) \leq C(d, N) \).

Checking the asymptotic complexity is much more straightforward. Consulting equations (A.5) and (A.6) shows that \( F(d, n) = O(d^N) \) whilst \( C(d, N) = \Omega(Nd^N) \). (And in fact as \( \binom{d+k-1}{k} \leq d^k \) then equation (A.2) demonstrates that \( C(d, N) = O(Nd^N) \).)

A.2. Logsignature bases.
A.2.1. Words, Lyndon words, and Lyndon brackets. Let $\mathcal{A} = \{a_1, \ldots, a_d\}$ be a set of $d$ letters. Let $\mathcal{A}^+ = \{a \in \mathcal{A}\}$ be the set of all words in these letters, of length between 1 and $N$ inclusive. For example $a_1 a_4 \in \mathcal{A}^+$ is a word of length two.

Impose the order $a_1 < a_2 < \cdots < a_d$ on $\mathcal{A}$, and extend it to the lexicographic order on words in $\mathcal{A}^+$ of the same length as each other, so that for example $a_1 a_2 < a_2 a_1$. Then a Lyndon word \(^4\) is a word which comes earlier in lexicographic order than any of its rotations. For example $a_2 a_3 a_4 a_2$ is a Lyndon word, as it is lexicographically earlier than $a_2 a_4 a_2 a_3$ and $a_3 a_4 a_2 a_2$.

Denote by $L(\mathcal{A}^+)$ the set of all Lyndon words of length between 1 and $N$.

Given any Lyndon word $w_1 \cdots w_n$ with $n \geq 2$ and $w_i \in \mathcal{A}$, we may consider its longest Lyndon suffix; that is, the smallest $j$ for which $w_j \cdots w_n$ is a Lyndon word. (It is guaranteed to exist as $w_n$ alone is a Lyndon word.) It is then a fact \(^4\) that $w_j \cdots w_n$ is also a Lyndon word. Given a Lyndon word $w$, we denote by $w^b$ its longest Lyndon suffix, and by $w^a$ the corresponding prefix.

Let $\text{span}$ denote the span with respect to $\mathbb{R}$, and let

$$\left[ \cdot, \cdot \right]: \text{span}(\mathcal{A}^+) \times \text{span}(\mathcal{A}^+) \to \text{span}(\mathcal{A}^+)$$

be the anticommutator given by

$$[w, z] = wz - zw.$$

Then define

$$\phi: \mathcal{L}(\mathcal{A}^+) \to \text{span}(\mathcal{A}^+)$$

by $\phi(w) = w$ if $w$ is a word of length one, and by

$$\phi(w) = [\phi(w^a), \phi(w^b)]$$

otherwise. For example,

$$\phi(a_1 a_2 a_2) = [[a_1, a_2], a_2] = [a_1 a_2 - a_2 a_1, a_2] = a_1 a_2 a_2 - 2a_2 a_1 a_2 + a_2 a_1 a_2.$$

Now extend $\phi$ by linearity from $\mathcal{L}(\mathcal{A}^+)$ to $\text{span}(\mathcal{L}(\mathcal{A}^+))$, so that

$$\phi: \text{span}(\mathcal{L}(\mathcal{A}^+)) \to \text{span}(\mathcal{A}^+)$$

is a linear map between finite dimensional real vector spaces, from a lower dimensional space to a higher dimensional space.

Next, let

$$\psi: \mathcal{A}^+ \to \text{span}(\mathcal{L}(\mathcal{A}^+))$$

be such that $\psi(w) = w$ if $w \in \mathcal{L}(\mathcal{A}^+)$, and $\psi(w) = 0$ otherwise. Extend $\psi$ by linearity to $\text{span}(\mathcal{A}^+)$, so that

$$\psi: \text{span}(\mathcal{A}^+) \to \text{span}(\mathcal{L}(\mathcal{A}^+))$$

is a linear map between finite dimensional real vector spaces, from a higher dimensional space to a lower dimensional space.
A.2.2. A basis for signatures. Next, recall that the signature transform maps between spaces as follows.

\[ \text{Sig}^N : \mathcal{S}(\mathbb{R}^d) \to \prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k}. \]

Let \( \{e_i \mid 1 \leq i \leq d\} \) be the usual basis for \( \mathbb{R}^d \). Then

\[ \{e_{i_1} \otimes \cdots \otimes e_{i_k} \mid i \leq i_1, \ldots, i_k \leq d\} \]

is a basis for \( (\mathbb{R}^d)^{\otimes k} \). An arbitrary element of \( \prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k} \) may be written as

\[ (A.8) \quad \left( \sum_{i_1, \ldots, i_k = 1}^{d} \alpha_{i_1, \ldots, i_k} e_{i_1} \otimes \cdots \otimes e_{i_k} \right)_{1 \leq k \leq N}, \]

for some \( \alpha_{i_1, \ldots, i_k} \).

Then \( A_{+N} \) may be used to represent a basis for \( \prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k} \). Identify \( e_{i_1} \otimes \cdots \otimes e_{i_k} \) with \( a_{i_1} \cdot \cdots \cdot a_{i_k} \). Extend linearly, so as to identify expression \( (A.8) \) with the formal sum of words

\[ \sum_{k=1}^{N} \sum_{i_1, \ldots, i_k = 1}^{d} \alpha_{i_1, \ldots, i_k} a_{i_1} \cdots a_{i_k}. \]

With this identification,

\[ (A.9) \quad \text{span}(A_{+N}) \cong \prod_{k=1}^{N} (\mathbb{R}^d)^{\otimes k}. \]

A.2.3. Bases for logsignatures. Suppose we have some \( x \in \mathcal{S}(\mathbb{R}^d) \). Using the identification in equation \( (A.9) \), then we may seek some \( x \in \text{span}(\mathcal{L}(A_{+N})) \) such that

\[ (A.10) \quad \phi(x) = \log \left( \text{Sig}^N(x) \right). \]

This is an overdetermined system. As a matrix \( \phi \) is tall and thin. However it turns out that \( \text{im (log)} = \text{im (\phi)} \) and moreover there exists a unique solution. (That it is an overdetermined system is typically the point of the logsignature transform over the signature transform, as it then represents the same information in less space.)

If \( x = \sum_{\ell \in \mathcal{L}(A_{+N})} \alpha_{\ell} \ell, \) with \( \alpha_{\ell} \in \mathbb{R} \), then by linearity

\[ \sum_{\ell \in \mathcal{L}(A_{+N})} \alpha_{\ell} \phi(\ell) = \log \left( \text{Sig}^N(x) \right), \]

so that \( \phi(\mathcal{L}(A_{+N})) \) is a basis, called the Lyndon basis, of \( \text{im (log)} \). The collection of \( \alpha_{\ell} \) are what we may seek to compute when computing the logsignature transform, and indeed, this is what is done by \texttt{iisignature}. See [14] for details of this procedure, which in particular involves solving the linear system \( (A.10) \).

However, it turns out that this is unnecessarily expensive. In deep learning, it is typical to apply a learnt linear transformation after a nonlinearity - in which case
we do not care in what basis we represent the logsignature, and we can find a more efficient one.

It turns out that the Lyndon basis exhibits a particular triangularity property \cite[Theorem 5.1]{15}, \cite[Theorem 32]{13}, meaning that for all $\ell \in \mathcal{L}(A^+ N)$, then $\phi(\ell)$ has coefficient zero for any Lyndon word lexicographically earlier than $\ell$. This property has already been exploited by \textit{iisignature} to solve (A.10) efficiently, but we can in fact do better: it means that

$$\psi \circ \phi: \text{span} \left( \mathcal{L} \left( A^+ N \right) \right) \rightarrow \text{span} \left( \mathcal{L} \left( A^+ N \right) \right)$$

is a triangular linear map, and so in particular it is invertible, and defines a change of basis; it is this alternate basis that we shall use instead. Instead of seeking $x$ as in equation (A.10), we may now instead seek $z \in \text{span} \left( \mathcal{L} \left( A^+ N \right) \right)$ such that

$$(\phi \circ (\psi \circ \phi)^{-1})(z) = \log \left( \text{Sig}^N(x) \right).$$

But now by simply applying $\psi$ to both sides:

$$z = \psi \left( \log \left( \text{Sig}^N(x) \right) \right).$$

This is now incredibly easy to compute. Once $\log \left( \text{Sig}^N(x) \right)$ has been computed, and interpreted as in equation (A.9), then the operation of $\psi$ is simply to extract the coefficients of all the Lyndon words, and we are done.

\textbf{Appendix B. Further benchmarks.}

\textbf{B.1. Code for reproducability.} The benchmarks may be reproduced with the following code on a Linux system. First install everything. Note that numpy must be installed in a separate command before \textit{iisignature}, and PyTorch must be installed in a separate command before Signatory.

```
pip install numpy==1.18.0 matplotlib==3.0.3
pip install torch==1.3.1 iisignature==0.24 esig==0.6.31
pip install signatory==1.1.6.1.3.1
```

```
git clone https://github.com/patrick-kidger/signatory.git
cd signatory
```

The unusually long version number for Signatory is used to specify both the version of Signatory, and the version of PyTorch that it is for. The \texttt{git clone} is necessary as the benchmarking code is not distributed via \texttt{pip}. Then run

```
python command.py benchmark --help
```

for further details on how to run any particular benchmark. For example,

```
python command.py benchmark -m time -f sigf -t depths -o graph
```

will perform time benchmarks on the forward operation of the signature transform, for a series of increasing depths, and will output the result as a graph.

\textbf{B.2. Memory benchmarks.} Our benchmark scripts do offer some limited ability to benchmark memory consumption, with the \texttt{-m memory} flag to the benchmark scripts.

The usual approach to such benchmarking, using \texttt{valgrind’s massif}, necessarily includes measuring the set-up code. As this includes loading both the Python interpreter and PyTorch, measuring the memory usage of our code becomes tricky.

As such we use an alternate method, in which the memory usage is sampled at intervals, using the Python package \texttt{memory_profiler}, which may be installed via
pip install memory_profiler. This in turn has the limitation that it may miss a peak in memory usage; for small calculations it may miss the entire calculation. Furthermore, the values reported are inconsistent with those reported in [14].

Due to these limitations, we do not report memory benchmarks here.

**B.3. Signature transform benchmarks.** See Figure 5.1 for the graphs of the benchmarks for the signature transform. The precise values of the points on these graphs are as follows. Also shown is the ratio between the speed of Signatory and the speed of \textit{iisignature}.

| Signature forward, varying channels | Channels | 2 | 3 | 4 | 5 | 6 | 7 |
|-------------------------------------|----------|---|---|---|---|---|---|
| \textsc{esig}                      | 0.531    | 9.34 | - | - | - | - | - |
| \textsc{iisignature}               | 0.00775  | 0.0632 | 0.375 | 1.97 | 7.19 | 20.9 | - |
| Signatory CPU (no parallel)        | 0.00327  | 0.0198 | 0.101 | 0.402 | 1.45 | 3.8 | - |
| Signatory CPU (parallel)           | 0.00286  | 0.00504 | 0.00975 | 0.00777 | 0.21 | 1.22 | - |
| Signatory GPU                      | 0.0129   | 0.0135 | 0.0182 | 0.00222 | 0.0599 | 0.158 | - |
| Speedup CPU (no parallel)          | 2.37     | 3.19 | 3.71 | 4.89 | 4.95 | 5.49 | - |
| Speedup CPU (parallel)             | 2.71     | 12.5 | 38.5 | 34.1 | 34.2 | 17.0 | - |
| Speedup GPU                        | 0.602    | 4.68 | 20.6 | 88.7 | 120 | 132 | - |

| Signature forward, varying channels | Channels | 2 | 3 | 4 | 5 | 6 | 7 |
|-------------------------------------|----------|---|---|---|---|---|---|
| \textsc{esig}                      | 0.026    | 0.248 | 1.59 | 7.78 | 27.6 | 1.28e+02 | - |
| \textsc{iisignature}               | 0.000468 | 0.00145 | 0.00485 | 0.00199 | 0.0859 | 0.376 | 1.83 | 8.16 |
| Signatory CPU (no parallel)        | 0.000708 | 0.00129 | 0.00222 | 0.000705 | 0.0027 | 0.104 | 0.402 | 1.68 |
| Signatory CPU (parallel)           | 0.000722 | 0.00242 | 0.00279 | 0.00321 | 0.00546 | 0.0161 | 0.0408 | 0.381 |
| Signatory GPU                      | 0.00172  | 0.00326 | 0.00484 | 0.00735 | 0.0104 | 0.0132 | 0.0232 | 0.0773 |
| Speedup CPU (no parallel)          | 0.661    | 1.12 | 2.2 | 2.61 | 3.18 | 3.6 | 4.55 | 4.86 |
| Speedup CPU (parallel)             | 0.649    | 0.597 | 1.74 | 6.21 | 15.7 | 23.3 | 44.8 | 21.4 |
| Speedup GPU                        | 0.273    | 0.443 | 1.0 | 2.71 | 8.24 | 28.3 | 79.9 | 106 |

| Signature backward, varying depths | Depth | 2 | 3 | 4 | 5 | 6 | 7 |
|-------------------------------------|-------|---|---|---|---|---|---|
| \textsc{esig}                      | 0.0149 | 0.00438 | 0.0179 | 0.0054 | 0.366 | 1.59 | 7.72 | 34.7 |
| \textsc{iisignature}               | 0.00322 | 0.00518 | 0.0123 | 0.0347 | 0.109 | 0.437 | 1.8 | 6.31 |
| Signatory CPU (no parallel)        | 0.00354 | 0.00409 | 0.0089 | 0.0152 | 0.0563 | 0.175 | 0.839 | 4.06 |
| Signatory CPU (parallel)           | 0.00525 | 0.00916 | 0.015  | 0.0216 | 0.0324 | 0.05  | 0.144 | 0.495 |
| Speedup CPU (no parallel)          | 0.464   | 0.845 | 1.45 | 2.75 | 3.37 | 3.63 | 4.28 | 5.49 |
| Speedup CPU (parallel)             | 0.422   | 1.07  | 2.02 | 6.28 | 6.51 | 9.07 | 9.21 | 8.54 |
| Speedup GPU                        | 0.284   | 0.478 | 1.19 | 4.42 | 11.3 | 31.7 | 53.8 | 70.1 |