Motiflets - Fast and Accurate Detection of Motifs in Time Series

Patrick Schäfer
patrick.schaefer@hu-berlin.de
Humboldt-Universität zu Berlin
Berlin, Germany

Ulf Leser
leser@informatik.hu-berlin.de
Humboldt-Universität zu Berlin
Berlin, Germany

ABSTRACT

A time series motif intuitively is a short time series that repeats itself approximately the same within a larger time series. Such motifs often represent concealed structures, such as heart beats in an ECG recording, or sleep spindles in EEG sleep data. Motif discovery (MD) is the task of finding such motifs in a given input series. As there are varying definitions of what exactly a motif is, a number of different algorithms exist. As central parameters they all take the length l of the motif and the maximal distance r between the motif's occurrences. In practice, however, especially suitable values for r are very hard to determine upfront, and the found motifs show a high variability. Setting the *wrong* input value will result in a motif that is not distinguishable from noise. Accordingly, finding an interesting motif with these methods requires extensive trial-and-error.

In this paper, we present a different approach to the MD problem. We define k-Motiflets as the set of exactly k occurrences of a motif of length l, whose maximum pairwise distance is minimal. This turns the MD problem upside-down: The central parameter of our approach is not the distance threshold r, but the desired size k of a motif set, which we show is considerably more intuitive and easier to set. Based on this definition, we present exact and approximate algorithms for finding k-Motiflets and analyze their complexity. To further ease the use of our method, we describe statistical tools to automatically determine the *right/suitable* values for its input parameters. Thus, for the first time, extracting meaningful motif sets without any a-priori knowledge becomes feasible.

By evaluating several real-world use cases and comparison to four state-of-the-art MD algorithms, we show that our proposed algorithm is (a) quantitatively superior, finding larger motif sets at higher similarity, (b) qualitatively better, leading to clearer and easier to interpret motifs, and (c) has the lowest runtime.

KEYWORDS

motif, time series, set, concealed, frequent, unsupervised

ACM Reference Format:
Patrick Schäfer and Ulf Leser. 2018. Motiflets - Fast and Accurate Detection of Motifs in Time Series. In *Woodstock '18: ACM Symposium on Neural Gaze Detection, June 03–05, 2018, Woodstock, NY*. ACM, New York, NY, USA, 14 pages. https://doi.org/10.1145/1122445.1122456

Woodstock '18, June 03–05, 2018, Woodstock, NY
© 2018 Association for Computing Machinery.
ACM ISBN 978-1-4503-XXXX-X/18/06…$15.00
https://doi.org/10.1145/1122445.1122456

1 INTRODUCTION

Time series (TS) are sequences of real values ordered along a specific dimension, with time as the most important dimension. The concept of time series motif discovery (TSMD, or MD in short) was first described in [21] and has since then emerged as an important primitive for exploring and analyzing TS [7, 14, 19, 21, 28, 29]. Intuitively, MD is the problem of finding patterns, i.e., short time series, that repeat themselves approximately the same within a given TS. These motifs often reflect concealed structures in the process generating the TS, such as heart beats in an ECG recording [22] or sleep spindles and k-Complexes in EEG sleep data [10]. Applications of MD exist across many domains, such as seismic signals [27], electric household devices [26], DNA sequences [5], electrocardiography data [16], wind generation turbines [9], or audio signal analysis [6]. MD is also important as a pre-processing step for classification, clustering, anomaly detection, and rule discovery in TS [28]. For example, identified motifs can help to speed up feature extraction in TS classification [11].

Though intuitively easy to describe, the specific definitions of the MD problem for a TS T differ notably between existing works. Several tools focus only on *motif pairs* [19, 29], which are defined as the most similar pair(s) of subsequences of T of user-defined length l. However, real-world motifs typically do not only occur in pairs; for example, heartbeats in ECG recordings are all similar to each other. A more general and arguably more natural approach to MD is the search for *motif sets*, defined as the largest set of short TS approximately contained in T and in *some sense* close to each other. At least four different definitions exist for this *in some sense*, namely (by date of publication): k-Motifs [21], Range Motif (RM) [19], Learning Motif (LM) [7], and VALMOD Motif Sets [15][1]. All of these methods require users to provide two central parameters: the motif length l, and a distance threshold r. While the former can often be estimated using domain knowledge, the latter is very hard to set. Yet, no algorithms are known for learning the input parameters from the data. This creates the need of extensive manual tuning by trial-and-error when using these methods in practice. Notably, all existing algorithms for motif sets are heuristics, and the exact complexity of the underlying problem is often unknown. For RM, there actually exists no algorithm yet.

In this paper, we introduce k-Motiflets, a novel definition for motif set discovery that turns the problem upside-down. Instead of requesting a user to define the threshold r, k-Motiflets take the desired size k of the motif set as parameter. On the other hand r is a real number for which intuition is very difficult to obtain, it cannot be learned, and failure to provide the *right* value will result in motifs indistinguishable from noise. Yet, k is an integer with an easily understood interpretation. Additionally, we provide, for

[1] For precise definitions, see Section 2

the first time, two algorithms to learn the input parameters of k-Motiflets. This reduces the time and efforts in exploratory analysis considerably. Based on our new definition, we provide exact and approximate algorithms for finding k-Motiflets and show that the approximate version leads to better motifs than four state-of-the-art competitors, is notably faster, and finds motifs that are close to the known motifs on all data sets we studied.

To illustrate the consequences of this approach in relation to prior work, Figure 1 (top) shows a TS from the Long Term Atrial Fibrillation (LTAF) database [22], which is often used for demonstrations in MD [3]. The problem is particularly difficult for MD as actually two motifs exists: The first half of the TS contains a rectangular calibration signal with 6 occurrences, and the second half shows ECG heartbeats with 16 to 17 occurrences. We applied our novel k-Motiflets to this problem and compared results to those of VALMOD [15], two implementations of k-Motifs - namely EMMA [17] and Set Finder [1] - and Learning Motifs (LM) [7])[2]. Such comparisons are actually difficult to make, due to the different parameterizations, and the previously mentioned inevitable yet complex tuning process; we will provide a systematic evaluation in Section 6. In Figure 1 (b), we show the positions of the motif occurrences (after tuning) for the two best motif sets found by each method; Figure 1 (c) shows examples for the actual shape of the occurrences. k-Motiflets (orange line in Figure 1 (b)) clearly identified all 16 heartbeats and all 6 calibration waves. Next in Figure 1b), Set Finder finds 11 heartbeats as TOP-1 motif and 5 calibration waves as TOP-2 motif. The third method, EMMA, is not able to handle this TS adequately and returns a blurred and too large calibration signal set as Top-1 motif set, and a too small calibration set as second best. Also VALMOD stays locked with the calibration signal without actually finding the optimal set. Finally, LM discovered up to 14 ECG waves and all 6 calibration signals.

In summary, the contributions of this paper are as follows:

(1) We define k-Motiflets, a novel definition for MD in time series. In contrast to all previous works, this definition is based on the desired size k of the motif set, not the maximum distance r between occurrences of a motif.
(2) We present exact and approximate algorithms for finding k-Motiflets. As k-Motiflet can be considered as an extension of the RM definition of motif sets, we thereby also provide the first implementation of this definition.
(3) We analyze the complexity of both algorithms and show that our polynomial-time approximate method is a 2-approximation to our exponential-time exact algorithm.
(4) To further ease the use of the new method, we present extensions of the algorithms, that can automatically learn the *right* values for the two input parameters, namely motif size k and length l, to discover interesting motifs. This considerably reduces the time and effort needed in exploratory analysis.
(5) We perform extensive quantitative and qualitative evaluation of our new methods on 5 real-world TS and compare them to four state-of-the-art competitors. We show that our approximate algorithm finds larger motif sets given the same distance threshold and motif sets with smaller pairwise distances given the motif set size k. By means of several use cases, we furthermore illustrate that k-Motiflets lead to motifs that are clearer and easier to interpret. Experiments also show that our approximate algorithm is faster than any of the competitors.

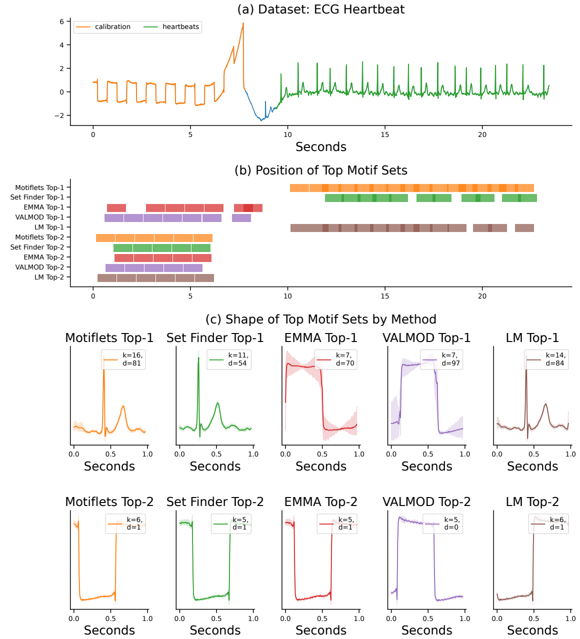


Figure 1: A comparison of MD algorithms on an ECG heartbeat TS from the LTAF database [22]. The TS contains two motifs. It starts with 6 repetitions of a calibration signal, followed by roughly 16 full heartbeats. We report the two TOP (largest) found motif sets. Two algorithms (EMMA and VALMOD) found the calibration wave as TOP-1 and TOP-2 motif set. k-Motiflets, Set Finder and LM identify both heartbeats and calibration. Still, only k-Motiflets identify all 16 heartbeats and 6 calibrations.

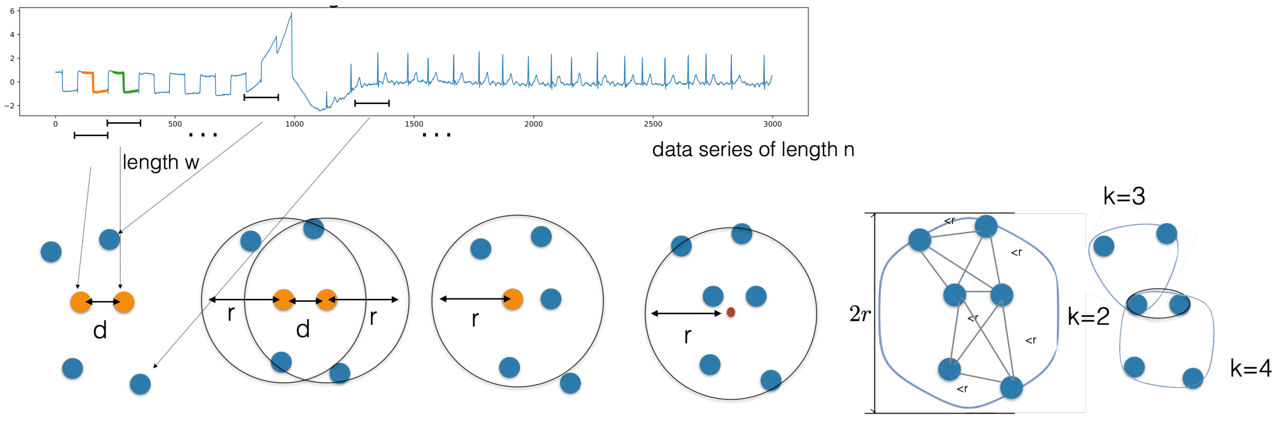
The remainder of this paper is organized as follows: Section 2 explains commonalities and differences between existing MD definitions and introduces our new approach, k-Motiflets. Section 3 presents related work. Section 4 introduces an exact and an approximate algorithm for finding k-Motiflets and analyzes their properties. Section 5 describes two extensions to learn the input parameters l and k from the data, respectively. Section 6 presents our experimental evaluation. Section 7 concludes the paper.

2 BACKGROUND AND DEFINITIONS

In this section, we first formally define time series (TS) and the z-normalized Euclidean distance, which we (like all prior work) will use throughout this work. Next, we introduce the four existing MD definitions and show their differences using a geometric metaphor. We then introduce k-Motiflets by derivation from Range Motifs (RM), and relate them to the prior work.

Definition 2.1. Time Series: A time series $T = (t_1, t_2, \ldots, t_n)$ of length n is an ordered sequence of n real-values $t_i \in \mathbb{R}$.

[2] To date, no implementation following the RM definition exists; see Section 2



(a) (Top) Pair Motif
support=2
extent=$d \in \mathbb{R}$

(b) Valmod Motif Sets
support=depends on D
extent=r=$D \cdot d \in \mathbb{R}$

(c) k-Motifs
support depends on r
extent=$r \in \mathbb{R}$

(d) Learning Motifs
support depends on r
extent=$r \in \mathbb{R}$

(e) Range Motifs
support depends on r
extent=pairwise <$2r \in \mathbb{R}$

(f) k-Motiflets
support=$k \in \mathbb{N}$
extent depends on k

Figure 2: Illustration of the six different concepts of motif discovery. We consider six subsequences of fixed length as potential motif set and plot them in a 2-dimensional space. From left to right: (a) PM, (b) VS, (c) K-Motif, (d) LM, (e) RM, (f) k-Motiflets, for $k \in [2, 3, 4]$. Geometrically, VS, LM and K-Motif are (unions of) hyperspheres; RM and k-Motiflets are Reuleaux polygons.

Note that time series sometimes are also called data series, for instance in [14].

Definition 2.2. Subsequence: A subsequence $S_{i;l}$ of a time series $T = (t_1, \ldots, t_n)$, with $1 \leq i \leq n$ and $1 \leq i + l \leq n$, is a time series of length l consisting of the l contiguous real-values from T starting at offset i: $S_{i;l} = (t_i, t_{i+1}, ..., t_{i+l-1})$.

Works in MD typically exclude overlapping subsequences from consideration for motifs, as their distance is naturally low.

Definition 2.3. Overlapping subsequences (Trivial Match): Two subsequences $S_{i;l}$ and $S_{j;l}$ of length l of the same time series T overlap iff they share at least $l/2$ common offsets of T: $(i - l/2) \leq j \leq (i + l/2)$.

In the context of MD, the similarity of two subsequences is (almost exclusively) measured using the *z-normalized Euclidean distance.*

Definition 2.4. z-normalized Euclidean distance (z-ED): Given two subsequences $S_l^{(1)} = (s_1^{(1)}, \ldots, s_l^{(1)})$ with mean $\mu^{(1)}$ and standard-deviation $\sigma^{(1)}$ and $S_l^{(2)} = (s_1^{(2)}, \ldots, s_l^{(2)})$ with $\mu^{(2)}$ and $\sigma^{(2)}$, both of length l, their z-normalized Euclidean distance (z-ED) is defined as:

$$z\text{-}ED(S_l^{(1)}, S_l^{(2)}) = \sqrt{\sum_{t=1}^{l} \left(\frac{s_t^{(1)} - \mu^{(1)}}{\sigma^{(1)}} - \frac{s_t^{(2)} - \mu^{(2)}}{\sigma^{(2)}} \right)^2} \qquad (1)$$

Using this distance function, we may now introduce a notion for the approximate matching of subsequences as basis for MD.

Definition 2.5. r-match: Two subsequences $S_{i;l}$ and $S_{j;l}$ of T are called r-matching iff (a) $z\text{-}ED(S_{i;l}, S_{j;l}) \leq r \in \mathbb{R}$ and (b) they are *non-overlapping*. A set S of subsequences of T is called r-matching, iff all subsequences in S are pairwise r-matching.

2.1 Pair Motifs and Motif Sets

We next define the two basic approaches to MD: *pair motifs* and *motif sets*. A geometrical and intuitive explanation of their differences is shown in Figure 2. Note that the original definitions of LM, VS and K-Motifs left it undefined whether the subsequences in a motif set must be pairwise non-overlapping or not. As such, the K-Motif reference implementation [17] discovers sets of pairwise overlapping subsequences. In this work, we require (by definition of r-matching) all sequences in a motif set to be non-overlapping.

Definition 2.6. Top Pair Motif (PM) [19]: The top pair motif of length $l \in \mathbb{N}$ of T is the pair of non-overlapping subsequences of length l of T with minimal distance.

Obviously, two PMs may share the same distance. To solve ties when enumerating PMs, the PMs are typically returned in the order of appearance in the TS. Next, we present the four different definitions of motif sets that capture approximately repeated subsequences of a TS.

Definition 2.7. Top K-Motif [21]: Given radius $r \in \mathbb{R}$ and length $l \in \mathbb{N}$, the top K-Motif is the largest set S of subsequences of length l of T for which the following holds: There exists a subsequence $S_{i,l}$ of T which is r-matching to all members of S. We call $S_{i,l}$ the core of S, and S the motif set (or just motif).

Note that this definition requires that the core of the motif itself is a subsequence of T. This constraint is lifted in the following definitions; in the latest and most liberal definition, i.e., the range motif (see below), actually no core must exist anymore.

Definition 2.8. Top Learning Motif (LM) [7]: Given a time series T, radius $r \in \mathbb{R}$ and length $l \in \mathbb{N}$, the top LM of T is the largest set S of subsequences of length l of T for which the following holds: There exists a core sequence C which is r-matching to all members of S.

The only difference between k-Motifs and Learning Motifs is that for the latter the core of S must not be a subsequence of T itself. For this reason, LM motifs are also called latent motifs [7].

An alternative definition for MD was introduced by VALMOD.

Definition 2.9. VALMOD Motif Set (VS) [15]: Given a time series T, its pair motif $S_{i;l}, S_{j;l}$, distance $r \in \mathbb{R}$ and length $l \in \mathbb{N}$, the VS of T is the set of subsequences that are $r - matching$ to $S_{i;l}$ or $S_{j;l}$.

Thus, the VS always computes the top pair motif first and then iteratively extends its two subsequences with close neighbours. Accordingly, the pairwise distances of subsequences in a VS motif may be up to $3r$.

The to-date most liberal definition of MD is that of [19], which does not require a core to exist. While it is more than a decade old, no algorithm for computing such motifs has been published yet.

Definition 2.10. Top Range Motif (RM) Set [19]: Given a time series T, distance $r \in \mathbb{R}$ and length $l \in \mathbb{N}$, the top RM of T is the largest set of subsequences S from T that are pairwise $2r$-matching.

Figure 2 shows a geometrical explanation for the differences between the five MD definitions based on the TS from Figure 1. For illustration, we represent subsequences of T as points in 2-dimensional space. Geometrically, the LM set forms a hypersphere with radius r around a latent core S_l. K-Motifs form a hyper-sphere of radius r around a core $S_{i;j}$ of T. VS is the union of two hyperspheres of radius r around the pair motif. Finally, RM forms a so-called Reuleaux Polygon: A shape created by the union of circles of radius r around the subsequences of the motif.

Observe that the circle of diameter $2r$ as defined by a LM is a special case of a Reuleaux Polygon and consequently of a RM. All points inside the LM have pairwise distance smaller than or equal to its diameter $2r$. In fact, RM returns the same shape as LM iff a circular shape covers the most subsequences among all possible shapes defined by Reuleaux Polygons. The opposite is not true, as a Reuleaux Triangle of width $2r$ cannot be covered by a circle with diameter $2r$. Therefore, the RM is a more general definition than LM; nevertheless, it is still under-researched. The computational complexities of finding the exact LM or RM are unknown. Solving PM and K-Motifs problem is quadratic in the TS length n. A list of existing implementations of the different definitions can be found in Table 1.

2.2 k-Motiflets

All of the aforementioned MD definitions have in common that their motif sets depend on two parameters, i.e., the length l of subsequences and the distance threshold r. Especially r is very hard to set in practice, as it is very difficult to get an intuition regarding a threshold on the z-normalized distance of subsequences of a TS. Furthermore, already slight variations of its value may lead to grossly different motifs which makes tuning rather brittle. Yet, no methods for learning the parameters from the data are known. In contrast, k-Motiflets, which will be defined in the following, is independent of r. Instead, it requires users to set an integer parameter k that defines the size of the motif set to be discovered. This measure is easy to understand, has much less possible values (integer versus real), can be learned from the data (Section 5), and inherently leads to smoothly growing motif sets in experimentation (see Figure 5 for an example). Before introducing k-Motiflets, we first have to define the *extent* of a motif.

Definition 2.11. Extent: Consider a TS T and a set S of subsequences of T of length l. The *extent* of S is the maximal pairwise distance of elements from S:

$$extent(S) = \max_{(S^{(1)},S^{(2)})\in S\times S} (z\text{-}ED(S^{(1)}, S^{(2)}))$$

We next define k-Motiflets. These could actually build on any of the existing motif set definitions; we use RM to achieve maximal flexibility.

Definition 2.12. Top k-Motiflet: Given a time series T, cardinality $k \in \mathbb{N}$ and length l, the top k-Motiflet of T is the set S with $|S| = k$ subsequences of T of length l for which the following holds: All elements of S are pairwise r-matching, and there exists no set S' with $extent(S') < extent(S)$ also fulfilling these constraints.

Note that the top k-Motiflet is not unique if two (or more) sets of subsequences with k-subsequences share the same smallest distance. In our current implementation, ties are broken by returning the motif set with the earlier occurrence in the TS. However, an extension to return all k-Motiflets would be simple. Geometrically, a k-Motiflet is the smallest Reuleaux polygon that covers k subsequences. For $k = 2$ this is equal to the Pair Motif definition. For any $k \geq 2$ this represents the RM of size k with smallest r. Figure 2 illustrates 2, 3, 4-Motiflets in comparison to the other definitions.

3 RELATED WORK

Motif discovery in TS has been researched intensively for approximately 20 years. The first publication we are aware of was studied in the context of summarizing and visualizing massive TS datasets [17]. In the following, we shall first discuss recent approaches to pair MD and then focus on methods for the discovery of motif sets.

The MK algorithm [19] from Mueen et al. published in 2009 is likely the most widely used baseline for pair MD. However, it is outperformed by more recent methods in terms of runtime, in particular QUICK MOTIF [12], STOMP [31], SCRIMP [30], and VALMOD [14]. QUICK MOTIF first builds a summarized representation of the data using Piecewise Aggregate Approximation (PAA) and arranges these summaries in Minimum Bounding Rectangles within a Hilbert R-Tree index for pruning. STOMP and SCRIMP are based on the computation of the matrix profile [29], which represents the 1-nearest-neighbor (1-NN) subsequence to each subsequence of a TS. The subsequence pair with smallest distance among all is the motif pair. VALMOD [14] addresses the limitation that previous works always assumed a user-defined motif length l. Instead, they proposed an efficient algorithm for finding best pairs within a range $[l_{min} \dots l_{max}]$[3]. VALMOD was extended to return motif sets by performing a range-query around the two pair motif sequences. A common characteristic of algorithms for pair MD is a complexity of up to $O(n^2 l)$, for a TS of length n and a fixed motif length l (compare Table 1). Using SCRIMP to compute the pairwise distance matrix, this may be reduced to $O(n^2)$. Our implementation of k-Motiflets is based on the fast formulation of this problem as in SCRIMP [4, 30], but extended for k-NN distances; it will be described in more detail in Section 4.

[3] In our evaluation in Section 6, we shall use VALMOD for fixed length l only.

Motif Type	Name	Worst Case Complexity	Properties	Exact?
Motif Pairs [19]	MK [19]	$O(ln^2)$	Admissible Pruning	Yes
	SCRIMP [30]	$O(n^2)$	Runtime independent of l	Yes
	VALMOD [14]	$O((l_{max} - l_{min}) \cdot n^2)$	Variable length over ranges	Yes
K-Motifs [17]	EMMA [17]	$O(ln^2)$	SAX-based, produces trivial-matches	Heuristic
	GrammarViz [24, 25]	$O(n^2)$	Discretization (SAX), variable length	Heuristic
	ScanMK [1]	$O(ln^2)$		Heuristic
	ClusterMK [1]	$O(ln^2)$	Hierarchical Clustering	Heuristic
	SetFinder [1]	$O(ln^2)$		Heuristic
Learning Motifs [7]	Learning Motifs [7]	$O(ln)$	Non-convex Gradient Desc.	Heuristic
VALMOD Motif Sets [14]	VALMOD [14]	$O((l_{max} - l_{min}) \cdot n^2)$	Variable length	Exact
Range Motifs [19]	None	-	No known implementation.	-

Table 1: Overview of state-of-the-art Pair Motif and Motif Set discovery definitions and implementations, given a motif length l and TS of length n. Notably, no Range Motif discovery algorithm was published to-date. There are four different formal MD definitions for Motif Sets we are aware of.

EMMA [17] was the first K-Motif discovery algorithm. It is based on the discretization of subsequences using SAX. In short, Symbolic Aggregate approXimation (SAX) [13] transforms an input TS into a string (word) based on computing mean values over intervals, and the discretization of these mean values. The SAX words are then hashed into buckets, where similar subsequences hash into similar buckets, and the buckets are subsequently post-processed to obtain the final motif sets. Also GrammarViz [24, 25] is based on SAX, on which it applies a linear-time algorithm Sequitur [20] for grammar inference. From the detected grammar rules, SAX words are derived that represent reoccurring subsequences of the TS. Like EMMA, the method is heuristic, as both mine motifs in the discretized SAX space, which can lead to two similar subsequences being considered as different.

ScanMK, ClusterMK, and SetFinder have been proposed by the same authors [1] as solutions to K-Motif discovery. ScanMK initializes set motif candidates with pair-motifs that are within a distance lower than r. From these two subsequences all nearby subsequences within r are queried and added to the set motif candidate. Finally, the set is condensed to remove subsequences that are more than $2r$ apart. ClusterMK is based on a bottom-up hierarchical clustering of the best-matching pairs of clusters within distance r. First, the closest pairs of subsequences are merged to form initial clusters. A cluster is then represented by averaging its members. Clustering terminates once the distance between clusters is larger than r. SetFinder directly searches the r-matches of every subsequence and outputs the highest cardinally set.

The concept of Learning Motif (LM) was introduced by Grabocka et al. [7] to better deal with noisy TS. The paper approaches LM discovery as a process which, starting from a random initialization, iteratively modifies a motif core S' to increase its frequency, i.e., the size of the surrounding motif, while keeping its radius fixed. As the frequency function is not differentiable, they propose a smooth Gaussian-kernel approximation that allows to use gradient ascent to find the hopefully best hidden motif cores. The LM solution is a heuristic, as the optimization problem is non-convex and the gradient ascent might get stuck in a local optimum.

Range Motif (RM) discovery was defined in [19]. It is the most liberal definition (see Section 2.1), as it does not require a motif core to exist anymore. To-date, no algorithm has been published implementing this RM concept. However, k-Motiflets are based on RM, as for any $k \geq 2$ we return the RM with smallest r to cover exactly k subsequences (see also previous Section). Our algorithms for computing k-Motiflets could thus easily be turned into a solution for the original RM problem by running them for increasing values of k until the distance threshold is violated.

4 EXACT AND APPROXIMATE K-MOTIFLET DISCOVERY

In this section we will present two algorithms solving the k-Motiflet problem. The first algorithm, presented in Section 4.2, is an efficient heuristic with polynomial runtime. Furthermore, we show that it is a 2-approximation of the exact solution. The second algorithm, presented in Section 4.3, is exact but has exponential runtime in k, and uses the heuristic solution as initial solution for pruning. Before describing the concrete algorithms, we first give an intuition of their inner working in Section 4.1.

Both algorithms expect parameters l and k to be given. While we share the necessity to set l manually with all other methods except VALMOD, we replace the usual parameter r (distance threshold) with k (size of the motif set). Although k is much easier to understand, setting it nevertheless might require time-consuming exploratory analysis. To reduce these efforts, we shall present two bespoke methods for learning both parameters l and k from the data in Section 5.

4.1 Intuition of Approximate Solution

Given a motif length l and a motif size k, the algorithmic idea of our algorithms for computing k-Motiflets is the following: we start by building motif set candidates by joining each subsequence of a TS T with its non-overlapping $(k-1)$-NNs. Next, we compute for each of these sets of cardinality k the *extent*, i.e. the maximum over all pairwise distances. Note that the subsequences in each set must not be pairwise as similar to each other as both are to the core S, as two neighbours of S may be on opposite sites of the hyperspace centered

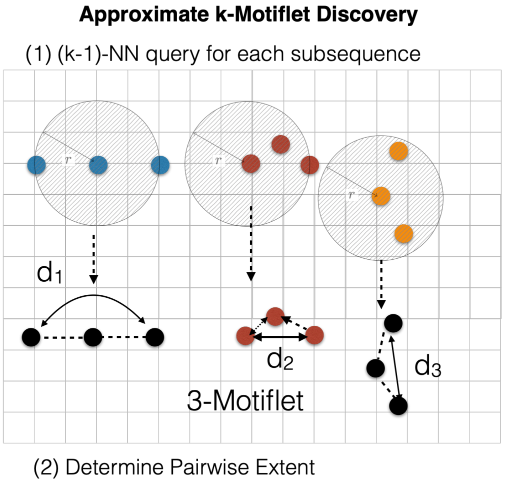

Approximate k-Motiflet Discovery
(1) (k-1)-NN query for each subsequence
r
r
r
d1
d2
d3
3-Motiflet
(2) Determine Pairwise Extent

Figure 3: Depicted are three sets (blue, red, orange) with radius r around a query. k-Motiflet discovery involves two steps: (1.) (k-1)-NN search around each query subsequence, and (2.) determine the extent of each set, i.e. d_1, d_2, d_3. Finally, the top k-Motiflet with smallest extent d_2 is returned.

Algorithm 1 Compute Approximate k-Motiflets

```
1:  procedure GET_K_MOTIFLETS($T$, $k$, $l$)
2:      $D_{i,j} \leftarrow$ CALC_DISTANCE_MATRIX(T, l)
3:      $(motiflet, d) \leftarrow (\{\}, inf)$                ▷ bsf of extent
4:      for $i \in [1, \ldots, (\text{len(T)} - l + 1)]$ do
5:          $idx \leftarrow$ ARGWHERE$(D_i < d) \cup \{i\}$
6:          if $len(idx) \geq k$ then
7:              $candidate \leftarrow$ NON_TRIVIAL_KNN$(k, idx)$
8:              $dist \leftarrow$ PAIRWISE_EXTENT$(D, candidate, d)$
9:              if $dist < d$ then
10:                 $(d, motiflet) \leftarrow (dist, k\_subset)$
11:             end if
12:         end if
13:     end for
14:     return $(motiflet, d)$
15: end procedure
```

around S. Thus, to find the best k-Motiflet, we cannot simply pick the smallest $(k-1)$-NN distance, but must explicitly determine the motif set with smallest extent. This process is illustrated in Figure 3, from $(n-1)$-NN search (top) to computing the extent (bottom) and choosing the motif set with smallest extent. Furthermore, without further modifications this method is a heuristic, as it only considers Motiflets built from the $k-1$-NNs of a core from T.

We will first outline an approximate solution to the k-Motiflet problem. We will show in Section 4.2.2 that this solution is a 2-approximation and present an exact algorithm in 4.3.

4.2 Approximate k-Motiflet Algorithm

Algorithm 1 takes as an input the TS T, the size of the motiflet $k \in \mathbb{N}$ and motif length $l \in \mathbb{N}$. First, we compute the pairwise z-normalized distance matrix (line 2). The algorithm applies admissible pruning to reduce the number of candidate sets using an upper bound on the best-so-far extent d (see line 3). It iteratively checks if there are at least k subsequences within a d-range (line 6). If *true*, we extract the closest non-trivial k subsequences (line 8), and determine the pairwise extent of this set (line 9). In PAIRWISE_EXTENT(_, _, d) we apply admissible pruning, too, by stopping the computation once any pairwise distance exceeds d. If the overall extent $dist$ is smaller than the best-so-far, we update the k-Motiflet (lines 10–13). Finally the k-Motiflet and its extent d are returned.

The presented algorithm is greedy and approximates the extent of the optimal set of subsequences in line 8, assuming that the NNs of a query are also the ones in the k-Motiflet. In NON_TRIVIAL_KNN() we order the subsequences by their distance to the query and return the closest non-trivial neighbours. Figure 3 illustrates the idea of the algorithm and the steps involved in computing a 3-Motiflet. We iteratively perform two steps for each subsequence q: (1) search for the $(k-1)$-NN of q, and (2) determine their pairwise extent of the candidate set. Finally, the set with minimal extent is returned (in red).

4.2.1 Complexity. The runtime of GET_K_MOTIFLETS(T, k, l) is dominated by the computation of the pairwise z-normalized distance matrix (line 2). Our implementation is based on an efficient formulation of this problem from [4, 30], extended for k-NN distances. This requires only $O(n^2)$-time, which is independent of the motif length l. Next, the algorithm iterates through all cells of the distance matrix in lines 5–6 with $O(n^2)$-time. Checking for non-trivial matches in line 8 requires k-times searching for the minimum over one row of the matrix with a complexity of $O(k \cdot n^2)$ over all n rows. We can compute the maximum of k pairwise distances in $O(k^2)$ (line 9). Accordingly, the for-loop is in $O(n \cdot k^2)$. Thus, the overall *worst case* runtime complexity is:

$$O(k \cdot n^2) + O(n \cdot k^2)$$

In the *best case*, due to admissible pruning, the first subsequence (first row of the matrix) is the top k-Motiflet and we can prune all further computations in the first cell of each subsequent row. The *best case* runtime complexity is thus:

$$O(n^2) + O(k^2)$$

4.2.2 2-Approximation.

Algorithm 1 only computes an approximate solutions, as it only considers Motiflets built from the $(k-1)$-NNs of a core from T, whereas the top k-Motiflet may not contain this core. In the following, we will first show that our method precisely is a 2-approximation, for $k = 3$, by constructing a worst-case instance, and then extend it to the case of $k > 3$

Case $k = 3$. Figure 4 illustrates such a worst case example for 3-Motiflets in both the xy-plane (for ease of illustration) and xyz-plane. The blue dots and red dots represent subsequences that are equally distributed on a grid with an offset of r. The offset between the red dot and the blue dots in the xy-plane shall be $r + \epsilon$, for an arbitrarily small $\epsilon \in \mathbb{R}^+$.

In the case of 3-Motiflets our approximate algorithm searches for 2-NNs of each subsequence, which in this example are always one unit of r away (illustrated by the hyperspheres). Thus, the pairwise extent is at most $d = 2r$ for two subsequences on the diameter. However, the optimal 3-Motiflet can be seen in the center of the

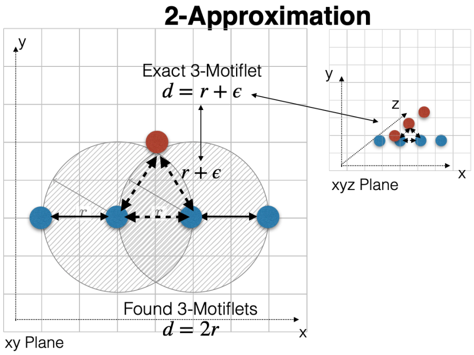


Figure 4: Worst case example for k=3 on xy and xyz-plane. Our approximate algorithm will return a 3-Motiflet with extent $2r$. However, the optimal 3-Motiflets has extent $r + \epsilon$.

figure: for each of the blue dots, the first 2-NNs are r away, and only their 3-NN (red dot) is $r + \epsilon$ away. Thus, the top 3-Motiflet has a pairwise distance of $d = r + \epsilon$, and consists of two blue dots and one red dot. This example is also the worst case instance for $k = 3$. The factor is largest when ϵ is close to 0, maximizing the difference of $2d$ and $\epsilon + r$. Increasing or decreasing epsilon will reduce the factor of the approximation as it is either not a part in the k-Motiflet $\epsilon > r0$ or is found by our approximate algorithm (for $\epsilon < 0$). The worst case instance is thus the case, when the red dot touches the intersections of the circles.

Case $k > 3$. We now extend this worst case example to $k > 3$ (using L_1 distance for the sake of simplicity): Assume we have a subsequence in $n \geq k + 2$-dimensional space $S = (0, 0, \ldots, 0)$ with $k-1$-neighbours $B^i, i \in [1, \ldots, k-1]$, where only the i-th dimension is set to r. E.g.: $B^1 = (r, 0, \ldots, 0)$ and $B^2 = (0, r, \ldots, 0)$. S and all B^i constitute a k-Motiflet with extent $d = 2r$. Now, we hide a single subsequence $R_0 = (r/2 + \epsilon, r/2 + \epsilon, 0, \ldots, 0)$ at the intersections of the hypersphere (as in Figure 4 for $k = 3$). R_0 has a distance of $r + \epsilon$ to S and B_1. Finally, we add $k - 1$ additional subsequences $R^i, i \in [3, \ldots, k+1]$, where the first two dimensions are set to $r/2+\epsilon$ and the i-th dimension is set to r. E.g. $R^3 = (r + \epsilon, r/2 + \epsilon, r, \ldots, 0)$. These are all distance r away from R_0, and at least $2r$ away from S.

Thus, the top k-Motiflets consists of the subsequences R_i and S with total extent $r + \epsilon$, but the found k-Motiflet has extent $2r$ with B_i and S.

Accordingly, our algorithm is a 2-approximation of the exact solution. Note that 2 is the maximal error; we actually observe much smaller factors on our real-world use cases, typically lower than 1.1 also for much higher k (see Section 6.3).

4.3 Exact k-Motiflets

The approximate algorithm gives an upper bound on the extent d of the optimal k-Motiflet solution. The algorithmic idea of our exact algorithm is based on an enumeration of all subsets of subsequences of T of size k combined with aggressive pruning. The pruning is based on the observation that the k-Motiflet must be within range d of a subsequence S in TS, as all other subsequences are within pairwise distance of at most d to S. To obtain the overall smallest set in terms of its extent, we hence may prune the d-range candidate sets to return the smallest k-element set. However, enumerating all subsets of k subsequences from a set of $\hat{k} > k$ elements is a combinatorial problem, which has exponential growth in $\mathbb{O}(\hat{k}^k)$.

Algorithm 2 Compute Exact k-Motiflets

```
1:  procedure GET_EXACT_K_MOTIFLETS($T$, $k$, $l$)
2:      $D_{i,j}$ ← CALC_DISTANCE_MATRIX(T, l)
3:      $(motiflet, d)$ ← GET_K_MOTIFLETS$(T, k, l)$        ▷ approximation
4:      for $i \in [1, \ldots, (\text{len(T)} - l + 1)]$ do
5:          $idx$ ← ARGWHERE$(D_i < d) \cup \{i\}$
6:          if $len(idx) \geq k$ then
7:              for $k\_subset \in$ NON_TRIVIAL_SUBSETS$(k, idx)$ do
8:                  $dist$ ← PAIRWISE_EXTENT$(D, k\_subset, d)$
9:                  if $dist < d$ then
10:                     $(d, motiflet)$ ← $(dist, k\_subset)$
11:                 end if
12:             end for
13:         end if
14:     end for
15:     return $(motiflet, d)$
16: end procedure
```

Algorithm 2 applies admissible pruning by using the best-so-far extent d. It initializes d by the result of our approximate algorithm in line 3. We iterate over all subsets of subsequences and return those within d-range. For choosing candidate subsequences, we have to check each subset of size k and compute its extent (line 7–9). Overall, there are $\mathbb{O}(n^k)$ in the worst case. The k-element motif set with lowest extent is the top k-Motiflet.

Thus, if we compare the approximate (Algorithm 1) and the exact solution (Algorithm 2), the main difference is in the enumeration of the candidate subsequences. Unfortunately, the exact algorithm has an exponential growth in the worst case, which makes it infeasible for even small k's, which we will show in the experimental section. There are also good reasons to believe that the k-Motiflet problem is NP-hard, but a formal proof still has to be found. However, we will show that our approximate k-Motiflets algorithm gives good results in our experimental evaluation in Section 6.

5 PARAMETER SELECTION

In this section, we present methods to automatically find suitable values for the motif length l and set size k so, that meaningful concealed structures of an input TS are found without domain knowledge. No comparable method exists for any of the competitor definitions. As MD in TS is an unsupervised problem, we cannot claim to find optimal values under all circumstances. For instance, the methods we present will not produce meaningful results when applied to entirely random TS, as in those simply no "suitable" k or l exist at all. However, we found them to be very effective and helpful in our experiments (Section 6). Our methods for determining values for k and l are based on an analysis of the extent function:

Definition 5.1. Extent Function (EF): Assume a fixed length l and a time series T. Let S_k be the top k-Motiflet with length l of T. Then, the *extent function EF* for T is defined as $EF(k) = extent(S_k)$.

Note that EF can be efficiently computed when starting from the largest value to be considered, as $extent(S_{k+1})$ is a (usually rather

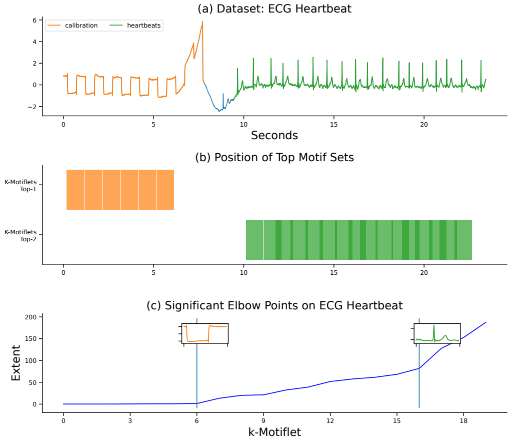


Figure 5: The *EF* (center) is a function of the cardinality of k-Motiflets to the extent. Elbow points represent large changes in similarity of the found motif set, indicative of a concept change from calibrations signal to heartbeats.

tight) bound for $extent(S_k)$, which allows for aggressive pruning in all cases but the first.

When considering the curve of the EF, we can observe the following: First, EF is monotonically increasing in k. Second, if the slope of *EF* increases *slowly* from k to $k+1$, then S_k can be extended to S_{k+1} with a motif that is very similar to the subsequences of S_k. A longer interval $[k, \ldots, k+n]$ for which EF increases only slowly and that cannot be extended (i.e., $EF(k-1)$ is considerably smaller than $EF(k)$ and $EF(k+n+1)$ is considerably larger than $EF(k+n)$) very probably stem from a set of $n+1$ subsequences of T whose k most similar elements build S_k[4] and where for every increment of k another highly similar subsequence from T exists and is added to build the next top motiflet. On the other hand, if $EF(k+1) - EF(k)$ is large, i.e., if we have a steep increase between k and $k+1$ - we call this an *elbow point* - then very probably the k-Motiflet could not be exceeded with further, highly similar subsequences. In such cases, the $k+1$ motiflet very likely is formed by an entirely new motif - with more occurrences, but at the price of a larger extent. Examples for both observations, i.e., long flat stretches and elbow points, can be found in Figure 5. These considerations lead to the following ideas:

(1) Elbow points in the *EF* indicate changes of motifs. The last value of k before the elbow indicates a maximal motiflet, which we consider a particularly meaningful value for k. We study these points in Section 5.1.
(2) Long flat stretches of the EFs indicate a high number of occurrences of a motif, but depend on the motif length l. Accordingly, we consider values of l leading to long flat stretches as particularly meaningful. Section 5.2 describes how we find such values.

5.1 Learning meaningful k

Elbow points, i.e. points with a notable increase in slope of the *EF* between two values k and $k+1$, indicate that the k-Motiflet cannot be extended to $k+1$ without a strong increase in its extent. Consider Figure 5 as an example. We set the motif length to 1 sec, i.e. 60 bpm. We observed the following: the *EF* (Figure 5 center) is flat until 6 repetitions of the calibration signal have been found. This stretch ends with a notable increase in slope until $k = 16$, where another elbow point exists. These two points are characteristic for this TS. The corresponding motifs are depicted at the bottom of the figure, with 6 and 16 occurrences, respectively.

We tested different methods for finding elbow points, such as [23] or scipy[5]. We found that a simple threshold α on the slope of the *EF* performed best for the particular shapes that *EF* typically exhibit. Given a list of $k-1$ extents $p = [d_i]_{i=2}^{k}$, we thus define elbow points as follows:

$$elbow(p(i), p(i+1)) = \left\{ \begin{array}{ll} 1, & iff\, m1/m2 > \alpha \\ 0, & else \end{array} \right\}$$

$$with\ m1 = (p(i+1) - p(i)) + \epsilon\ and$$

$$m2 = (p(i) - p(i-1)) + \epsilon$$

A small constant $\epsilon \in \mathbb{R}^+$ is added to the slope to avoid dividing by 0. An elbow is found, if the slope between neighboring indices rises by a factor of α. In our experiments (see next section), we used a constant value of $\alpha = 5$. Further evaluations of this method on more data sets can be found on our supporting web page [8].

5.2 Learning Motif Length l

As described before, the length of a flat stretch in the *EF* corresponds to a maximal motiflet. The existence and lengths of such stretches depend on l. For instance, if we set l exactly to the periodicity of the heartbeat or of the calibration wave in Figure 2, the *EF* contains two long flat stretches each corresponding to a (high) number of occurrences of the respective motif. Learning a suitable motif length thus can be approached by searching values for l that create long flat stretches in the *EF*.

Accordingly, one could find l by computing EFs for a range of l values and chose the one where the EF contains the longest flat stretch. This, however, would have two drawbacks: (1) we would assume that only a single motif exists, and (2) stretches of different lengths may also exhibit different (small) slopes and are thus hard to compare, i.e., given a single threshold for "flat" would be difficult. Instead, we determine l by calculating a normalized *area under the EF*, abbreviated as EF_AU, as steeper stretches or smaller stretches - necessarily ending with an elbow point and thus an increase in slope - lead to larger areas under *EF*.

For a given length l, let $EF^{(l)}$ be the list of the $k-1$ extents $p^{(l)} = [d_i^{(l)}]_{i=2}^{k}$ and $e^{(l)}$ be the number of identified elbows. The

[4] Note that this is not mandatory, as there could also be sets of subsequences of sizes $k, k+1, \ldots$ that are (a) disjoint and (b) each forms a top motiflet for its value of k.

[5] https://www.scipy.org

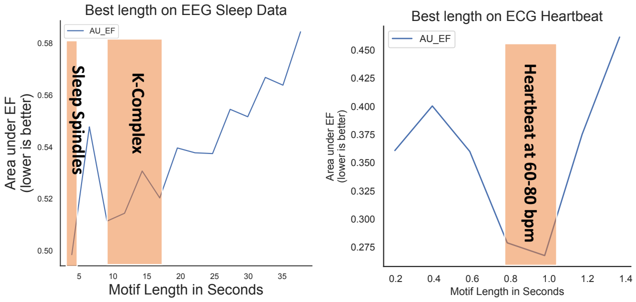


Figure 6: The *Area Under the EF (AU_EF)* captures the frequency of approximate repeats. The minima roughly capture known motifs in the two datasets, corresponding to the sleep spindles and K-Complex in sleep data (left) and heartbeats at a rate of 60 **to** 80 **bpm in ECG data (right).**

AU_EF score for length l is defined as:

$$AU\_EF(p^{(l)}) = \frac{1}{e^{(l)}} \sum_{i=2}^{k} \frac{(d_i^{(l)} - min(p^{(l)}))}{(max(p^{(l)}) - min(p^{(l)}))} \in [0, 1]$$

$$and$$

$$best = \min_{l \in [l\_min, l\_max]} AU\_EF(p^{(l)})$$

I.e., in our implementation we iterate over reasonable values for l and choose the value where $AU\_EF()$ is minimal.

Figure 6 shows two plots of the *AU_EF* for a range of discrete motif lengths $l \in [25, \dots, 200]$ for our running ECG example (left) and also an EEG sleep data set (right). The AU_EF has its minimum around $l = 0.8s$ to $l = 1s$, equal to a heartbeat rate of 60-80 bpm. The resulting motif sets are shown in Figure 5. In EEG sleep data the local minima correspond to sleep spindles at $5s$ and K-Complexes at $10 - 20s$ in sleeping cycles. Further evaluations of this method on more data sets can be found on our supporting web page [8].

6 EXPERIMENTAL EVALUATION

Our experimental evaluation is three-fold:

(1) In Section 6.1, we compare our approximate k-Motiflet algorithm against four state of the art MD methods in a quantitative analysis on five data sets. In this analysis, we disregard any known motifs in the data but instead compute the extents and cardinality of motif sets at given combinations of extent and k, or respectively r.
(2) In Section 6.2, we compare our approximate k-Motiflet algorithm against four state-of-the-art methods in a qualitative analysis on four data sets - those for which motifs are known from the literature. We evaluate methods by their ability to find these motifs.
(3) Finally, we compare our approximate and exact k-Motiflet algorithms regarding quality of results and both against the competitors in terms of runtime in Section 6.3,

Competitors: We compare our new algorithm to VALMOD [15], EMMA [17], Set Finder [1], and Learning Motifs (LM) [7]. We used the original implementation of EMMA and Set Finder but performed some runtime optimizations. In EMMA we improved the computation of means and stds from $\mathbb{O}(nl)$ to $\mathbb{O}(n)$ using a sliding window implementation. For Set Finder, we improved the filtering of trivial matches by sorting the indices first and then searching for overlaps in sorted indices, rather than checking all pairs of indices. We used our own python re-implementation of VALMOD because the reference implementation is for pair motifs only. For LM, we used the JAVA implementation provided by the authors.

Data Sets: We collected five challenging real-life data sets to assess the quality and scalability of MD algorithms. For three out of these, the literature describes motifs which we shall use for evaluating the MD algorithms in Section 6.2. An overview can be found in Table 2. The five data sets are the following:

Muscle Activation was collected from professional in-line speed skating [18] on a large motor driven treadmill with Electromyography (EMG) data of multiple movements. It consists of 29.899 measurements at $100Hz$ corresponding to $30s$ in total. The known motifs are the muscle movement and a recovery phase.

ECG Heartbeats contains a patient's (ID 71) heartbeat from the LTAF database [22]. It consists of 3.000 measurements at $128Hz$ corresponding to $23s$. The heartbeat rate is around 60 to 80 bpm. There are two motifs: A calibration signal and the actual heartbeats.

Physiodata - EEG sleep data contains a recording of an afternoon nap of a healthy, nonsmoking person, between 20 to 40 years old [10]. Data was recorded with an extrathoracic strain belt. The dataset consists of 269.286 points at $100hz$ corresponding to $45min$. Known motifs are so-called sleep spindles and k-complexes.

Industrial Winding Process is a snapshot of a process where a plastic web is unwound from a first reel (unwinding reel), goes over the second traction reel and is finally rewound on the the third rewinding reel [2]. The recordings correspond to the traction of the second reel angular speed. The data contains 2.500 points sampled at $0.1s$, corresponding to $250s$. No documented motifs exist.

Functional near-infrared spectroscopy (fNIRS) contains brain imaginary data recorded at $690nm$ intensity. There are 208.028 measurements in total. The data is known to be a difficult example, as it contains four motion artifacts, due to movements of the patient, which dominate MD [3]. No documented motifs exist.

Setting parameters r, l, and k: A direct comparison of k-Motiflets to the other methods is impossible as we use a different approach to the MD problem: Competitors rely on the motif length l and radius r as input parameters, whereas k-Motiflets require the length l and the number k of motif occurrences. Regarding l, we used the known value if a value was known (see Table 2) and otherwise learn l as described in Section 5.2. In any case, the value of l was the same for all methods in all experiments. In contrast, the method for setting k / r are necessarily different in the different evaluations and are thus described individually in the respective sections.

Hardware: All scalability experiments were carried out on a single server running LINUX with 2xIntel Xeon E5-2630v3 and 64GB RAM, using python version 3.8.3.

Reproducibility: To ensure reproducible results and to foster follow-up work, we provide the k-Motiflets source code, Jupyter-Notebooks, visualizations of the datasets, additional analysis, and the raw measurement sheets on our website [8].

	Length	Known Motifs	Motif Length l	Range for k
Muscle Activation	29899 (30s)	Gluteus Muscle Activation and Recovery	Known: ~ 120 ms	$ks = [2 \ldots 20]$
ECG Heartbeats	3000 (23s)	Calibration and Heartbeats	Known: ~ $0.8 - 1$ s	$ks = [2 \ldots 20]$
EEG Sleep Data	269286 (45 min)	Sleep Spindles and K-Complex	Known: 1-6s and 30s	$ks = [2 \ldots 20]$
Industrial Winding	2499 (250s)	None	Learned: $l \in \{2, 3, \ldots, 15\}$	$ks = [2 \ldots 12]$
fNIRS	208028	"medically significant" condition [3]	Learned: $l \in \{1000, 1200, \cdots, 4000\}$	$ks = [2 \ldots 20]$

Table 2: Properties of real world use cases.

6.1 Quantitative Analysis

We first compare the results of the approximate k-Motiflet algorithm to that of four state-of-the-art competitors using five datasets. For these comparisons we performed an unbiased computation of extents and cardinalities of found motif sets at equivalent values of r (respectively $d = 2 \cdot r$) and k. In this evaluation, we find an MD method M_1 better than an MD method M_2, when M_1 finds larger motif sets at the same radius, smaller radii for the same motif cardinality, or both. The meaningfulness of the motif sets as found by different methods will be discussed in Section 6.2.

We first ran each competitor for increasing values of r and counted the cardinality k and real extent of the found top motif sets, generating pairs of (k, r). We then ran k-Motiflets for increasing values of k and measured the extent of the found top motif set(s). which generates comparable pairs. Finally, we plotted the achieved extents by growing cardinality for each method. A good method finds motif sets with small extents even with increasing cardinalities, i.e. its line would be rather flat (parallel to x-axis). Figure 7 shows that k-Motiflets in this regard shows the best performance of all methods. For each value of k in each data set, it finds a motif set that has smaller than or at least equally small extent as all competitors; in turn, for each possible extent, it finds a larger or at least equally large motif set. Despite its different definitions, there is no clear second place among the other competitors, and we saw a different ranking on each of the use cases presented.

6.2 Qualitative Analysis

In this section we discuss the quality of the discovered motif sets by comparing them to known motifs in those datasets where such a standard exists. The purpose is to compare methods not only by the size and extent of found motifs as in the previous section, but also to consider whether these motifs are actually meaningful, i.e., correspond to important events in the process producing the TS.

The literature provides motifs for three of our five data sets, i.e., EEG sleep data, ECG heartbeats, and muscle activation. However, for none of them the precise motif occurrences are annotated in the respective time series: Instead, only their rough shape and rough length are described in the form of pair motifs. We used this information for creating a silver standard of motif sets by exploiting k-Motiflets unique ability to automatically learn meaningful values for k and l (see Section 5). Specifically, we learned values for k and l directly from the data and compared the results with the descriptions from the papers. In all cases, the two Top-2 motifs corresponded very well to the descriptions as did the corresponding motif lengths. Therefore, we decided to use the results of k-Motiflets as silver standard for these data sets and compared the ability of the other methods to recover the respective motifs. To enable such a comparison, we provided the competitors with proper r- and l-values derived from the silver standard. Note that in this setting our method had to recover meaningful motifs without any additional knowledge, while the competitors were provided with proper values for r and l.

EEG sleep data: This dataset contains two main motifs, namely the so-called K-Complex and the so-called sleep spindles [19]. Accordingly, we consider the two top motifs found by each methods. Results are shown in Figure 8, using the Top-2 k-Motiflet as silver standard. The two largest motif sets found by the k-Motiflet algorithm correspond very well to K-Complexes (with $k = 16$) and sleep spindles (with $k = 15$), respectively. Also, EMMA and LM find both motifs, but LM finds them in reverse order and both identify notably less occurrences. SetFinder and VALMOD find only subsets of the K-complex motif, both as top-1 and as top-2 motif.

ECG Heartbeats: This data set was used as running example throughout this paper. The Top-2 motif sets as computed by the different methods are shown in (Figure 1). Our novel algorithm identified 16 heartbeats and 6 calibration waves. SetFinder and LM also find both motifs but both with less occurrences (11/5 and 14/6, respectively). EMMA returns blurred version of the calibration signal as top-1 and top-2 motif. Also VALMOD stays locked with the calibration signal.

Muscle Activation: The two top motifs present in this dataset are the activation (top-1) and the recovery phase (top-2) of the Gluteus Maximus muscle and have 13 and 12 occurrences, respectively. k-Motiflets and Set Finder are the only to identify the activation phase as top-1 motif, but only k-Motiflets with $k = 13$ and Set Finder with only $k = 11$ occurrences. All five methods identify the recovery phase either as top-1 or top-2 motif. While Valmod and LM find all $k = 12$ recovery phases as top-1 motif, their extent d is at least 50% larger than that of k-Motiflets ($d = 180$).

6.3 Runtimes and exact k-Motiflets

In the previous section, we evaluated the quality of the approximate k-Motiflet algorithm compared to four state-of-the-art MD methods. We did, however, not yet consider the exact k-Motiflet algorithm, because (a) its runtime is exponential in the size of the motif set and thus probably infeasible for larger values of k, and (b) we did not expect the motif sets found by the approximate version to be much worse than that found by the exact version. In this section, we

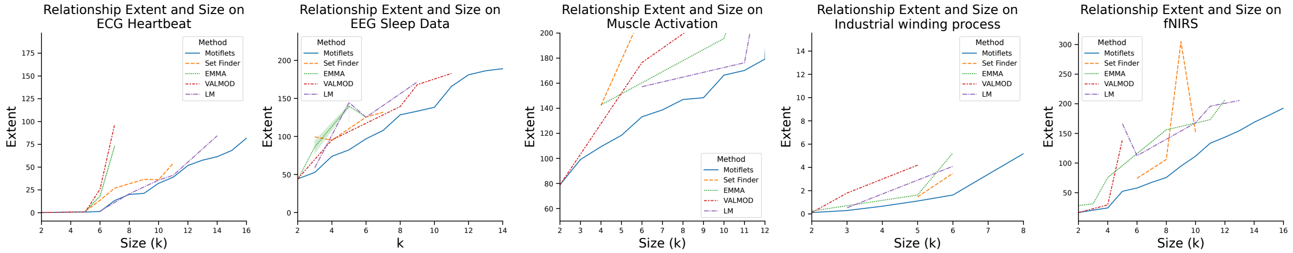


Figure 7: Relationship between cardinality (size) and extent of the motif sets found by each method. The curves of k-Motiflets are always below all competitors, e.g., it returns the largest motif set with highest similarity on all datasets by far.

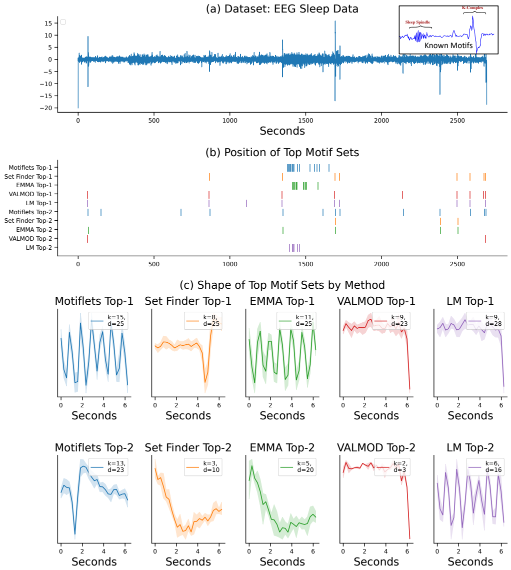


Figure 8: Top-2 Motif Sets found for the EEG Sleep dataset. For the competitors, we derived $l = 6s$ and $d' = 25 \approx 2r$ (TOP-1) and $d'' = 13 \approx 2r$ (TOP-2) from the k-Motiflet's results. Top-lane: Parts of the time series at low resolution; the right part shows occurrences of the two known motifs in a higher resolution. Second lane: The two top-2 motifs found by the different methods. The top-2 k-Motiflets precisely correspond to the *k-Complex* with 16 repetitions and *sleep spindles* with 15 repetitions. All other methods perform worse.

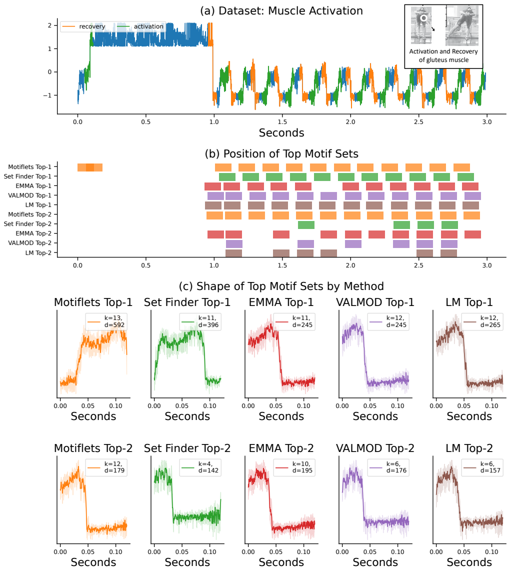


Figure 9: Top motif sets found for Muscle Activation dataset. For the competitors, we derived $l = 120ms$ and $d' = 200 \approx 2r$ (TOP-2) and $d'' = 600 \approx 2r$ (TOP-1) from the k-Motiflet's results. The top-1 motif set found by k-Motiflets corresponds very well to the *activation phase* and the top-2 motif to the *recovery phase*. All methods find the *recovery phase*, but either with less occurrences or with a 50% larger extent.

experimentally verify both of these assumptions and subsequently also compare their runtimes to that of all competitors.

Scalability of approximate and exact k-Motiflet algorithms: We first study the scalability of the approximate and the exact k-Motiflet algorithm regarding the length n of a time series and the cardinality k of the motif sets. To this end, we use the largest time series from our data sets (fNIRS), encompassing $n = 269.286$ time points.

Figure 10 (left) shows runtimes with growing TS length n, measured with fixed $k = 5$. Interestingly, the runtimes of both methods are almost equal, resulting in 11 minutes for the full TS. Figure 10 (right) shows runtimes for growing values of k at a fixed length $n = 10.000$. Exact and approximate algorithms differ extremely for values of $k > 7$, where the exponential complexity of the exact version results in a steep increase of the runtime. For instance, the runtime for $k = 7$ is 4 seconds, 5.7 minutes for $k = 8$, and already close to 12 days for $k = 9$. Thus, the exact algorithm becomes untraceable for larger k, even with the admissible pruning we implemented. In contrast, the runtime of the approximate algorithm remains below 2 minutes even for $k = 30$.

Quality of approximation: We next studied the difference in results produced by the approximate and the exact k-Motiflet algorithms, depending on the length of a TS and on the chosen value of k. We first ran both algorithms on a growing prefix of all datasets for a fixed value $k = 5$ and measured the ratio of the extents of the approximate to the exact solution over n (i.e,. higher values

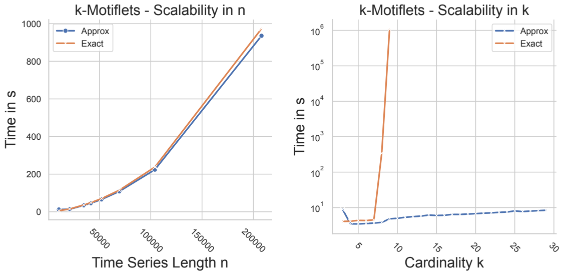


Figure 10: Runtime of the approximate vs. exact Algorithm 1 with motif length $l = 100$. Left: as a function of the TS length n, with fixed cardinality $k = 5$. Right: as a function of k with fixed TS length $n = 10000$. Both scale quadratic in n but the exact algorithm is exponentially in k.

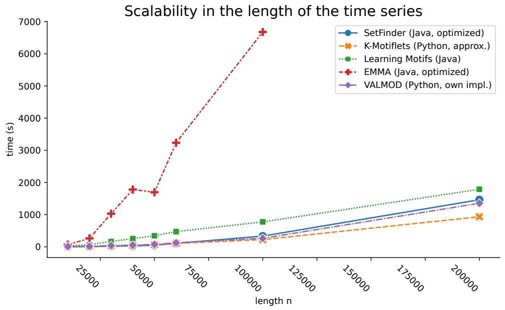


Figure 11: Scalability of different MD approaches in length n, with motif length $l = 100$. While a fair comparison among two programming languages (Java, Python) is difficult, k-Motifets is fastest.

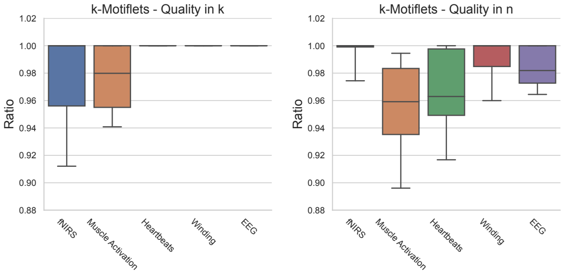


Figure 12: Quality as a ratio of the extents of the top-1 motif sets of the approximate to the exact algorithm. Left: Boxplot over fractions of the full length n, $n' \in [1/8\%, 1/7\%, \ldots, 100\%]$ of full TS length n with fixed cardinality $k = 5$. Right: Boxplot over ratio as a function of $k \in [2, ..., 9]$ with fixed length TS $n = 10000$.

mean that the approximate version is closer to the optimal solution). Results are shown in the box-plot in Figure 12 (right). For some datasets when varying k, the approximate and exact solution always returned the same motifs, such as for heartbeats, window and EEG Figure 12 (left). Overall, we observed that the ratio is consistently over 91% for varying k, and 89% for varying n. This means that the approximate version finds motif sets close to the same extent as the exact algorithm. We performed an in-depth analysis of the differences of results between the two methods. Interestingly, we found that they mostly come from cases where the parameter k was set smaller than the actual number of motif occurrences, which lead to the two methods finding different subsets of the same motif, which in turn led to slightly different extents. If the motif had e.g. 8 occurrences, and we require $k = 4$ occurrences, the approximate solution might find other 4 (of the 8) subsequences than the exact solution. When we move to the full frequency $k = 8$ of the motif however, these differences in extent faded away.

Runtime of competitors: Finally, we compared the scalability of the approximate k-motiflet algorithm to its four competitors using the (largest) fNIRS dataset. For a fair comparison given different input parameters, we first set $k = 5$, determined the extent of the top motif set as found by k-Motiflets, and used the corresponding radius as input for all competitors. We emphasize that the runtimes nevertheless are difficult to compare as the implementations use different languages (Java versus Python) and also show different efforts for runtime optimization. Under these circumstances, Figure 11 shows that our implementation of k-Motiflets is faster than all competitor implementations we tested (despite being programmed in Python), though the differences to all methods except EMMA are rather small (less than factor 2).

7 CONCLUSION

Often the first step in analyzing unlabelled time series is motif discovery, used to derive hypotheses from the data based on similar, frequent subsequences. However, existing tools for MD show a high variance in the discovered motifs depending on the given input parameter. If these parameters are set incorrectly this leads to the discovery of pure noise. In this paper, we presented a novel definition for motif set discovery, named k-Motiflets, which are the sets of subsequences with exactly k approximate repeats and highest similarity in a given time series. We argued that the value of k is much easier to set by a user than the usually used parameter r, which is the maximal similarity of a motif set. We presented an approximate and an exact algorithm for finding k-Motiflets and proved that the former is a 2-approximation of the latter, which has exponential runtime in k. We also presented two algorithms along with our k-Motiflets for automatically learning appropriate values for l and k without any a-priori knowledge of the motifs. By qualitative and quantitative evaluation on up to five real-world use cases, we showed that the approximate algorithm produces better motifs than all its competitors at lower runtimes, and that its results come very close to the exact algorithm despite an exponentially lower runtime. Future work will consider variable length or multivariate motif discovery.

8 ACKNOWLEDGMENTS

We wish to thank Themis Palpanas, Rafael Moczalla, Arik Ermshaus, and Leonard Clauß for their input and fruitful discussions.

REFERENCES

[1] A. Bagnall, J. Hills, and J. Lines. Finding motif sets in time series. *arXiv preprint arXiv:1407.3685*, 2014.

[2] T. Bastogne, H. Noura, A. Richard, and J.-M. Hittinger. Application of subspace methods to the identification of a winding process. In *1997 European Control Conference (ECC)*, pages 2168–2173. IEEE, 1997.

[3] H. A. Dau and E. Keogh. Matrix profile v: A generic technique to incorporate domain knowledge into motif discovery. In *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, pages 125–134, 2017.

[4] I. Dokmanic, R. Parhizkar, J. Ranieri, and M. Vetterli. Euclidean distance matrices: essential theory, algorithms, and applications. *IEEE Signal Processing Magazine*, 32(6):12–30, 2015.

[5] E. Eden, D. Lipson, S. Yogev, and Z. Yakhini. Discovering motifs in ranked lists of dna sequences. *PLoS Comput Biol*, 3(3):e39, 2007.

[6] E. F. Gomes and F. Batista. Classifying urban sounds using time series motifs. *Advanced Science and Technology Letters*, 97:52–57, 2015.

[7] J. Grabocka, N. Schilling, and L. Schmidt-Thieme. Latent time-series motifs. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 11(1):1–20, 2016.

[8] k-Motiflets Source Code and Raw Results. https://github.com/patrickzib/motiflets, 2022.

[9] C. Kamath and Y. J. Fan. Finding motifs in wind generation time series data. In *2012 11th International Conference on Machine Learning and Applications*, volume 2, pages 481–486. IEEE, 2012.

[10] J. Kohlmorgen, K.-R. Müller, J. Rittweger, and K. Pawelzik. Identification of nonstationary dynamics in physiological recordings. *Biological Cybernetics*, 83(1):73–84, 2000.

[11] N. K. Lee, F. L. Azizan, Y. S. Wong, and N. Omar. Deepfinder: An integration of feature-based and deep learning approach for dna motif discovery. *Biotechnology & Biotechnological Equipment*, 32(3):759–768, 2018.

[12] Y. Li, M. L. Yiu, Z. Gong, et al. Quick-motif: An efficient and scalable framework for exact motif discovery. In *2015 IEEE 31st International Conference on Data Engineering*, pages 579–590. IEEE, 2015.

[13] J. Lin, E. Keogh, L. Wei, and S. Lonardi. Experiencing sax: a novel symbolic representation of time series. *Data Mining and knowledge discovery*, 15(2):107–144, 2007.

[14] M. Linardi, Y. Zhu, T. Palpanas, and E. Keogh. Matrix profile x: Valmod-scalable discovery of variable-length motifs in data series. In *Proceedings of the 2018 International Conference on Management of Data*, pages 1053–1066, 2018.

[15] M. Linardi, Y. Zhu, T. Palpanas, and E. Keogh. Valmod: A suite for easy and exact detection of variable length motifs in data series. In *Proceedings of the 2018 International Conference on Management of Data*, pages 1757–1760, 2018.

[16] B. Liu, J. Li, C. Chen, W. Tan, Q. Chen, and M. Zhou. Efficient motif discovery for large-scale time series in healthcare. *IEEE Transactions on Industrial Informatics*, 11(3):583–590, 2015.

[17] J. Lonardi and P. Patel. Finding motifs in time series. In *Proc. of the 2nd Workshop on Temporal Data Mining*, pages 53–68, 2002.

[18] F. Mörchen and A. Ultsch. Efficient mining of understandable patterns from multivariate interval time series. *Data mining and knowledge discovery*, 15(2):181–215, 2007.

[19] A. Mueen, E. Keogh, Q. Zhu, S. Cash, and B. Westover. Exact discovery of time series motifs. In *Proceedings of the 2009 SIAM international conference on data mining*, pages 473–484. SIAM, 2009.

[20] C. G. Nevill-Manning and I. H. Witten. Linear-time, incremental hierarchy inference for compression. In *Proceedings DCC'97. Data Compression Conference*, pages 3–11. IEEE, 1997.

[21] P. Patel, E. Keogh, J. Lin, and S. Lonardi. Mining motifs in massive time series databases. In *2002 IEEE International Conference on Data Mining, 2002. Proceedings.*, pages 370–377. IEEE, 2002.

[22] S. Petrutiu, A. V. Sahakian, and S. Swiryn. Abrupt changes in fibrillatory wave characteristics at the termination of paroxysmal atrial fibrillation in humans. *Europace*, 9(7):466–470, 2007.

[23] V. Satopaa, J. Albrecht, D. Irwin, and B. Raghavan. Finding a" kneedle" in a haystack: Detecting knee points in system behavior. In *2011 31st international conference on distributed computing systems workshops*, pages 166–171. IEEE, 2011.

[24] P. Senin, J. Lin, X. Wang, T. Oates, S. Gandhi, A. P. Boedihardjo, C. Chen, and S. Frankenstein. Grammarviz 3.0: Interactive discovery of variable-length time series patterns. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 12(1):1–28, 2018.

[25] P. Senin, J. Lin, X. Wang, T. Oates, S. Gandhi, A. P. Boedihardjo, C. Chen, S. Frankenstein, and M. Lerner. Grammarviz 2.0: a tool for grammar-based pattern discovery in time series. In *Joint European conference on machine learning and knowledge discovery in databases*, pages 468–472. Springer, 2014.

[26] H. Shao, M. Marwah, and N. Ramakrishnan. A temporal motif mining approach to unsupervised energy disaggregation. In *Proceedings of the 1st International Workshop on Non-Intrusive Load Monitoring, Pittsburgh, PA, USA*, volume 7, 2012.

[27] M. A. Siddiquee, Z. Akhavan, and A. Mueen. Seismo: Semi-supervised time series motif discovery for seismic signal detection. In *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, pages 99–108, 2019.

[28] S. Torkamani and V. Lohweg. Survey on time series motif discovery. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery*, 7(2):e1199, 2017.

[29] C.-C. M. Yeh, Y. Zhu, L. Ulanova, N. Begum, Y. Ding, H. A. Dau, D. F. Silva, A. Mueen, and E. Keogh. Matrix profile i: all pairs similarity joins for time series: a unifying view that includes motifs, discords and shapelets. In *2016 IEEE 16th international conference on data mining (ICDM)*, pages 1317–1322. Ieee, 2016.

[30] Y. Zhu, C.-C. M. Yeh, Z. Zimmerman, K. Kamgar, and E. Keogh. Matrix profile xi: Scrimp++: time series motif discovery at interactive speeds. In *2018 IEEE International Conference on Data Mining (ICDM)*, pages 837–846. IEEE, 2018.

[31] Y. Zhu, Z. Zimmerman, N. S. Senobari, C.-C. M. Yeh, G. Funning, A. Mueen, P. Brisk, and E. Keogh. Matrix profile ii: Exploiting a novel algorithm and gpus to break the one hundred million barrier for time series motifs and joins. In *2016 IEEE 16th international conference on data mining (ICDM)*, pages 739–748. IEEE, 2016.

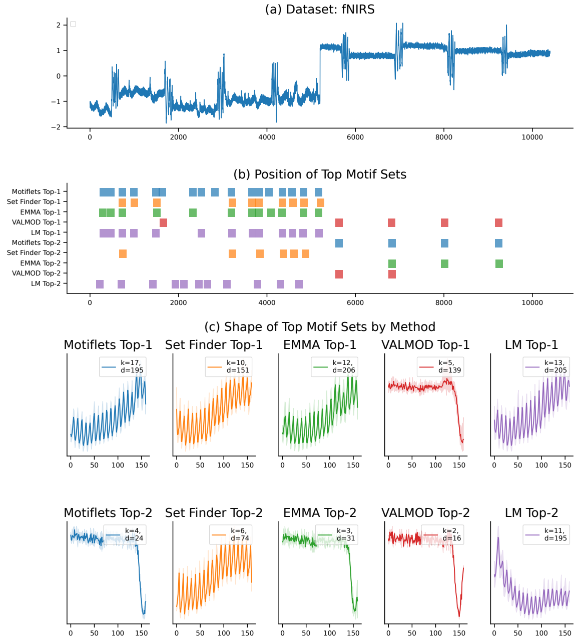


Figure 13: The top motif sets found on the *fNIRS dataset* using length 80. The found motif was also reported in [3]. *k*-Motiflets finds the highest number of repeats.

9 APPENDICES

9.1 Addition Data Sets

9.1.1 Functional near-infrared spectroscopy (fNIRS).

This fNIRS dataset contains brain imaginary data recorded at 690*nm* intensity.

Known Motifs: The data is known to be a difficult example, as it contains eight motion artifacts, due to movements of the patient, which dominate MD [3]. These motion artifacts are clearly visible in the signal by higher magnitude waves. The authors in [3] addressed this by including additional accelerometer data into MD.

Known Motifs: As no documented motifs exist in literature, we first applied our motif length selection to the data and found a minimum in the AU_EF corresponding to $l = 160$ time stamps. Figure 13 shows the TOP-2 motif sets for this length $l = 160$.

(1) The TOP-1 motif found by most methods is very similar, except for VALMOD, which found the motion artifact. Motiflets found 17 repetitions and the others much less from 10 to 13. This motif found by all methods was also reported in [3] after pre-processing the data. It shows a "medically significant" [3] motif. Thus, while the other methods do find this motif set, their precision is much less.

(2) The motion artifact, as presented in [3], was found as TOP-2 motif set all but two methods. k-Motiflets found all 4 repetitions in the latter halve of the signal, yet the others only 2 to 3. VALMOD found 5 repetitions of this signal as TOP-1 motif though.

Overall, k-Motiflets was the only to not only find both (a) the motion artifact and the (b) "medically significant" motif, but also with the highest frequency.