

UNIVERSITY OF TARTU
FACULTY OF MATHEMATICS AND COMPUTER SCIENCE
INSTITUTE OF COMPUTER SCIENCE

Egon Elbre
Parallel Pattern Discovery
Master's Thesis

Supervisor: Prof. J. Vilo

Tartu May 6, 2013

Contents

1	Introduction	4
1.1	Motivation and background	4
1.2	Contributions of this work	5
1.3	Structure of the thesis	5
2	Definitions	7
2.1	Sequence and Dataset	7
2.2	Pattern	8
2.3	Query	8
2.3.1	Query features	9
2.4	Pool	9
2.5	Pattern Discovery	10
3	Overview	11
3.1	Algorithms	11
3.1.1	SPEXS	11
3.1.2	TEIRESIAS	12
3.1.3	Verbumculus	13
3.1.4	MobyDick	13
3.1.5	RSAT	13
3.1.6	Other	13
3.2	Reviews	14
3.3	Problems	14

better
title
needed

4	SPEXS Generalization	15
4.1	Algorithm	15
4.2	Pools	17
4.3	Filtering	17
4.4	Extending	17
4.4.1	Sequences	18
4.4.2	Groups	19
4.4.3	Star	20
4.4.4	Optimizations	21
4.5	Summary	21
5	Parallelization	22
5.1	Process	22
5.2	Extending	23
5.3	Distributed processes	24
6	Implementation	27
6.1	Architecture	27
6.2	Configuration	28
6.3	Input and Output	29
6.4	Alphabet and Database	29
6.5	Pools	29
6.6	Features and Filters	30
6.7	Synchronized Tree Traversal	31
6.8	Debugging	34
7	Applications and experimental results	36
7.1	Examples	36
7.1.1	DNA sequences	36
7.1.2	Protein sequences	36
7.1.3	Text mining	36
7.1.4	Code mining	37

7.2 Performance	37
8 Conclusions	38
Bibliography	39
A spexs2	43
A.1 source	43
B Reference Implementation	45

Chapter 1

Introduction

write at least 3-4 pages

1.1 Motivation and background

One of the problems arising in dataset analysis is the discovery of interesting patterns. These patterns can show how the dataset is formed, how it repeats itself or can be characteristic to some particular subset of the data.

For example a protein motif in a genomic sequence could predict disease. Patterns in medical diagnoses could show relations between diseases. Repeating pattern in source code could show how code could be minimized.

Research in pattern discovery is mainly driven by biology, which means most of the discovery algorithms have been designed for genomic sequences in mind. The techniques could be potentially useful elsewhere, so the algorithms should be generic as possible.

With genomic sequences there is another problem, the amount of data[GC95]. The data collected are growing with increasing speed, which means we need to use more computational resources to analyse them. This means the pattern discovery algorithms should take advantage of multicore processors, dis-

cite
some-
thing

cite
some-
thing

tributed systems and highly parallel computers.

write a priori vs some prior knowledge

write broad examples from nat processing, code

write usual limitations, alphabet, pattern language...

1.2 Contributions of this work

We have derived a new parallel algorithm called SPEXS2 for discovering interesting patterns from a set of sequences. We describe SPEXS2 in a generic way and show how to extend it further.

The practical and "ideal" versions of an algorithm can often diverge due to performance and implementation details, therefore we also explain problems and possible solutions with implementing such algorithm. We also have provided a concise implementation of the algorithm that captures the generic description more closely.

Then we show some possible applications for the algorithm and analyse parallelization benefits.

The practical implementation *spexs2* is already being used in several projects ...

write about current use

1.3 Structure of the thesis

In this thesis we explore an algorithm for parallel pattern discovery. We choose an existing algorithm SPEXS[Vil02] and show how it can be parallelized.

The problem of algorithm parallelization can usually be divided into generalization and reification. Usually algorithms are designed in some particular setting, which they are constrained by their data structures, input and output; and specialized to some particular case to increase the performance.

Generalization means that we relax as many constraints as possible, trying to get a mathematical formulation of the algorithm. Also we try decompose the algorithm into independent parts that could be analysed separately.

Reification means that we can parallelize the algorithm by replacing these "abstract" notions by parallel algorithms, data-structures and run the decomposed parts in parallel (if possible).

In Chapter 2 we introduce the terminology. In Chapter 3 we give an overview of already existing algorithms and discuss why SPEXS[Vil02] was chosen as a base for parallelization. We generalize the SPEXS algorithm in Chapter 4 and reify it in Chapter 5. We discuss an implementation of the parallelized algorithm in Chapter 6 and in Chapter 7 show its possible applications and performance characteristics. The conclusions are presented in Chapter 8.

Chapter 2

Definitions

Pattern discovery is a research area aiming to discover unknown patterns in a given set of data structures that are frequent and interesting according to some measure. In this chapter we formally define necessary terms used in this thesis.

2.1 Sequence and Dataset

We use Σ to denote the set of tokens in the dataset, an *alphabet*. The *size* of the alphabet is $|\Sigma|$. *Tokens* can be numbers, letters, words or sentences - any symbol.

Any sequence $S = a_1a_2...a_n, \forall a_i \in \Sigma$ is called a *sequence* over the token set Σ . If the length of the string is 0, it is called an empty sequence or ϵ .

Example 2.1.1. `ACGTGCCATC` is a sequence where $\Sigma = \{\text{A}, \text{C}, \text{G}, \text{T}\}$.

A *dataset* is a collection of sequences.

Example 2.1.2. In a document sentences can be considered as a *dataset*, where a single sentence is a *sequences* and each word is a *token* in the alphabet. Text `This is some example. This is an other example.` has sequences $\{ [\text{This is an example}], [\text{This is an other example}] \}$ and the alphabet is $\Sigma = \{\text{this}, \text{is}, \text{an}, \text{example}, \text{other}\}$.

2.2 Pattern

Our aim is to discover repetitive and common structures in data. We call such structures *patterns*. A generic way to define a *pattern* is as a set of all the sub-structures it represents. This means we can say whether some data sub-structure is represented by a pattern.

The *pattern structure* is usually dependent on the data-structures which it represents. For example sequence patterns are usually represented sequences, graph patterns are represented as graphs; but sequence patterns could also be represented as a graph.

We denote the set of structures that a pattern structure p defines as $all(p)$. If $\alpha \in all(p)$, where α is a structure then we say that structure α *matches exactly* pattern p . We say that α *matches* p if any of structure $all(p)$ is a sub-structure of α .

In this thesis we only consider sequential pattern structures and use *pattern* to mean *sequential pattern structure*. We represent such patterns with regular expressions.

write about regexps

cite
regex

Pattern size is the length of the pattern sequence.

Example 2.2.1. `. [AT]` is a pattern of size 2 and denotes a set $\{ \text{AA}, \text{AT}, \text{CA}, \text{CT}, \text{GA}, \text{GT}, \text{TA}, \text{TT} \}$; it matches `CCTC` and exactly matches `AT`.

We denote the set of all pattern p *matches* in a dataset D as $matches(p, D) = \{match(p, \alpha) | \alpha \in D, matches(p, \alpha)\}$.

2.3 Query

We need to somehow understand where given pattern p is located in a dataset D . This compound structure $q = \langle D, p, matches(p, D) \rangle$ is called a *query*.

Example 2.3.1. Let our dataset be $D = [\text{ACGT}, \text{TXCGA}]$ and our pattern be $p = \text{C.}$. The corresponding query is $\langle D, p, \{[1, 3], [2, 4]\} \rangle$, which means

that the pattern p ends in sequence 1 at position 3 and in sequence 2 at position 4.

2.3.1 Query features

When we talk about how "interesting" a pattern is, we are actually evaluating the query, since the pattern requires a context where it can be "interesting".

Queries can have different properties: length, number of matches in the dataset, pattern textual representation etc. Such properties can be represented by a function that take a query as an input and return the property. Formally a *query feature* is a function $f : \text{Query} \mapsto \text{Any}$.

We also need to see how "interesting" one query is compared to the others. *Query interestingness* is a function $f : \text{Query} \mapsto \text{Value}$ where the *Value*s are well-ordered. This gives a measure to compare two different queries. Often we can represent such interestingness measures as a real number.

We should also be able to somehow specify criterias for query. *Query filter* is a function $f : \text{Query} \mapsto \text{Boolean}$ and shows whether the query matches the criteria.

Example 2.3.2. Pattern occurrences in a document is a interestingness measure. Whether query pattern is at least 3 tokens is a query filter.

2.4 Pool

Pool is an abstract datatype for a collection of queries. The pool allows queries to be stored. The only operations that pool must provide is "push", for adding a query, and "pop", for getting a query.

Example 2.4.1. Stacks and queues both satisfy the pool requirement. We could also define a pool that stores the queries on the disk; also it could pack or reorder the queries for performance reasons.

2.5 Pattern Discovery

In this thesis *pattern discovery* is a process of finding the most interesting subset, according to a query interestingness, of sequential patterns, that conform to some criteria, in a sequence dataset.

Example 2.5.1. Let our search problem be "Finding most common nucleotide patterns that are at least 3 nucleotides long from a shotgun sequencing output.", then *most common* defines our interestingness measure. *At least 3 nucleotides* is the pattern subset criteria. *Sequencing output* is our dataset and *nucleotides* define the token alphabet.

Chapter 3

Overview

better
title
needed

Work in progress

In this chapter we give a overview of different algorithms used for pattern discovery.

Reorganize
some-
how

3.1 Algorithms

Overview of different combinatorial algorithms.

3.1.1 SPEXS

SPEXS is an pattern discovery algorithm described in "Pattern Discovery from Biosequences"[Vil02]. This algorithm finds patterns from a sequence. We take this as our basis for developing a new parallel algorithm. In this chapter we describe original algorithm so that we can later show the changes made to this algorithm.

We describe the general representation of the SPEXS algorithm. The original algorithm was as follows:

move algorithm to generalization

Algorithm 1 The SPEXS algorithm

Input: String S , pattern class \mathcal{P} , output criteria, search order, and fitness measure \mathcal{F}

Output: Patterns $\pi \in \mathcal{P}$ fulfilling all criteria, and output in the order of fitness \mathcal{F}

```
1: Convert input sequences into a single sequence
2: Initiate data structures
3: Root  $\leftarrow$  new node
4: Root.label  $\leftarrow \epsilon$ 
5: Root.pos  $\leftarrow (1,2,\dots,n)$ 
6: enqueue( $\mathcal{Q}$ , Root, order)
7: while  $N \leftarrow$  dequeue( $\mathcal{Q}$ ) do
8:   Create all possible extensions  $p \in \mathcal{P}$  of  $N$  using  $N$ .pos and  $S$ 
9:   for extension  $p$  of  $N$  do
10:    if pattern  $p$  and position list  $p$ .pos fulfill the criteria then
11:       $N$ .child  $\leftarrow p$ 
12:      calculate  $\mathcal{F}(p, S)$ 
13:      enqueue( $\mathcal{Q}$ ,  $p$ , order)
14:      if  $p$  fulfills the output criteria then
15:        store  $p$  in output queue  $\mathcal{O}$ 
16: Report the list of top-ranking patterns from output queue  $\mathcal{O}$ 
```

The main idea of the algorithm is that first we generate a pattern and a query that matches all possible positions in the sequence. We then put this query into a queue for extending. Extending a query means finding all queries whose patterns length is longer by 1. If any of the queries is fit, by some criteria, it will be put into the main queue, for further extension, and output queue for possible output.

3.1.2 TEIRESIAS

TEIRESIAS[RF98] is an algorithm for the discovery of rigid patterns in biological sequences.

write more

TEIRESIAS operates in two phases: scanning and convolution. Scanning phase identifies elementary patterns that are frequent. During convolution these elementary patterns are combined to make larger patterns.

This method is a divide and conquer method to only consider frequent patterns.

patterns with any symbol

[write more](#)

3.1.3 Verbumculus

Verbumculus[AGL03] is...

statistical analysis, pattern matching

no complex patterns

[write more](#)

3.1.4 MobyDick

MobyDick[BLS00]... statistical prediction of frequent

no complex patterns

[write more](#)

3.1.5 RSAT

RSAT[Tho+08] is ...

matrix based pattern

[write more](#)

3.1.6 Other

[RSK09; Jen+06]

3.2 Reviews

[P+00; DD07; SD06]

write about some reviews

3.3 Problems

Work in progress

Algorithms are fixed and hard to extend with new pattern types, structures and optimizations. Generalization usually comes at the cost of performance and complexity.

write more

Sequential algorithms do not take advantage of multicore processors.

write more

Data that exceeds computer memory can't work efficiently... can't be distributed efficiently.

write more

Chapter 4

SPEXS Generalization

Work in progress

In this chapter we show how to make SPEXS algorithm more abstract by allowing flexibility through function composition and finding minimal requirements for the data-structures.

4.1 Algorithm

The algorithm in a more conventional view is:

Algorithm 2 The spexs2 algorithm

Input: *dataset*, *in* and *out* are pools, *extend* is an extender function, *extend?*, *output?* are filters

Output: Patterns satisfying filters and *extender* are in *out* pool

```
1: function SPEXS2(dataset, in, out, extend, extend?, output?)
2:    $\epsilon \leftarrow \text{NewEmptyQuery}(\text{dataset})$ 
3:   in.put( $\epsilon$ )
4:   while  $q \leftarrow \text{in.pop}()$  do
5:     extended  $\leftarrow \text{extend}(q, \text{dataset})$ 
6:     for  $qx \in \text{extended}$  do
7:       if  $\text{extend?}(qx)$  then
8:         in.push( $qx$ )
9:       if  $\text{output?}(qx)$  then
10:        out.push( $qx$ )
11:    postprocess( $q$ )
```

When the algorithm starts we create an empty pattern query ϵ and put into the *in* pool. The *in* pool contains queries whose patterns should be further examined.

We pick a query from the *in* pool for extending. The extending means generating all queries whose pattern size is larger by one. There can be several such queries.

If any of the queries should be further examined as defined by the *extendable* query filter, it will be put into the *in* pool.

If the query is suitable for output as defined by the *outputtable* filter, it will be put into the *out* pool.

If we extend each pattern at each step by one we guarantee that we examine all the patterns that conform to our criteria as defined by *extendable* filter.

4.2 Pools

It has no guarantees on how the queries are stored internally and in which order they are taken out. This gives an option to store on disk the queries if needed.

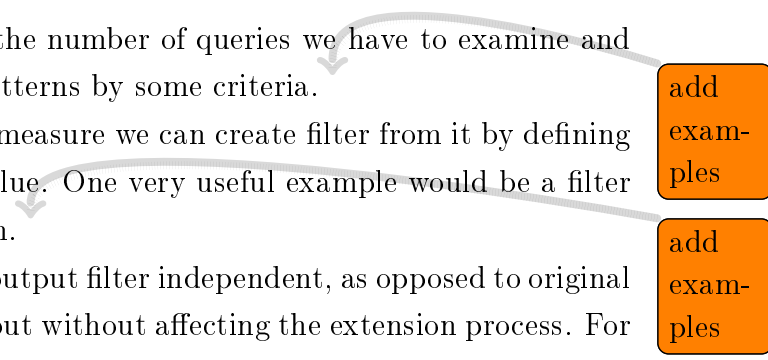
In practice this means we can use any collection such as list, set, queue as a pool. This gives us different performance and memory characteristics.

4.3 Filtering

Filtering allows us to reduce the number of queries we have to examine and allows to select a subset of patterns by some criteria.

If we have interestingness measure we can create filter from it by defining it's minimum or maximum value. One very useful example would be a filter for limiting the pattern length.

By making extension and output filter independent, as opposed to original SPEXS, we can still limit output without affecting the extension process. For example if we wish to see only patterns of length 3 we cannot do it with one filter, since we still would need to extend patterns of length 0, 1 and 2.



add
exam-
ples

add
exam-
ples

4.4 Extending

The extending process is at the core of the algorithm and there are several ways of doing it.

write motivation

write comments

The idea of extending method is:

Algorithm 3 SPEXS2 extender

Input: q query, $walk$ function

Output: result contains queries that have been extended by one

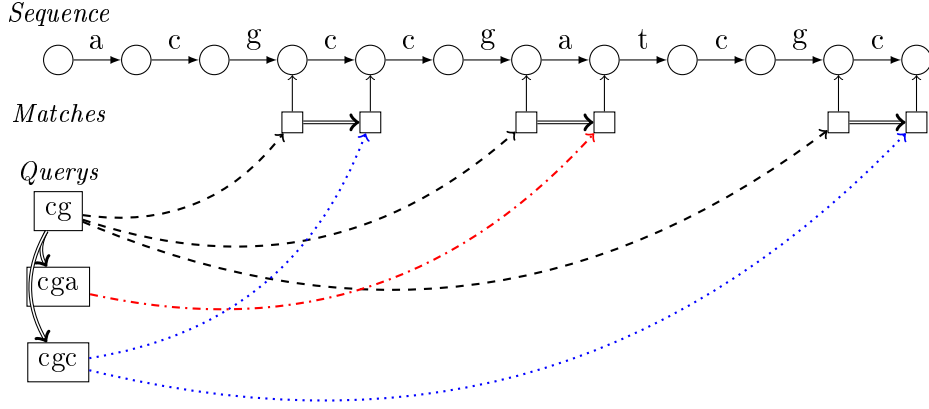
```
1: steps  $\leftarrow$  new collection([Token, Pos])
2: for pos  $\in$  positions( $q.matches$ ) do
3:   [token, loc]  $\leftarrow$  walk( $q.document$ , pos)
4:   steps.add([token, pos])
5: matches  $\leftarrow$  new map(Token  $\mapsto$  [Pos])
6: for [token, loc]  $\in$  steps do
7:   if matches[token] doesn't exist then
8:     matches[token]  $\leftarrow$  empty set
9:   matches[token]  $\leftarrow$  matches[token] + loc
10: queries  $\leftarrow$  new collection([Query])
11: for (token, positions)  $\in$  matches do
12:    $qx \leftarrow$  new query
13:    $qx.document \leftarrow q.document$ 
14:    $qx.pattern \leftarrow q.pattern + token$ 
15:    $qx.positions \leftarrow positions$ 
16:   queries.add( $qx$ )
```

The behavior of *extender* depends on how *next* is implemented, we shall look at different ways how to implement it. The different implementations can capture more complex patterns, but often at the cost of performance.

4.4.1 Sequences

The simplest case how the next function behaves is when we are only looking for simple sequences – the alphabet for patterns and sequences is the same.

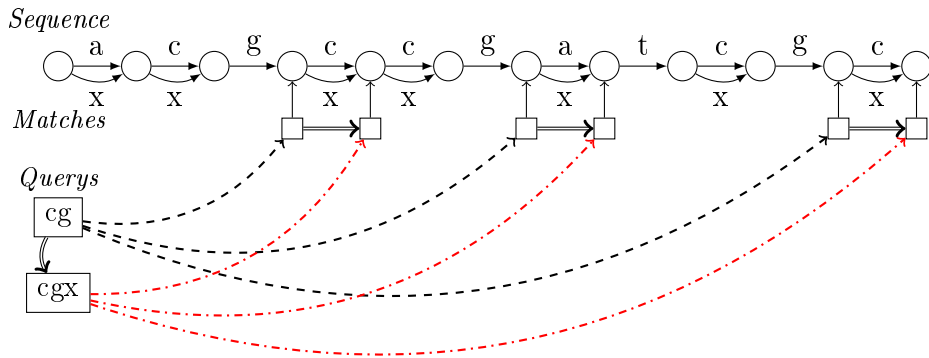
Let's consider a sequence *ACGCCGATCGC* and a pattern *CG*.



Initially we have matches only for query *CG*. Then by taking the *next* token from the sequence we can build up queries *CGA* and *CGC*.

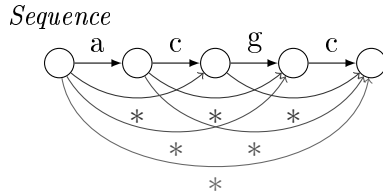
4.4.2 Groups

One common addition in a pattern language is capturing a group of tokens. For example we can use $X = [AC]$ to denote both tokens *A*, *C*. By adding where either one transitions we can capture such groups in the extension process.



4.4.3 Star

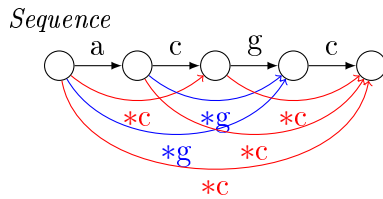
Another possible extension is the *dot-star* or more simply capturing a run of elements. Here we just show the expanded sequence with * symbol.



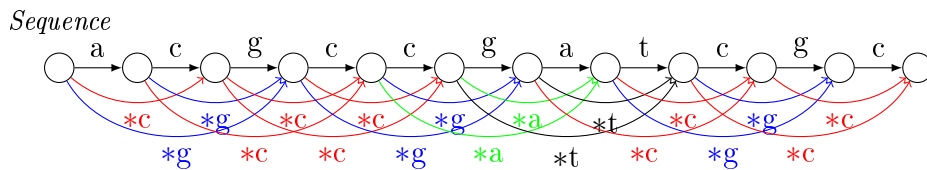
Here we immediately notice how the complexity increases by introducing pattern token.

write properly

We can skip this intermediary step isn't necessary we can instead extend with $*Y$, where Y is some other token. This means we avoid this single large query and have multiple smaller queries.



We can also limit the length of the run.



Here we have limited the run length to be either 2 or 3.

4.4.4 Optimizations

We can further optimize *group next* by inferring the positions from simple *sequence next*. We can see that the positions of a group extension is the same as the union of positions by the group tokens.

If we have a group token γ that contains $tokens(\gamma)$ then the *matches* for such group is

$$matches(p\gamma, D) = \bigcup_{t \in tokens(\gamma)} matches(pt, D)$$

4.5 Summary

write what follows, how used

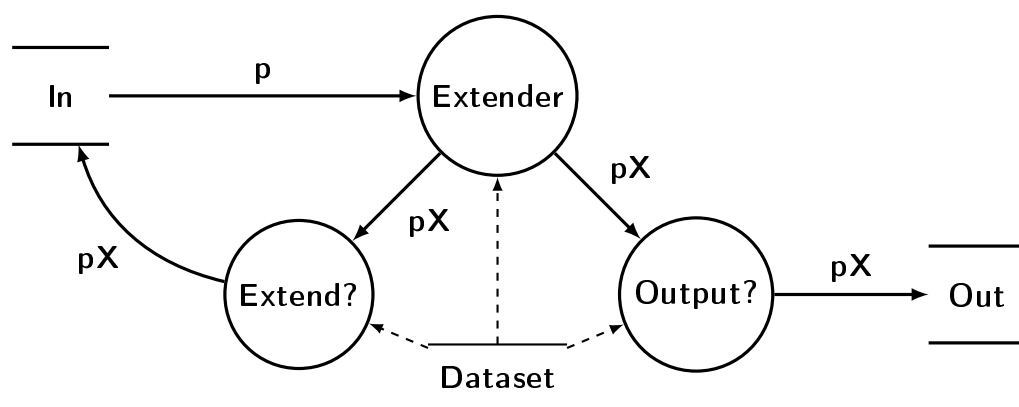
Chapter 5

Parallelization

Here we discuss different ways how we can partition the algorithm to support parallelism.

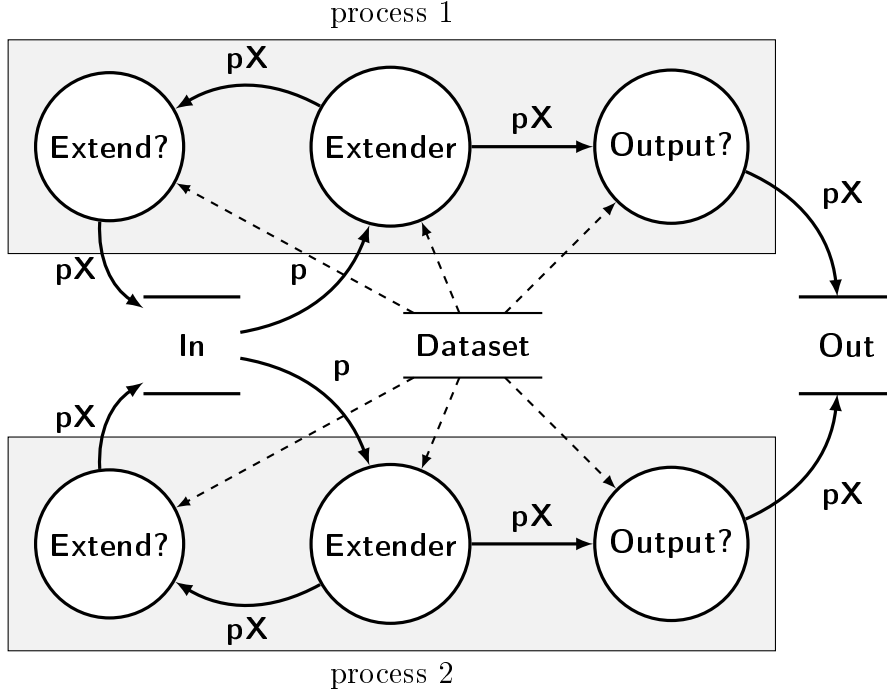
5.1 Process

The main process of the algorithm as described by dataflow diagram.[Kah74; LP95] Circles denote processes and unfinished rectangles denote data stores.



We can see that the different query extensions do not share a dependency, except the dataset. Since dataset itself is read-only for a given process, it

means we can use multiple extender processes. The same applies for extendability and output filter.



We can add more processes in a similar fashion without affecting the end result. Although this will introduce a source of indeterminism.

5.2 Extending

Extender can be parallelized by using MapReduce concepts[Doe09; DG08; Jr09]. We use Clojure[Hic08] reducers library to show how this can be implemented.

Algorithm 4 Parallel extender

```
1 (require '[clojure.core/reducers :as r])
2
3 ; fold-join based grouping function
4 (defn group-map-by [g f coll]
5   (r/fold
6     (r/monoid (partial merge-with into) (constantly {}))
7     (fn [ret x]
8       (let [k (g x)]
9         (assoc ret k (conj (get ret k []) (f x))))))
10    coll))
11
12 (defn extend [dataset query]
13   (let [steps (r/mapcat #(walk dataset %) (:positions query))
14         grouped (group-map-by :token :position steps)]
15     (r/map #(child-query q %) grouped))))
```

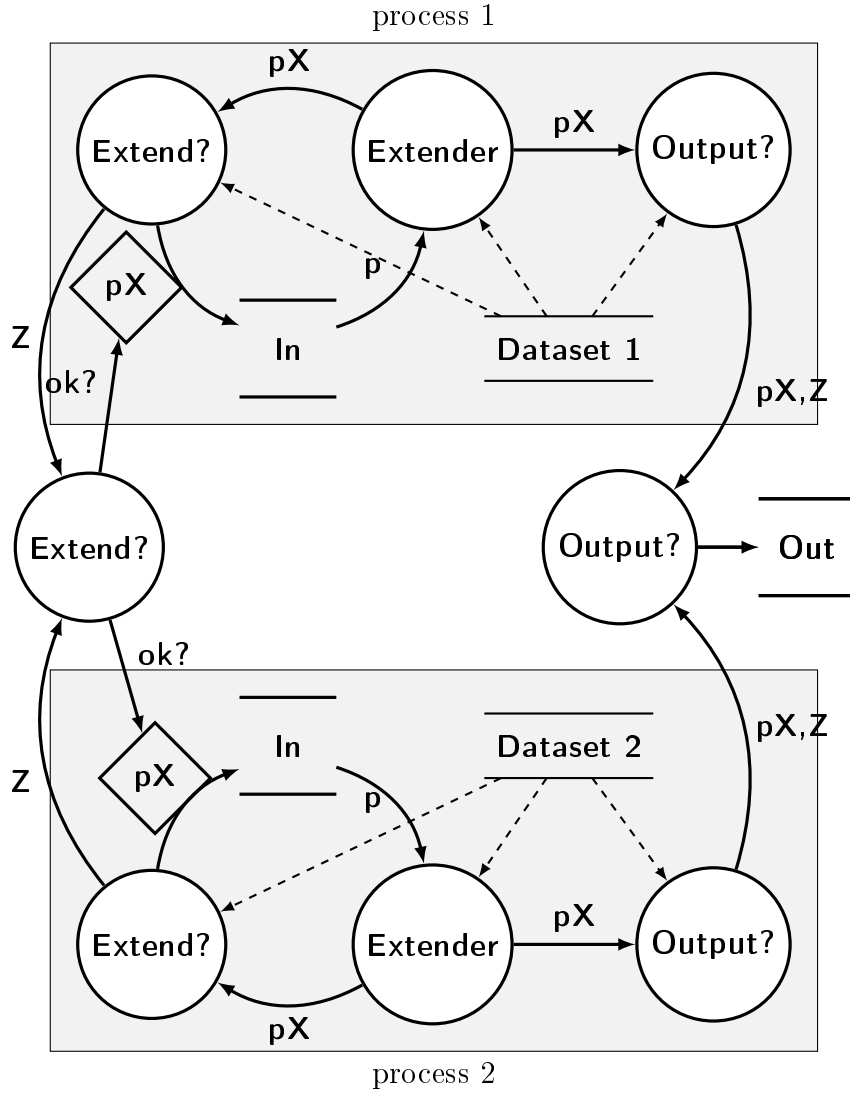
This may not give much improvement on desktop CPUs, since we already can process multiple queries at the same time. This parallelization could be beneficial for highly parallel processors such as GPGPUs or FPGAs.

5.3 Distributed processes

Since the dataset and the process memory consumption can get quite it would also be beneficial to be able to partition the dataset between multiple machines.

The extension results for a given query stays inside the sequence which means we can partition by dividing sequences to separate datasets.

The whole dataset is required only for filtering, since even one of the simplest operations ("counting matches in dataset") requires full knowledge of all matches over the dataset. We can use partial results (Z) to reduce the communication overhead.



For example to see whether some query is over some count limit we first count matches in the partial datasets, then send the partial results to a process that adds these results together. Depending on that result we can decide whether it needs further processing.

Chapter 6

Implementation

Here we discuss a practical implementation, *spexs2*, for pattern discovery in sequences.

In this chapter we will discuss a practical implementation, *spexs2*, for pattern discovery in sequences. We only discuss parts that we consider non-trivial or interesting and could be useful in implementing other algorithms.

Information about the full source code is in the Appendix B and C.

6.1 Architecture

The main criteria for designing program have been described in D. Parnas paper "On the Criteria To Be Used in Decomposing Systems into Modules"[Par72]. It suggests decomposing into isolated units and parts that are likely to change together.

We chose the following module decomposition for the application:

Configuration structure for holding the configuration data

Setup based on the configuration initializes data-structures and functions for the algorithm

Reader reads in the data from files

Database a collection of datasets

Algorithm the SPEXS2 algorithm

Printer prints the result queries

The program starts by interpreting flags, then it marshals configuration file onto an internal structure, this configuration is given into setup module. Setup module initializes (as defined by configuration) a reader, a printer and also prepares structures for algorithm. Then the reader reads input to the database. Then the algorithm is activated and finally it is printed out with Printer.

This structure is universal for algorithm implementations and allows easily to add more configuration options, different input formats and different output formats. By changing the configuration, reader and printer we could make it a web service instead of running it on a command line.

6.2 Configuration

One problem with flexible algorithms is that there are a lot of ways to be run. This can lead to having tens or hundreds of command-line flags for the application.

To avoid this problem we first decided to use a *json* file for the program configuration. Using *json* requires exact placement of commas and quotes that caused a lot of problems, hence we started using *yaml* that is more suitable for human input.

write Short example of a configuration file.

When running the program from command line it can be uncomfortable to make little changes to the configuration files. In these cases a command line flag would be much easier. To solve this problem we added markup into the json files so they could be replaced with a flag.

For example, inside the configuration file:

```
"Datasets" : {  
  "fore" : { "File" : "$input:main$"  
  ...
```

Using *spexs2 -conf conf.json input=other* would replace the "File" value with "other". If there is no flag from command line is given, it will be replaced with "main".

The configuration file can be problematic for running the first time. You first need to find a configuration file for your application. To remedy this problem the application could provide sample configuration files that can be used directly from the command line.

6.3 Input and Output

write about importance of separating the input reader and output printer from the algorithmic code

6.4 Alphabet and Database

write about problems with large alphabets and datasets

6.5 Pools

There can be different performance characteristics when using a particular implementation. Most importantly to support parallelism they should be ideally lock-free, but we can use locked version as well.

remove the lock-free stuff

If we use a fifo queue as the in pool the algorithm does a breadth first search of patterns. This can be problematic since we would need a lot of memory to hold all the patterns in memory.

A lifo queue for in pool is a more reasonable choice for memory problems since we need to hold less patterns in memory.

A priority queue suits for the output pool since we can easily then use

some feature to sort the queue. A lock-free priority queue would be preferred, but it can be hard to get right.

link to
lock-
free
queues

Trivial solution would be to use locks for enqueueing and dequeuing, but under high contention it will become a bottleneck.

We know that most of the time we do not need all the results, but only the best. We also know that the result limit is usually several magnitudes smaller than the number of output candidates; this means most of the queries put into the result queue will be immediately discarded.

Uf the query is worse than the worst in the priority queue, it can be discarded immediately without doing push/pop. If we allow for that check to fail once in a while - we can make it mostly lock-free.

6.6 Features and Filters

write simpler and examples

One problem is that the amount of possible filters it's useful to construct them from some other features. Or if we wish to use multiple filters we can combine them.

We can use these features to find out something about the query. They each feature is defined as:

```
type Feature func(q *Query) (float64, string)
```

Most of features are in \mathfrak{R} , but for some there is some extended information that we may wish to know - hence the need for additional string value. One of the simplest is Pattern representation.

Also many of the features are defined in terms of multiple datasets. We can use a closure to easily define a more generic feature.

Example:

```
func Matches(dataset []int) Feature {  
    return func(q *Query) (float64, string) {
```

```

        matches := countf(q.Pos, dataset)
        return matches, ""
    }
}

```

Here the Matches function creates a feature function defined for dataset.

We can use the name in the configuration file as "Matches(fore)".

If a feature returns a floating point value we can easily turn that into a filter by specifying a minimum or/and maximum value.

For example to give a lower and higher limits to some feature:

```

func featureFilter(feature Feature, min float64, max float64) Filter {
    return func(q *Query) bool {
        v, _ := feature(q)
        return (min <= v) && (v <= max)
    }
}

```

Of course there are some filters that cannot be defined by features hence there is still possibility to make separate filters. Such as disallowing star symbol in the beginning of the pattern.

6.7 Synchronized Tree Traversal

spexs2 can be seen as a pattern tree traversal algorithm with some extra logic. Implementing search over a tree requires synchronization such that there are only a certain number of workers and that they wouldn't die of starvation.

Without synchronization the parallel version looks like:

Algorithm 5 Tree traversal

Output: All nodes in tree get processed with fn

```
1: function VISIT(tree, start, fn, examine?)
2:   unvisited  $\leftarrow$  { start }
3:   start workers
4:     while unvisited not empty do
5:       node  $\leftarrow$  unvisited.take()
6:       fn(node)
7:       for child  $\in$  children(node) do
8:         if examine?(child) then
9:           unvisited.put(child)
10:
11:   wait for workers
```

This would not work correctly with multiple workers since there are race conditions and the workers can die early due to starvation.

The solution is to control worker startup and only terminate workers if all have finished and there are no more items in unvisited set.

Algorithm 6 Synchronized graph traversal

Output: All nodes in *graph* get processed with *fn*

```
1: function VISIT(graph, start, fn, examine?)
2:   added  $\leftarrow$  new semaphore(0)
3:   terminate  $\leftarrow$  false
4:   mutex  $\leftarrow$  new mutex()
5:   workers  $\leftarrow$  0
6:   unvisited  $\leftarrow$  { start }
7:   added.signal()
8:   start workers
9:     while true do
10:       added.wait()
11:       mutex.lock()
12:       if terminate then
13:         added.signal()
14:         mutex.unlock()
15:         break
16:       node  $\leftarrow$  unvisited.take()
17:       workers  $\leftarrow$  workers + 1
18:       mutex.unlock()

19:       fn(node)

20:       for child  $\in$  children(node) do
21:         mutex.lock()
22:         if examine?(child) then
23:           unvisited.put(child)
24:           added.signal()
25:           mutex.unlock()

26:       mutex.lock()
27:       workers  $\leftarrow$  workers - 1
28:       if workers = 0 and unvisited = {} then
29:         terminate  $\leftarrow$  true
30:         added.signal()
31:       mutex.unlock()
32:
33:   wait for workers
```

We use *mutex* to protect variables and data structures. Semaphore *added* tracks how many items are in the *unvisited* set, if the process finally terminates it is turned into a turnstile on line 31 and 13. Variable *workers* tracks how many workers are busy.

6.8 Debugging

Seeing how the algorithm works is very useful to get an understanding how the algorithm works. This often can help to either improve the input configuration or debug the program itself. Often this is resolved by adding debug statements.

For example:

```

1 func Spexs(s *Setup) {
2     for q, ok := s.In.Pop(); ok {
3         trace("started extending %v", q)
4         extended := s.Extend(q)
5         trace("extension result %v", extended)
6         for qx := range extended {
7             if s.Extendable(qx) {
8                 trace("> extendable %v" qx)
9                 s.In.Push(qx)
10            }
11            if s.Outputtable(qx) {
12                trace("> outputtable %v" qx)
13                s.Out.Push(qx)
14            }
15        }
16    }
17 }
```

Such statements make it harder to read the actual code, also it's hard to modify the statements for debugging or provide different ways of debugging.

We can use lexical closures to make it simpler:

```

1 type Extender func(q Query) [] Query
2
3 func AddDebuggingStatements(s *Setup) {
4     fn := s.Extend
5     s.Extend := func(q Query) [] Query {
6         trace("started extending %v", q)
7         extended := fn(q)
8         trace("extension result %v", extended)
9     }
```

```

9
10         for qx := range extended {
11             trace(" > %v", qx)
12             trace(" > extendable %v", s.Extendable(qx))
13             trace(" > outputtable %v", s.Outputtable(qx))
14         }
15         return extended
16     }
17 }
18
19 func Spexs(s *Setup) {
20     for q, ok := s.In.Pop(); ok {
21         extended := s.Extend(q)
22         for qx := range extended {
23             if s.Extendable(qx) {
24                 s.In.Push(qx)
25             }
26             if s.Outputtable(qx) {
27                 s.Out.Push(qx)
28             }
29         }
30     }
31 }
32
33 func run(){
34     S := CreateSpexsSetup()
35     AddDebuggingStatements(S)
36     Spexs(S)
37 }

```

We have removed the debugging statements from the algorithm. We could define other such "debug statement injectors" that provide different levels of details. This method of course has a slight performance impact due to the additional indirection. This can be extended to provide user interaction and other features.

Chapter 7

Applications and experimental results

Work in progress

7.1 Examples

Here we show examples for the program:

7.1.1 DNA sequences

make an example

7.1.2 Protein sequences

make an example

7.1.3 Text mining

make an example

7.1.4 Code mining

make an example

7.2 Performance

make an example

Chapter 8

Conclusions

Work in progress

write results 1

write results 2

write context, compare

write strength + limitations

write speed

write so what? why is it important

write what is next?

write strong conclusions

write take home message

In this thesis we showed how by making an algorithm more abstract and general we can also make it parallel. We showed that this algorithm can find patterns from sequences.

Although we showed that we can apply this algorithm on NFAs we did not analyze the performance characteristics. This suggests that this algorithm may be able to work on trees and graph, but would require slight modifications.

We also demonstrated how to make the algorithm more concrete and work

well on some particular datasets. This also took into consideration further development and flexibility of the algorithm.

The SPEXS2 implementation currently is already used in biosequenceing and text mining.

Bibliography

- [AGL03] A. Apostolico, F. Gong, and S. Lonardi. “Verbumculus and the Discovery of Unusual Words”. In: *Journal of Computer Science and Technology* 19.1 (2003), pp. 22–41. URL: <http://www.cs.ucr.edu/~stelo/papers/verb03.ps.gz>.
- [BLS00] Harmen J. Bussemaker, Hao Li, and Eric D. Siggia. “Building a dictionary for genomes: Identification of presumptive regulatory sites by statistical analysis”. In: *Proceedings of the National Academy of Sciences* 97.18 (2000), pp. 10096–10100. DOI: 10.1073/pnas.180265397. eprint: <http://www.pnas.org/content/97/18/10096.full.pdf+html>. URL: <http://www.pnas.org/content/97/18/10096.abstract>.
- [DD07] Modan Das and Ho-Kwok Dai. “A survey of DNA motif finding algorithms”. In: *BMC bioinformatics* 8.Suppl 7 (2007), S21.
- [DG08] Jeffrey Dean and Sanjay Ghemawat. “MapReduce: simplified data processing on large clusters”. In: *Commun. ACM* 51.1 (Jan. 2008), pp. 107–113. ISSN: 0001-0782. DOI: 10.1145/1327452.1327492. URL: <http://doi.acm.org/10.1145/1327452.1327492>.
- [GC95] Mark S Guyer and Francis S Collins. “How is the Human Genome Project doing, and what have we learned so far?” In: *Proceedings of the National Academy of Sciences* 92.24 (1995), pp. 10841–10848.
- [Hic08] R. Hickey. “The Clojure programming language”. In: *Proceedings of the 2008 symposium on Dynamic languages*. ACM New York, NY, USA. 2008.
- [Hic12a] R. Hickey. *Anatomy of a Reducer*. May 2012. URL: <http://clojure.com/blog/2012/05/15/anatomy-of-reducer.html>.

- [Hic12b] R. Hickey. *Reducers - A Library and Model for Collection Processing*. May 2012. URL: <http://clojure.com/blog/2012/05/08/reducers-a-library-and-model-for-collection-processing.html>.
- [HN05] Maximilian Häußler and Jacques Nicolas. *Motif Discovery on Promotor Sequences*. Anglais. Rapport de recherche RR-5714. INRIA, 2005, p. 136. URL: <http://hal.inria.fr/inria-00070303>.
- [Jen+06] Kyle L. Jensen et al. “A generic motif discovery algorithm for sequential data”. In: *Bioinformatics* 22.1 (2006), pp. 21–28. DOI: 10.1093/bioinformatics/bti745. eprint: <http://bioinformatics.oxfordjournals.org/content/22/1/21.full.pdf+html>. URL: <http://bioinformatics.oxfordjournals.org/content/22/1/21.abstract>.
- [Jr09] Guy L. Steele Jr. “Organizing functional code for parallel execution or, foldl and foldr considered slightly harmful”. In: *ICFP*. 2009, pp. 1–2.
- [Kah74] G. Kahn. “The semantics of a simple language for parallel programming”. In: *Information processing*. Ed. by J. L. Rosenfeld. Stockholm, Sweden: North Holland, Amsterdam, Aug. 1974, pp. 471–475.
- [LP95] E.A. Lee and T.M. Parks. “Dataflow process networks”. In: *Proceedings of the IEEE* 83.5 (May 1995), pp. 773–801. ISSN: 0018-9219. DOI: 10.1109/5.381846.
- [P+00] Pavel A Pevzner, Sing-Hoi Sze, et al. “Combinatorial approaches to finding subtle signals in DNA sequences”. In: *Proceedings of the Eighth International Conference on Intelligent Systems for Molecular Biology*. Vol. 8. 2000, pp. 269–278.
- [Par72] D. L. Parnas. “On the criteria to be used in decomposing systems into modules”. In: *Commun. ACM* 15.12 (Dec. 1972), pp. 1053–1058. ISSN: 0001-0782. DOI: 10.1145/361598.361623. URL: <http://doi.acm.org/10.1145/361598.361623>.
- [RF98] I Rigoutsos and A Floratos. “Combinatorial pattern discovery in biological sequences: The TEIRESIAS algorithm.” In: *Bioinformatics* 14.1 (1998), pp. 55–67. DOI: 10.1093/bioinformatics/14.1.55. eprint: <http://bioinformatics.oxfordjournals.org/content/14/1/55.full.pdf+html>. URL: <http://bioinformatics.oxfordjournals.org/content/14/1/55.abstract>.

- [RSK09] Pedro Ribeiro, Fernando Silva, and Marcus Kaiser. “Strategies for network motifs discovery”. In: *e-Science, 2009. e-Science’09. Fifth IEEE International Conference on*. IEEE. 2009, pp. 80–87.
- [SD06] Geir Kjetil Sandve and Finn Drablos. “A survey of motif discovery methods in an integrated framework”. In: *Biol Direct* 1.11 (2006).
- [Tho+08] Morgane Thomas-Chollier et al. “RSAT: regulatory sequence analysis tools”. In: *Nucleic Acids Research* 36.suppl 2 (2008), W119–W127. DOI: 10.1093/nar/gkn304. eprint: http://nar.oxfordjournals.org/content/36/suppl_2/W119.full.pdf+html. URL: http://nar.oxfordjournals.org/content/36/suppl_2/W119.abstract.
- [Vil02] Jaak Vilo. “Pattern Discovery from Biosequences”. PhD thesis. University of Helsinki, 2002.

Appendix A

spexs2

The program can be found at github.com/egonelbre/spexs.

Several configurations can be found in the folder *examples*. It is best to start with an already existing configuration and modify it to your needs.

If the running *spexs2 -details* will print extended help about all the available features, filters, extenders.

A.1 source

The source code in *src* has the following structure:

```
src/
├── spexs .....algorithm definition
│   ├── extenders/ .....query extenders
│   ├── features/ .....query feature calculators
│   ├── filters/ .....filter implementations
│   ├── pool/ .....different queue implementations
│   ├── database.go .....sequence dataset definition
│   ├── query.go .....query definition
│   └── spexs.go .....algorithm implementation
├── spexs2 .....command-line utility
│   └── conf.go .....configuration reader
```

- dataset.go dataset reader
- features.go parses and creates feature functions
- help.go prints help for the program
- printer.go prints the final output
- runtime.go profiling and live-view setup
- setup.go prepares everything for algorithm
- spexs2.go main-entry point

There are also additional packages:

src/

- debugger/ debugger for concurrent processes
- stats/ statistical functions
 - binom/ binomial p-value calculation
 - hyper/ hypergeometric p-value calculation
- utils/ additional utility functions
- bit/ functions for bitmanipulation
- set/ set implementations
 - hash/ hash table with entry per value
 - bin/ hash table with bitvectors
 - trie/ 2-level hashtable with bitvectors

For compilation there are two scripts *make.bat* and *make.sh* that build the program into bin directory.

Appendix B

Reference Implementation

This is a concise implementation of the parallel spexs2 algorithm. It is presented in Clojure[Hic08].

```
1 (require '[clojure.core.reducers :as r])
2
3 ; a parallel grouping function
4 (defn group-map-by [g f coll]
5   (r/fold
6     (r/monoid (partial merge-with into) (constantly {})))
7     (fn [ret x]
8       (let [k (g x)]
9         (assoc ret k (conj (get ret k []) (f x)))))
10    coll))
11
12 ; these are the minimal requirements for a dataset
13 (defprotocol Dataset
14   (all [this] "return all possible positions on the dataset")
15   (walk [this pos] "return coll of Step from pos"))
16
17 (defrecord Query [pattern positions])
18 (defrecord Step [token position])
19
20 ; create an empty query for a dataset
21 (defn empty-query [dataset]
22   (Query. [] (all dataset)))
23
24 ; create a child query for parent given a token and positions
25 (defn child-query [parent [token positions]]
26   (Query. (conj (:pattern parent) token) positions))
27
28 ; declare our extension functions:
29 (defn walk-extend [dataset positions]
30   (let [steps (mapcat #(walk dataset %) positions)]
```

```

31     (group-map-by :token :position steps)))
32
33 ; function to combine multiple extension functions
34 (defn combine-extenders [extenders]
35   (fn [dataset positions]
36     (apply merge-with concat (map #(% dataset positions) extenders))))
37
38 ; finally the algorithm itself:
39 (defn spexs-step [ds q extend]
40   (map #(child-query q %) (extend ds (:positions q))))
41
42 (defn spexs [{
43   ds :dataset ; dataset
44   in :in      ; input coll
45   out :out     ; output coll
46   extend :extend ; position extender function
47   extend? :extend? ; query filter for further extension
48   output? :output? ; query filter for output
49 }]
50   (let [e (empty-query ds)]
51     (loop [in (conj in e)
52            out out]
53       (if-not (empty? in)
54         (let [[q & qs] in
55               querys (spexs-step ds q extend)
56               new-in (concat qs (filter extend? querys))
57               new-out (concat out (filter output? querys))]
58           (recur new-in new-out))
59         out))))
60
61 ; here is an example how to implement a dataset
62 (defn posify [row-index row-item]
63   (map (fn [pos] [row-index pos]) (range (count row-item))))
64
65 (defrecord SequenceDataset [items]
66   (token [this [row pos]]
67     (nth (nth (:items this) row) pos))
68
69   Dataset ; satisfy dataset interface
70   (all [this]
71     (mapcat posify (range) (:items this)))
72   (walk [this [row i]]
73     (let [row-item (nth (:items this) row)]
74       (if (> (count row-item) i)
75         [(Step. (token this [row i]) [row (inc i)])]
76         []))))
77
78 ; and how to use
79 (def simple-dataset (SequenceDataset. ["ACGT" "CGATA" "AGCTTCGA" "GCGTAA"]))
80
81 (spexs { :dataset simple-dataset :input [] :output []
82         :extend walk-extend

```

```
83      :extend? #(> (count (:positions %)) 3)
84      :output? #(> (count (:pattern %)) 2))}
```

Non-exclusive licence to reproduce thesis and make thesis public

I, Egon Elbre (date of birth: July 27, 1988),

1. herewith grant the University of Tartu a free permit (non-exclusive licence) to:
 - (a) reproduce, for the purpose of preservation and making available to the public, including for addition to the DSpace digital archives until expiry of the term of validity of the copyright, and
 - (b) make available to the public via the web environment of the University of Tartu, including via the DSpace digital archives until expiry of the term of validity of the copyright, "Parallel Pattern Discovery", supervised by Jaak Vilo.
2. I am aware of the fact that the author retains these rights.
3. I certify that granting the non-exclusive licence does not infringe the intellectual property rights or rights arising from the Personal Data Protection Act.

Tartu, May 6, 2013