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Parallel Pattern Discovery

Master's Thesis Draft

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Contents

Chapter 1

Introduction

1.1 Motivation and background

Collecting new data has been increasing more rapidly than algorithms and computer processing power. The average size of each dataset has also been increasing. This suggests that the only way to keep up with analysis is to parallelize algorithms.

One of main drivers of such large datasets is analysis of genomic and proteomic sequences. Regularities in such data can give new insights into how these patterns form and how they are related to the other features of the data.

In this thesis we explore an algorithm for finding patterns and show how generalizations can make it scalable and flexible, and simpler both in theory and implementation compared with non-abstract version.

1.2 Structure of the thesis

In the the Chapter 2 we give definitions for terminology that is used to describe the alogrithm. In the Chapter 3 we investigate the original SPEXS algorithm and TEIRESIAS algorithm. We generalize the SPEXS algorithm to get a flexible algorithm in Chapter 4 and we partition the algorithm to

make it suitable for parallelization in Chapter 5. In Chapter 6 we discuss the implementation of SPEXS. In Chapter 7 we show possible applications for the algorithm.

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.

Since the discovery algorithms are highly dependent on the data structures, that are being searched, the algorithm must be minimal in the requirements on the dataset to be applicable as wide range as possible. This also means that the patterns found must be dependent on the initial data.

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* $S = a_1 a_2 ... a_n, \forall i \in \Sigma$ 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.

For example $ACGTGCCATC$ is a sequence where $\Sigma = \{A, C, G, T\}$.

A *dataset* is a set of sequences. For example a document can be considered as a dataset, where the sentences are sequences and each word is a token in the alphabet.

2.2 Pattern

A *pattern* is a structure that defines a set of sequences. This pattern usually is denoted by a squence with an extended alphabet.

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

The most commonly used pattern descriptions are regular expressions. For example $.[AT]$ can denote a set $\{AA, AT, CA, CT, GA, GT, TA, TT\}$ and this would match $CCTC$ and exactly match AT. A *match* is a location set where the pattern in the sequence ends.

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

A *query* is a compound structure $< D, p, matches(p, D) >$, where D is the dataset and p a pattern.

2.4 Query features

Query feature is a function $f : Q \mapsto A$, where Q is the query type. It gives information about the query such as the pattern representation, length, number of matches in the dataset.

Query interestingness is a function $f : Q \mapsto Ord$ of the query whose results are well-ordered. This functions result allows to say whether one query is more interesting than the other. For convenience it is useful to represent that value in $\Re$.

Query filter is a function $f : Q \mapsto Bool$ of the query whose result is a boolean.

2.5 Pattern Discovery

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

Chapter 3

Algorithms

There are many itemset discovery algorithms, but only few are general and can discover more complex patterns.

3.1 SPEXS

SPEXS is an pattern discovery algorithm described by Vilo et al. 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:

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 into sequences into a single sequence
2: Initiate data structures
3: Root ← newnode
4: Root.label ← ϵ
5: Root.pos ← (1, 2, ..., n)
6: enqueue(Q, Root, order)
7: while N ← dequeue(Q) do
8:     Create all possible extensions P ∈ 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 ← P
12:            calculate F(P, S)
13:            enqueue(Q, P, order)
14:            if P fulfills the output criteria then
15:                store P into ouput queue O
16: Report the list of top-ranking patterns from output queue O
```

The main idea of the algorithm is that first we generate a pattern and a query that match 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 result.

3.2 TEIRESIAS

write about it

Chapter 4

Generalization

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

4.1 Algorithm

The algorithm in a more convetional view is:

Algorithm 2 The SPEXS2 algorithm

Input: *dataset*, *in* pool, *out* pool, *extender*, *extendable* filter, *outputtable* filter, *postprocess* function
Output: Patterns satisfying filters and *extender* are in *out* pool

```
1: ε ← NewEmptyQuery(dataset)
2: in.put(ε)
3: while q ← in.take() do
4:     extended ← extender(q, dataset)
5:     for qx ∈ extended do
6:         if extendable(qx) then
7:             in.put(qx)
8:         if outputtable(qx) then
9:             out.put(qx)
10:    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 fit for output we 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.

4.2 Pools

Pool is an abstract datatype for a collection of queries. The pool allows queries to be put into it and taken from it, also we can ask whether the pool is empty or not.

It has no guarantees on how the queries are stored internally and in which order they are taken out.

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

This also means that pools can persist the queries if necesssary.

4.3 Filtering

Filtering allows us to reduce the number of queries we have to examine. It also allows to select only interesting 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 separating the extension and output filter, 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 need to extend patterns of length 0, 1 and 2.

4.4 Extending

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

The extending method is:

Algorithm 3 SPEXS2 extender

Input: q query, *next* function
Output: result contains queries that have been extended by one

```
1:  nexts ← new collection
2:  for pos ∈ positions(q.matches) do
3:      (token, loc) ← next(q.document, pos)
4:      nexts.put((token, pos))
5:  matches ← new map of token to position set
6:  for (token, loc) ∈ nexts do
7:      if matches[token] doesn't exist then
8:          matches[token] ← {}
9:      matches[token] ← matches[token] + loc
10: querys ← new collection
11: for (token, positions) ∈ matches do
12:     qx ← new query
13:     qx.document ← q.document
14:     qx.pattern ← q.pattern + token
15:     qx.positions ← positions
16:     querys.add(qx)
```

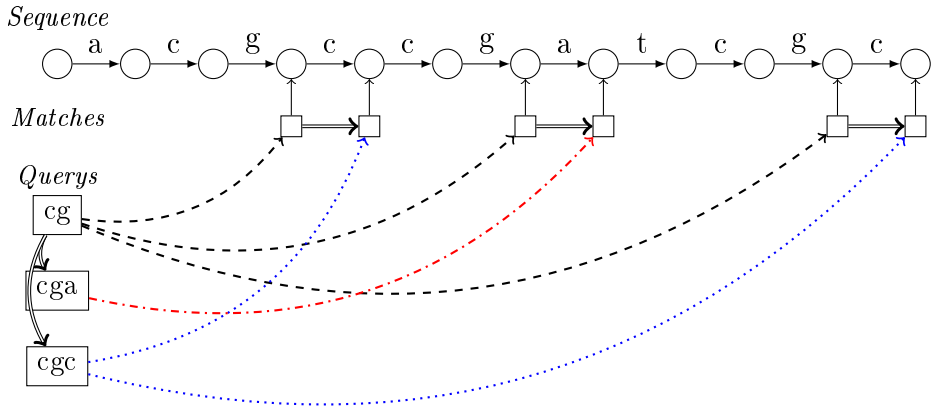
The behavior of *extender* depends on how *next* is implemented, we shall

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.

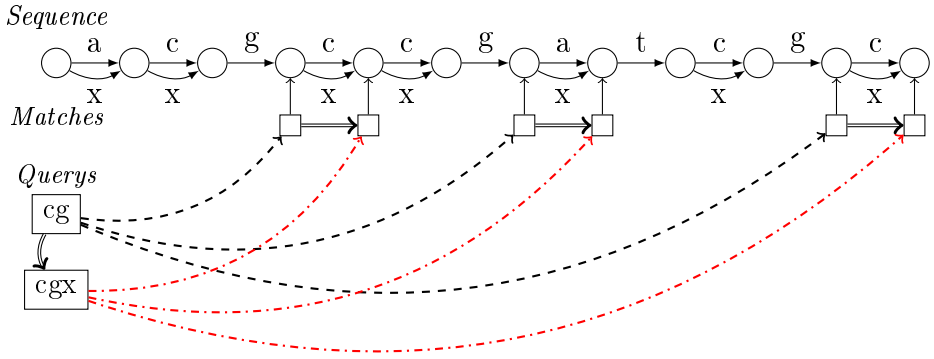
Let's consider a sequence $ACGCCGATCGC$ and a pattern CG.



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

4.4.2 Groups

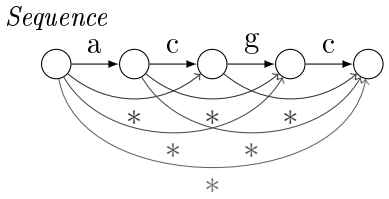
One common addition in pattern language is capturing a group of tokens. For example we can use $X = [AC]$ to denote both tokens A, T. By adding where either one transitions we can capture such groups in the extension process.



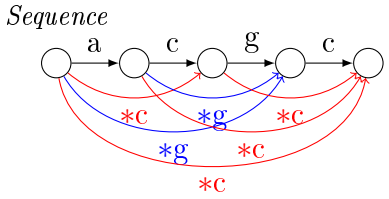
We shall omit the extension examples since the following of corresponding edges is trivial and anologous to previous examples.

4.4.3 Star

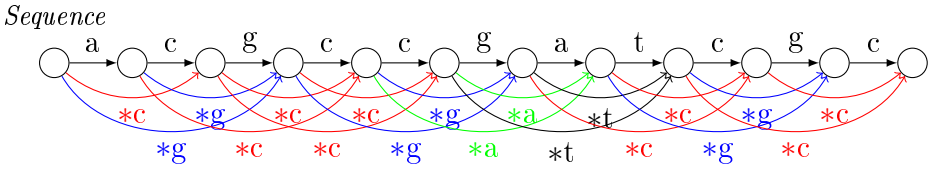
Another possible extension is the *dot-star* or more simply capturing a run of elements. Here we just show the expanded sequence with $*$ symbol.



Here we immediately notice how the complexity increases by introducing pattern token. Since this is a 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

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

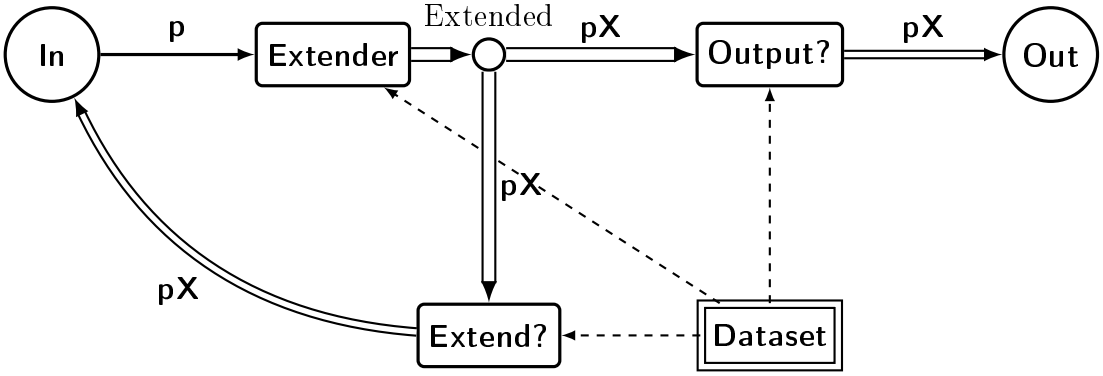
Chapter 5

Parallelization

Here we describe how we can partition the algorithm to support parallelism. A proof of concept for fully parallelized code can be seen in appendix A.

5.1 Process

The main process of the algorithm as described by dataflow diagram.[?, ?]



Here we can see that the only dependence between query extending is the original dataset.

use proper syntax for dataflow diagrams

5.2 Adding Nodes

We can have multiple *in* nodes if the *extender* knows from where to fetch the *querys*, which would require an additional scheduler.

This means that we can run several *extenders* in parallel without effecting the overall process. Although we introduce a source for indeterminism.

5.3 Extending

Since much of the work is done in *extender* we should also try to parallelize it as well:

Algorithm 4 Parallel Extender with Group optimization

Input: Query q, function $next : \mathcal{I} \rightarrow [(\mathcal{I}, \mathcal{P})]$
Output: Set of querys that have been extended by one step

1: $nexts \leftarrow map(next, positions(q.matches))$
2: $matches \leftarrow groupBy(fst, nexts)$
3: $result \leftarrow map(queryMaker(q), matches)$
4: $optimized \leftarrow map((x) \rightarrow (union(matches(x))), groups)$
5: $returnunion(result, optimized)$

figure out how to make it readable

5.4 Dataset partitioning

Since the dataset itself can be large it would be useful to divide it into parts.

As we can see the extender only needs that sequences are intact, hence we can do the extension on partitioned dataset.

If we look at where we need synchronization points if we partition the dataset. Whole parts of extension still apply for parts of dataset.

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. But many such features can be calculated on sharded dataset with map-reduce.

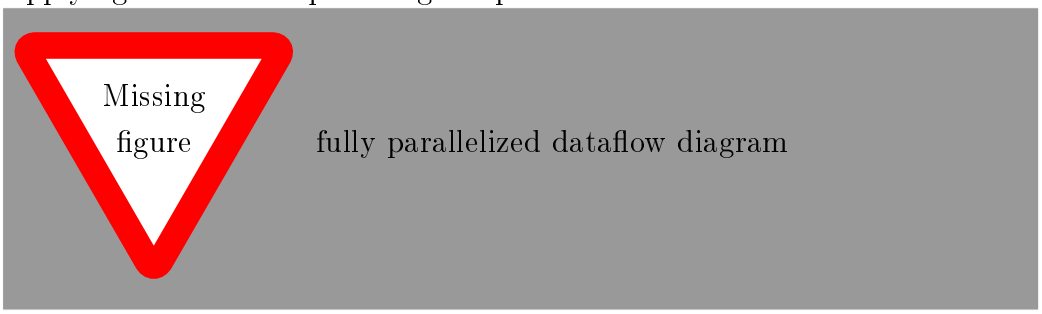
example how to do counting

There are also operations that require presence of all information or extended synchronization. One of the examples implemented in SPEXS is finding minimal p-value by splitting the data.

explain the optimal finding

5.5 Parallelized Process

Applying these techniques we get a parallel dataflow:



fully parallelized dataflow diagram

Chapter 6

Implementation

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

The actual implementation may need to diverge from the abstract definition for several reasons; mainly practicality, simplicity and performance. Many of the operations can be optimized for some particular type of datasets and configuration.

In this chapter we will discuss parts of program that the author considers non-trivial in it's design decisions. 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 Decomposition of Programs. It suggests decomposing into isolated units and parts that are likely to change together. [**?**]

We chose the following decomposition:

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

- **Pattern** represents a pattern
- **Query** stores the pattern with database and pattern
- **Set** stores matching positions
- **Pool** stores queries
- **Extender** drives algorithms extending step
- **Feature** computes a value from the Query
- **Filter** filters some queries

Printer prints the result queries

Debugging utilities for the program

It is a trivial decomposition for the algorithm part, since a lot of is derived directly from the algorithm definition.

The main criteria was to decompose things based on their behavior, whether there is a commonality between them or whether they change independently from the other parts. [**?**]

6.2 Configuration

One problem with flexible algorithms is that they a lot of ways to be run. This often would need having tens or hundereds of program flags. To avoid this problem we decided to use a *json* file for the program configuration.

Short example of a configuration file.

To properly represent configuration in a static language we marshal this file directly to the data-structure. This means we can be less worried about parsing when setting up our algorithm.

The problem with only using a json file is that when running from command line it may be more comfortable using flags. To solve this problem we added replacement strings into the json files that can be given in as a program argument.

```
"Datasets" : {
    "fore" : { "File" : "$inp$"
    ...
```

When using *spexs2 –conf conf.json input=filename* the input will be replaced by filename. Also there is optional default value if one wasn't given.

6.3 Setup and Database

Setup consumes the configuration and based on the values initializes pools; creates and combines features and filters; reads in the data; and creates the printer.

6.4 Reader and Printer

One problem with data is that it comes in many different forms. For example reading in words and single letters requires different behaviors.

One thing that may be helpful is supporting different binary formats.

6.5 Sets

Since we need a collection how to store the matching positions it suggests the need for a set datatype.

If we have predictable distribution we can pack the sets better.

Although such optimizations can be avoided, if during storing pools the sets are packed using some compression algorithm.

6.6 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.

For the pools we have several choices: lifo, fifo or priority.

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 out pool since we can easily then use some feature to sort the queue and choose only a limited amount. A lock-free priority queue would be preferred but it has many details to work correctly.

link to lock-free queues

One simple solution to make priority queue concurrent is to use mutexes when storing or retrieving values. This also would mean that, if the priority queue is used intensively, it can become a bottleneck.

We can use some knowledge about our priority-queue behavior. We know that we usually have a limited-size and the amount of patterns suitable for putting into the output queue is several magnitudes larger; this means most of the queries put into the result queue can be discarded.

So, if 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.

Algorithm 5 priority queue push

1: *worst* ← *current worst*
2: **if** *worst* > *new element* **then return**
3: *mutex.lock*
4: *queue.put*(*new element*)
5: **if** *queue.length* > *queue.limit* **then**
6: *current worst* ← *queue.pop*()
7: *mutex.unlock*

We assume the assignments to be atomic.

6.7 Features and Filters

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 $\Re$, 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.

6.8 Debugging

Debugging is a important part of development process hence the need for more information how the algorithm is working.

Often this is resolved by adding some debug statments:

```
for i := 0; i < 100; i += 1{
    printf("picking")
    a := pick()
    printf("picked %v", a)

    printf("picking")
    b := pick()
    printf("picked %v", b)

    out.put(a + b)
}
```

This can be harmful to the readability of the code. To fix this debugging problem we use closures.

```
type PickFunc func()Thing
func debuggable(fn PickFunc) PickFunc {
    return func() Thing {
        printf("start picking")
        p := fn()
        printf("picked %v" p)
        return p
    }
}

pick = debuggable(pick)
for i := 0; i < 100; i += 1{
    a := pick()
    b := pick()
    out.put(a + b)
}
```

As we can see the algorithm implementation is much more readable and we can inject different debugging statements without actually changing the algorithm.

Also we can now change the ways how to add debug info. One of would be a full stepwise debugger.

```
func debuggable(fn PickFunc) PickFunc {
    return func() Thing {
        mutex.lock()
        p := fn()
        while not continue
            interact with user
        mutex.unlock()
        return p
```

```
    }
}
```

Chapter 7

Applications and experimental results

Here we show examples for the program:

7.1 DNA sequences

make an example

7.2 Protein sequences

make an example

7.3 Text mining

make an example

7.4 Code mining

make an example

Chapter 8

Conclusions

results 1
results 2
context, compare
strength + limitations
so what? why is it important
what is next?
strong conclusions
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 and also NFAs.

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.

Appendix A

Exhaustive Parallel Pattern Search

This part assumes knowledge of *lisp* like languages. The code here is presented in Clojure and for an introduction see `clojure.org/getting_started`.

First we show reader macros that are different from other lisps. Then we present the algorithm with comments.

lists

sets

maps

lambdas

defn

map/reduce

write code

Appendix B

SPEXS2 Command Line Utility

Write

B.1 Configuration

Write

B.2 Running

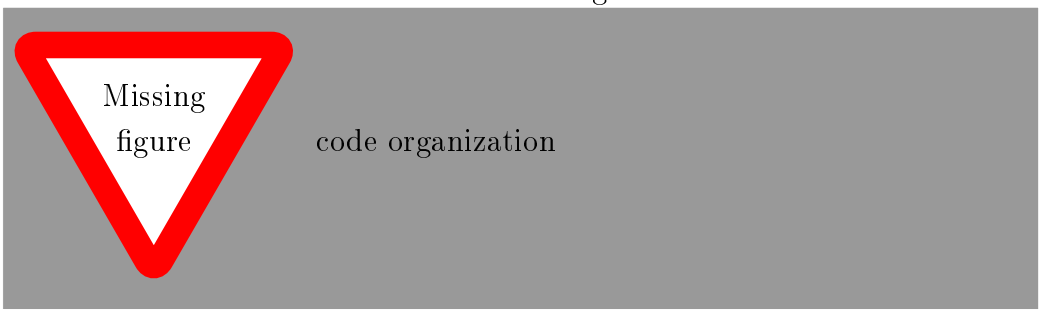
Write

Appendix C

SPEXS2 Source Code

The source code for the implementation of *SPEXS2* is available at `github.com/egonelbre/spexs`.

The source folder "src" has the following structure:



code organization