Module Interface Specification for SubLiMat

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1 Revision History

Date	Version	Notes
March 10, 2025	1.0	Document's first version
April 4th, 2025	1.1	Document's updates after changes on modular design
April 7th, 2025	1.2	Updated version after comments on modular design

2 Symbols, Abbreviations and Acronyms

See SRS Documentation at SRS Documentation

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3 Introduction

The following document details the Module Interface Specifications for the SubLiMatsoftware. The software is designed to evaluate the effect of given substitution matrices in the quality of the alignment of a set of DNA sequences.

Complementary documents include the System Requirement Specifications and Module Guide. The full documentation and implementation can be found at https://github.com/UGarCil/UGarcil_capstone.

Many components from the present documentation follow the template for a MIS for scientific computing software used in Patel (2023), Bicket (2017). These documentations were adapted from the MIS template.

4 Notation

This section is taken from the MIS template.

> The structure of the MIS for modules comes from Hoffman and Strooper (1995), with the addition that template modules have been adapted from Ghezzi et al. (2003). The mathematical notation comes from Chapter 3 of Hoffman and Strooper (1995). For instance, the symbol := is used for a multiple assignment statement and conditional rules follow the form $(c_1 \Rightarrow r_1|c_2 \Rightarrow r_2|...|c_n \Rightarrow r_n)$....

The following table summarizes the primitive data types used by the SubLiMatsoftware.

Data Type	Notation	Description
character	char	a single symbol or digit
float	$\mathbb{R}$	a real (i.e. non complex) number defined within (-∞, ∞), which common values between -3.0 to 3.0
natural number	$\mathbb{N}$	a number without a fractional component in [1, ∞)
str	char	string, represented as a chain of characters from the ASCII
dict	python dictionary	a data structure that stores only state variables

The specification of SubLiMat uses some derived data types: sequences, strings, and tuples. Sequences are lists filled with elements of the same data type. Strings are sequences of characters. Tuples contain a list of values, potentially of different types. In addition, SubLiMat uses functions, which are defined by the data types of their inputs and outputs. Local functions are described by giving their type signature followed by their specification.

5 Module Decomposition

The following table is taken directly from the Module Guide document for this project.

Level 1	**Level 2**
Hardware-Hiding	
Behaviour-Hiding	Alignment (Needleman-Wunsch) Interface Module Control Manager Module Sequence Data Structure Module
Software Decision	Substitution Matrix Module File Manager Module

Table 1: Module Hierarchy

It is important to highlight the categorization for the Alignment Interface Module in the table above. While the use of the Needleman-Wunsch algorithm sits at a high level behavior that defines the main architecture of the software, it is also a Software Decision, as future releases of the software may opt for other alignment algorithms. Its placement in the documentation as Behaviour-Hiding follows a functional justification by making the Needleman-Wunsch algorithm a high-behavior decision component.

6 MIS of Alignment (Needleman-Wunsch) Module

6.1 Module

alignment

```
ADT NeedlemanWunsch:
    - constructor (seq_a, seq_b, gap) → None
    - align(submat) → float       # Returns alignment score
    - get_aligned() → (str, str)  # Returns (aligned_a, aligned_b)
```

6.2 Uses

- **Sequence Data Structure Module**: For validated biological sequence input
- **Substitution Matrix Module**: For accessing substitution matrices and gap penalties

6.3 Syntax

6.3.1 Exported Constants

None

6.3.2 Exported Access Programs

Name	In	Out	Exceptions
`NeedlemanWunsch`	seq_a: str, seq_b: str, gap_penalty: float = -2	NeedlemanWunsch-instance	
`NeedlemanWunsch()`	submat: dict	float (alignment score)	AlignmentError
`align`	submat: dict	float (alignment score)	AlignmentError
`get_aligned_sequences`	-	tuple (str, str)	-

6.4 Semantics

6.4.1 State Variables

- `seq_a`: str (First input sequence)
- `seq_b`: str (Second input sequence)
- `gap_penalty`: float (Gap insertion penalty score)
- `submat`: dict (Active substitution matrix)

- `seq_a_aligned`: str (Aligned version of seq_a)
- `seq_b_aligned`: str (Aligned version of seq_b)

6.4.2 Environment Variables

None

6.4.3 Access Routine Semantics

NeedlemanWunsch.__init__(seq_a, seq_b, gap_penalty=-2):

- Initializes alignment processor with sequences and gap penalty
- Transition: Sets instance variables

NeedlemanWunsch.__call__(submat):

- Output: Alignment score $NeedlemanWunsch.align \rightarrow float$ is calculated by generating sequence pairwise comparison matrix F and traversing using the algorithm.
- Exception: AlignmentError if sequences cannot be aligned

NeedlemanWunsch.align(submat):

- Output: Final alignment score (float)
- Exception: AlignmentError if alignment fails

NeedlemanWunsch.get_aligned_sequences():

- Output: Tuple of aligned sequences (str, str)
- Requires: align() must have been called first

6.4.4 Local Functions

None

6.5 Considerations

- Time Complexity: O(mn) for sequences of length m and n
- Space Complexity: O(mn) for full matrix storage
- Handles both traditional and parameterized substitution matrices
- Inserts gap penalties through constant gap penalty

7 MIS of Control Manager Module

7.1 Module

main

7.2 Uses

- **File Manager Module**: For file I/O operations
- **Alignment Module**: For sequence alignment
- **Sequence Data Structure Module**: For sequence handling
- **Substitution Matrix Module**: For matrix operations

7.3 Syntax

7.3.1 Exported Constants

None

7.3.2 Exported Access Programs

Name	In	Out	Exceptions
main	seq_data: SequenceData, matrix_bench: SubMat	list[dict]	AlignmentError

7.4 Semantics

7.4.1 State Variables

None

7.4.2 Environment Variables

None

7.4.3 Access Routine Semantics

main(seq_data, matrix_bench):

- **Input**: SequenceData instance and SubMat instance
- **Output**: List of dictionaries containing alignment results
- **Exception**: Raises AlignmentError if alignment fails

7.5 Workflow

The control flow follows this sequence:

1. Sequence data is loaded via SequenceData module
2. Substitution matrices are loaded via SubMat module
3. For each substitution matrix:
   (a) Alignment is performed via NeedlemanWunsch
   (b) Results are collected
4. Results are exported via FileManager

7.6 Considerations

- Acts as the system's main coordinator
- Stateless - maintains no internal state between runs
- Delegates all specialized operations to other modules
- Handles the sequencing of operations but not their implementation

8 MIS of Sequence Data Structure Module

8.1 Module

sequence_data_structure

```
ADT SequenceData:
    constructor(file_path: str) → None
    validate_sequence(seq: str) → None
    get_sequences() → tuple[str, str]
```

8.2 Uses

- **File Manager Module**: For loading sequence data from files

8.3 Syntax

8.3.1 Exported Constants

None

8.3.2 Exported Access Programs

Name	In	Out	Exceptions
`SequenceData`	read_file_path: str	SequenceData instance	ValueError
`validate_sequence`	seq: str	-	ValueError
`get_sequences`	-	tuple (str, str)	-

8.4 Semantics

8.4.1 State Variables

- `seq_a`: str (First nucleotide sequence: 5' to 3')
- `seq_b`: str (Second nucleotide sequence: 5' to 3')

8.4.2 Environment Variables

None

8.4.3 Assumptions

- Underscore (_) represents gap characters
- sequence files are provided in fasta format

8.4.4 Access Routine Semantics

SequenceData.__init__(read_file_path: str):

- Loads sequences via `read_sequence_file()`
- Validates sequences using `validate_sequence()`
- Stores `seq_a` and `seq_b`
- **Exception**: Raises `ValueError` for:
  - Invalid FASTA format
  - Unequal sequence counts

validate_sequence(seq: str):

- Checks sequence validity
- **Exception**: Raises `ValueError` if:
  - Contains non-{A,T,G,C,-} characters
  - Zero-length sequence

get_sequences() → (str,str):

- **Output**: Returns (`seq_a`:str, `seq_b`:str)

8.4.5 Local Functions

None

8.5 Considerations

- Case-sensitive for nucleotide characters
- No support for ambiguous bases (N, R, Y, etc.)
- Gap character (-) must be explicitly included
- Validation occurs during initialization

9 MIS of Substitution Matrix Module

9.1 Module

substitution_matrix

```
ADT SubMat:
    constructor(filepath) → None       # Loads/validates matrices
    validate_benchmark(matrices) → None
    get_matrix_names() → list[str]  # Returns matrix IDs
```

9.2 Uses

- **File Manager Module**: For loading matrix data from files

9.3 Syntax

9.3.1 Exported Constants

- **penalizingCostOf_**: A 4x4 matrix representing the baseline penalizing costs for nucleotide comparisons.

9.3.2 Exported Access Programs

Name	In	Out	Exceptions
get_substitution_matrix	name: str	submat: dict	InvalidMatrixError
validate_benchmark	benchmark: list[dict]	-	InvalidMatrixError
get_matrix_names	-	list[str]	-

9.4 Semantics

9.4.1 State Variables

- `data`: List of matrix dictionaries containing:
  - `NAME`: str (String identifier)
  - `PENALIZING_COSTS`: 4x4 float matrix

9.4.2 Environment Variables

None

9.4.3 Access Routine Semantics

get_substitution_matrix(name: str) → dict:

- Retrieves matrix dictionary by name from `data`
- **Output**: Dictionary with keys:
  - `NAME`: Matrix identifier
  - `PENALIZING_COSTS`: 4x4 scoring matrix

validate_benchmark(benchmark: list[dict]):

- **Exception**: Raises `InvalidMatrixError` if:
  - Any matrix is not 4x4
  - Contains non-numeric values

  Returns boolean indicating validity

get_matrix_names() → list[str]:

- **Output**: List of all loaded matrix names

9.4.4 Local Functions

None

10 MIS of File Manager Module

10.1 Module

file_manager

10.2 Uses

- **Software Hardware Module**: For interaction with I/O services
- **Control Manager Module**: For file management operations and file path information

10.3 Syntax

10.3.1 Exported Constants

- None

10.3.2 Exported Access Programs

Name	In	Out	Exceptions
read_sequence_file	file_path: str	tuple (str, str)	ValueError
read_submat_file	file_path: str	list[dict]	ValueError
export	data: list[dict], file_path: str	-	IOError

10.4 Semantics

10.4.1 State Variables

None

10.4.2 Environment Variables

None

10.4.3 Access Routine Semantics

read_sequence_file(file_path: str) → tuple:

- Reads and validates FASTA file
- **Output**: Tuple of two nucleotide sequences (str, str)
- **Exception**: Raises `ValueError` if:

  - Missing sequence headers
  - Invalid number of sequences
  - Zero-length sequences

read_submat_file(file_path: str) → list[dict]:

- Loads and validates substitution matrices
- **Output**: List of matrix dictionaries with:
  - `NAME`: String identifier
  - `PENALIZING_COSTS`: 4x4 numerical matrix
- **Exception**: Raises `ValueError` if:
  - Non-square matrices
  - Non-numeric values
  - Incomplete matrix data

export(data: list[dict], file_path: str):

- Writes benchmark results to CSV
- **Output**: None (creates file at specified path)
- **Exception**: Raises `IOError` if file cannot be written

10.4.4 Local Functions

None

10.5 Considerations

- UTF-8 encoding enforced for all text files
- CSV output includes headers: "matrix" and "score"
- Paths are resolved relative to user's designated directory

References

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