

DNATool

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Chapter 1

eda-lvl5-dnatool

- Fecha de entrega: 10/05/2022
- Grupo: 7
 - DALZOTTO, Rafael
 - HEIR, Alejandro Nahuel

22.08 - Algoritmos y Estructuras de Datos - Ingeniería Electrónica - ITBA

1.1 Respuestas

1.1.1 Mejores alineamientos para los mystery genomes:

- Mystery genome 1 - OV806939
 - Delta B.1.617.2 - OM202516
 - Puntaje óptimo: 29826
- Mystery genome 2 - MT345875
 - Beta B.1.351 - MZ314996
 - Puntaje óptimo: 29865
- Mystery genome 3 - OU772970
 - Delta B.1.617.2 - OM202516
 - Puntaje óptimo: 29840

Los alineamientos óptimos correspondientes se encuentra en `/resources/test/results/`

1.2 Bonus points

- La complejidad computacional del algoritmo Needleman-Wunsch es $O(mn)$ debido a que el calculo de las direcciones (o scores) de la matriz de alineacion depende de los largos de ambas secuencias
- Al cambiar los valores en el sistema de puntaje, cambia el puntaje final de alineamiento óptimo y tambien puede cambiar el alineamiento optimo en si
- Comparamos los genomas de SARS-CoV-2003 y MERS-CoV con Wuhan reference genome
 - Puntaje de MERS-CoV vs Wuhan reference genome: 7240
 - Puntaje de SARS-CoV-2003 vs Wuhan reference genome: 18645

Chapter 2

Class Index

2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

DirCell		
DirCell	contains 4 directions in a single byte	7
DirectionMat	8

Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

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Chapter 4

Class Documentation

4.1 DirCell Struct Reference

[DirCell](#) contains 4 directions in a single byte.

```
#include <DirectionMat.h>
```

Public Attributes

- `uint8_t d0`: 2
- `uint8_t d1`: 2
- `uint8_t d2`: 2
- `uint8_t d3`: 2

4.1.1 Detailed Description

[DirCell](#) contains 4 directions in a single byte.

4.1.2 Member Data Documentation

4.1.2.1 d0

```
uint8_t DirCell::d0
```

4.1.2.2 d1

```
uint8_t DirCell::d1
```

4.1.2.3 d2

```
uint8_t DirCell::d2
```

4.1.2.4 d3

```
uint8_t DirCell::d3
```

The documentation for this struct was generated from the following file:

- [DirectionMat.h](#)

4.2 DirectionMat Class Reference

```
#include <DirectionMat.h>
```

Public Member Functions

- [DirectionMat](#) (const size_t rows, const size_t cols)
Constructs a new Direction Mat object.
- [~DirectionMat](#) ()
Destroys the Direction Mat object.
- uint8_t [at](#) (size_t row, size_t col)
Reads a given DirectionMap cell.
- void [set](#) (uint8_t val, size_t row, size_t col)
Writes a given DirecitonMat cell.
- void [print](#) ()
Prints the given [DirectionMat](#), used for debugging.

Public Attributes

- const size_t [rows](#)
- const size_t [cols](#)

4.2.1 Constructor & Destructor Documentation

4.2.1.1 DirectionMat()

```
DirectionMat::DirectionMat (
    const size_t rows,
    const size_t cols )
```

Constructs a new Direction Mat object.

Parameters

<i>rows</i>	Total rows
<i>cols</i>	Total cols

4.2.1.2 ~DirectionMat()

```
DirectionMat::~~DirectionMat ( )
```

Destroys the Direction Mat object.

4.2.2 Member Function Documentation**4.2.2.1 at()**

```
uint8_t DirectionMat::at (
    size_t row,
    size_t col )
```

Reads a given DirectionMap cell.

Parameters

<i>row</i>	
<i>col</i>	

Returns

uint8_t

4.2.2.2 print()

```
void DirectionMat::print ( )
```

Prints the given [DirectionMat](#), used for debugging.

Parameters

<i>mat</i>	initialized DirectionMat
------------	--

4.2.2.3 set()

```
void DirectionMat::set (
    uint8_t val,
    size_t row,
    size_t col )
```

Writes a given DirecitonMat cell.

Parameters

<i>val</i>	Data to store
<i>row</i>	
<i>col</i>	

4.2.3 Member Data Documentation

4.2.3.1 cols

```
const size_t DirectionMat::cols
```

4.2.3.2 rows

```
const size_t DirectionMat::rows
```

The documentation for this class was generated from the following files:

- [DirectionMat.h](#)
- [DirectionMat.cpp](#)

Chapter 5

File Documentation

5.1 Aligner.cpp File Reference

Genetic sequence aligner, based on Needleman-Wunsch algorithm.

```
#include "Aligner.h"
#include <iostream>
#include <cstdlib>
#include <algorithm>
#include <vector>
```

Enumerations

- enum [Direction](#) { [VERTICAL](#) , [DIAGONAL](#) , [HORIZONTAL](#) }

Functions

- void [initMat](#) ([DirectionMat](#) &mat)
Initializes a [DirectionMat](#) for storing Needleman-Wunsch directions.
- int32_t [fillMat](#) ([DirectionMat](#) &mat, const string &seq1, const string &seq2)
Completes a [DirectionMat](#) based on two given genetic sequences.
- void [buildAlignment](#) ([DirectionMat](#) &mat, const string &seq1, const string &seq2, array< string, 3 > &output)
Builds the optimal alignment for two genetic sequences and an already filled [DirectionMat](#).
- int32_t [getGlobalAlignment](#) (const string &seq1, const string &seq2, array< string, 3 > &alignment)
Runs aligner for two acgt-like strings.

5.1.1 Detailed Description

Genetic sequence aligner, based on Needleman-Wunsch algorithm.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.1.2 Enumeration Type Documentation

5.1.2.1 Direction

enum [Direction](#)

Enumerator

VERTICAL	
DIAGONAL	
HORIZONTAL	

5.1.3 Function Documentation

5.1.3.1 buildAligment()

```
void buildAligment (
    DirectionMat & mat,
    const string & seq1,
    const string & seq2,
    array< string, 3 > & output )
```

Builds the optimal alignment for two genetic sequences and an already filled [DirectionMat](#).

Parameters

<i>mat</i>	
<i>seq1</i>	String with one acgt-like genetic sequence.
<i>seq2</i>	String with one acgt-like genetic sequence.
<i>output</i>	3-string array to store the optimal alignment.

5.1.3.2 fillMat()

```
int32_t fillMat (  
    DirectionMat & mat,  
    const string & seq1,  
    const string & seq2 )
```

Completes a [DirectionMat](#) based on two given genetic sequences.

Parameters

<i>mat</i>	
<i>seq1</i>	String with one acgt-like genetic sequence.
<i>seq2</i>	String with one acgt-like genetic sequence.

Returns

int32_t Optimal score

5.1.3.3 getGlobalAlignment()

```
int32_t getGlobalAlignment (  
    const string & seq1,  
    const string & seq2,  
    array< string, 3 > & alignment )
```

Runs aligner for two acgt-like strings.

Parameters

<i>seq1</i>	String with one acgt-like genetic sequence.
<i>seq2</i>	String with one acgt-like genetic sequence.
<i>alignment</i>	3-string array to store the optimal alignment.

Returns

int32_t Optimal alignment score

5.1.3.4 initMat()

```
void initMat (
    DirectionMat & mat )
```

Initializes a [DirectionMat](#) for storing Needleman-Wunsch directions.

Parameters

<i>rows</i>	
<i>cols</i>	

5.2 Aligner.h File Reference

Genetic sequence aligner, based on Needleman-Wunsch algorithm.

```
#include <string>
#include <array>
#include "DirectionMat.h"
```

Functions

- void [initMat](#) ([DirectionMat](#) &mat)
Initializes a [DirectionMat](#) for storing Needleman-Wunsch directions.
- int32_t [fillMat](#) ([DirectionMat](#) &mat, const std::string &seq1, const std::string &seq2)
- void [buildAlignment](#) ([DirectionMat](#) &mat, const std::string &seq1, const std::string &seq2, std::array< std::string, 3 > &output)
- int32_t [getGlobalAlignment](#) (const std::string &seq1, const std::string &seq2, std::array< std::string, 3 > &alignment)

5.2.1 Detailed Description

Genetic sequence aligner, based on Needleman-Wunsch algorithm.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.2.2 Function Documentation

5.2.2.1 buildAligment()

```
void buildAligment (
    DirectionMat & mat,
    const std::string & seq1,
    const std::string & seq2,
    std::array< std::string, 3 > & output )
```

5.2.2.2 fillMat()

```
int32_t fillMat (
    DirectionMat & mat,
    const std::string & seq1,
    const std::string & seq2 )
```

5.2.2.3 getGlobalAlignment()

```
int32_t getGlobalAlignment (
    const std::string & seq1,
    const std::string & seq2,
    std::array< std::string, 3 > & alignment )
```

5.2.2.4 initMat()

```
void initMat (
    DirectionMat & mat )
```

Initializes a [DirectionMat](#) for storing Needleman-Wunsch directions.

Parameters

<i>rows</i>	
<i>cols</i>	

5.3 Aligner.h

[Go to the documentation of this file.](#)

```
1
11 #ifndef ALIGNER_H
12 #define ALIGNER_H
13
14 #include <string>
15 #include <array>
16
17 #include "DirectionMat.h"
18
19 void initMat(DirectionMat &mat);
20
21 int32_t fillMat(DirectionMat &mat, const std::string &seq1, const std::string &seq2);
22
23 void buildAlignent(DirectionMat &mat, const std::string &seq1, const std::string &seq2,
24                  std::array<std::string, 3> &output);
25
26 int32_t getGlobalAlignment(const std::string &seq1, const std::string &seq2,
27                          std::array<std::string, 3> &alignment);
28
29 #endif
```

5.4 DirectionMat.cpp File Reference

Implements 2 bit-size matrix cells.

```
#include "DirectionMat.h"
```

5.4.1 Detailed Description

Implements 2 bit-size matrix cells.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.5 DirectionMat.h File Reference

Implements 2 bit-size matrix cells optimized for memory usage.

```
#include <iostream>
```

Classes

- struct [DirCell](#)
DirCell contains 4 directions in a single byte.
- class [DirectionMat](#)

5.5.1 Detailed Description

Implements 2 bit-size matrix cells optimized for memory usage.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.6 DirectionMat.h

[Go to the documentation of this file.](#)

```
1
11 #ifndef DIRECTIONMAT_H
12 #define DIRECTIONMAT_H
13
14 #include <iostream>
15
16 typedef struct
17 {
18     uint8_t d0 : 2;
19     uint8_t d1 : 2;
20     uint8_t d2 : 2;
21     uint8_t d3 : 2;
22 } DirCell;
23
24 class DirectionMat
25 {
26 public:
27     DirectionMat(const size_t rows, const size_t cols);
28     ~DirectionMat();
29
30     uint8_t at(size_t row, size_t col);
31     void set(uint8_t val, size_t row, size_t col);
32     void print();
33
34     const size_t rows;
35     const size_t cols;
36
37 private:
38     DirCell *data;
39     size_t compactCols;
40 };
41
42 #endif
```

5.7 GBReader.cpp File Reference

Sequence extractor for GenBank-like files.

```
#include "GBReader.h"  
#include <algorithm>
```

Functions

- bool [isNotACGT](#) (char c)
Checks if a given character is not 'a', 'c', 'g' or 't'.
- bool [getSequence](#) (string &output, istream &file)
Extracts an acgt-like string from a GenBank file.

5.7.1 Detailed Description

Sequence extractor for GenBank-like files.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.7.2 Function Documentation

5.7.2.1 [getSequence\(\)](#)

```
bool getSequence (  
    string & output,  
    istream & file )
```

Extracts an acgt-like string from a GenBank file.

Parameters

<i>output</i>	String to store the acgt sequence
<i>file</i>	istream file handler.

Returns

true Success
false Failure

5.7.2.2 isNotACGT()

```
bool isNotACGT (
    char c )
```

Checks if a given character is not 'a', 'c', 'g' or 't'.

Parameters

<i>c</i>	
----------	--

Returns

true It's not
false It is

5.8 GBReader.h File Reference

Sequence extractor for GenBank-like files.

```
#include <iostream>
```

Functions

- bool [getSequence](#) (std::string &output, std::istream &file)

5.8.1 Detailed Description

Sequence extractor for GenBank-like files.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.8.2 Function Documentation

5.8.2.1 getSequence()

```
bool getSequence (
    std::string & output,
    std::istream & file )
```

5.9 GBReader.h

[Go to the documentation of this file.](#)

```
1
12 #ifndef GBREADER_H
13 #define GBREADER_H
14
15 #include <iostream>
16
17 bool getSequence(std::string &output, std::istream &file);
18
19 #endif
```

5.10 main.cpp File Reference

Runs the genetic sequence aligner.

```
#include <iostream>
#include <fstream>
#include <chrono>
#include "GBReader.h"
#include "Aligner.h"
```

Functions

- void [printElapsedFrom](#) (time_point< steady_clock > ×tamp)
- int [main](#) (int argc, char **argv)

5.10.1 Detailed Description

Runs the genetic sequence aligner.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.10.2 Function Documentation

5.10.2.1 main()

```
int main (
    int argc,
    char ** argv )
```

5.10.2.2 printElapsedFrom()

```
void printElapsedFrom (
    time_point< steady_clock > & timestamp )
```

5.11 main_test.cpp File Reference

Tests for the genetic sequence aligner.

```
#include <iostream>
#include <string>
#include <array>
#include <fstream>
#include <sstream>
#include "GBReader.h"
#include "Aligner.h"
```

Functions

- bool `testMatInit` (`DirectionMat` &mat, `DirectionMat` &expectedMat)
- bool `testFillMat` (`DirectionMat` &mat, const string &s1, const string &s2, int32_t expectedScore, `DirectionMat` &expectedMat)
- bool `testAlignment` (`DirectionMat` &mat, const string &s1, const string &s2, array< string, 3 > &expectedAlignment)
- int `main` ()

5.11.1 Detailed Description

Tests for the genetic sequence aligner.

Authors

DALZOTTO, Rafael; HEIR, Alejandro - Grupo 7

Version

0.1

Date

2022-05-08

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5.11.2 Function Documentation

5.11.2.1 `main()`

```
int main ( )
```

5.11.2.2 `testAlignment()`

```
bool testAlignment (
    DirectionMat & mat,
    const string & s1,
    const string & s2,
    array< string, 3 > & expectedAlignment )
```

5.11.2.3 testFillMat()

```
bool testFillMat (
    DirectionMat & mat,
    const string & s1,
    const string & s2,
    int32_t expectedScore,
    DirectionMat & expectedMat )
```

5.11.2.4 testMatInit()

```
bool testMatInit (
    DirectionMat & mat,
    DirectionMat & expectedMat )
```

5.12 README.md File Reference

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