

DNATool

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Chapter 1

eda-lvl5-dnatool README

- 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
 - Wuhan reference genome - NC_045512.2
 - Puntaje óptimo: 29885
- 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.

Sin embargo logramos reducir sustancialmente el uso de memoria, gracias a aprovechar cada bit en los elementos de la matriz de direcciones ([DirectionMat](#)) y debido a que no usamos una matriz de scores, resultando en un uso de memoria de no mas de 250 MB para comparar dos secuencias de unos 30000 pares de base (resultados experimentales). En cambio al usar una matriz de scores de `int32_t`, el uso de memoria se eleva a mas de 3 GB.

- 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
 - Los alineamientos óptimos correspondientes se encuentran en `/resources/test/results/`

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 )
```

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