Bilkent University

CS481 | cs583 - Bioinformatics Algorithms

Fall 2022

Homework Assignment #3

General Instructions

FAILURE TO FULFILL ANY OF THE FOLLOWING ITEMS WILL RESULT IN A GRADE SCORE OF \circ (zero) WITHOUT ANY CHANCE OF REDEMPTION.

- You must **write your code yourself**. Sufficient evidence of plagiarism will be treated the same as for plagiarism or cheating.
- **C / C++, Python or Java** will be used as programming language. STL is allowed. The assignments are created with C / C++ in mind, so using other languages would require minimum tweaking.
- Your code must **compile**.
- · Your code must be complete.
- Your code must run on dijkstra.cs.bilkent.edu.tr server.
- Your code must make use of argument parsing.
 Refer to: https://docs.google.com/presentation/d/1rU0DhBg6yVXbfEtNuK73pjc1yWSPG90YnGNH-b-kklQ
- Submit your answers **ONLY** through the Moodle page.
- Zip your files and send them in only one zipped file.
- File name format surname_name_hw#.zip.
- The zip file must contain the following items:
 - All the source files.
 - Makefile to compile the source code and produce the binary. Even if you use Python, include this Makefile.
 - A README.txt file that briefly describes how your program works.
- All submissions must be made **strictly before the stipulated deadline**.
- A **bonus** will be given for the fastest code that solves the assignment successfully.

1) MULTIPLE SEQUENCE ALIGNMENT

Aim: In this assignment, you will learn about multiple sequence alignment using pair-wise alignment and center-star alignment.

1.1 Data

- · Input
 - 1. A FASTA file containing **MULTIPLE**, **MULTILINE** sequences. The file is given using the -i switch.

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2. The scoring function for the match, mismatch and gap penalties. The scores are given using the -s switch, separated by ":".

Output

1. A text file containing multiple sequence alignment in PHYLYP format (http://scikit-bio.org/docs/0.2.3/generated/skbio.io.phylip.html. Given by the switch -o.

1.2 Tasks

Perform Multiple Sequence Alignment using Center-Star Algorithm. The sequences to be aligned are in the input FASTA file. Save the alignment output as PHYLIP format in an output file.

2) EXAMPLE 1

The numbers presented in the example are not necessarily correct. They just show how the program should output the information.

2.1 Input

```
user@dijkstra$ cat input.fasta
> S1_____a

MPE

> S2____b

MKE

> S3__c

MSKE

> S4____d

SKE
```

2.2 Execution

```
user@dijkstra$ ./hw3 -i input.fasta -o output.phy -s 1:-1:-5
```

2.3 Output

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3) EXAMPLE 2

The numbers presented in the example are not necessarily correct. They just show how the program should output the information.

3.1 Input

```
user@dijkstra$ cat input.fasta
   >gi|3212
2
   \tt MGIKGLTGLLSENAPKCMKDHEMKTLFGRKVAIDASMSIYQFLIAVRQQDGQMLMNESGDVTSHLMGFFY
   RTIRMVDHGIKPCYIFDGKPPELKGSVLAKRFARREEAKEGEEEAKETGTAEDVDKLARRQVRVTREHNE
   ECKKLLSLMGIPVVTAPGEAEAQCAELARAGKVYAAGSEDMDTLTFHSPILLRHLTFSEAKKMPISEIHL
   DVALRDLEMSMDQFIELCILLGCDYLEPCKGIGPKTALKLMREHGTLGKVVEHIRGKMAEKAEEIKAAAD
   EEAEAEAEAEKYDSDPENEEGGETMINSDGEEVPAPSKPKSPKKKAPAKKKKIASSGMQIPEFWPWEEAK
   OLFLKPDVVNGDDLVLEWKOPDTEGLVEFLCRDKGFNEDRVRAGAAKLSKMLAAKOOGRLDGFFTVKPKE
   PAAKDAGKGKGKDTKGEKRKAEEKGAAKKKTKK
   >gi|3211
10
   MGIKGLTQVIGDTAPTAIKENEIKNYFGRKVAIDASMSIYQFLIAVRSEGAMLTSADGETTSHLMGIFYR
   TIRMVDNGIKPVYVFDGKPPDMKGGELTKRAEKREEASKQLVLATDAGDAVEMEKMNKRLVKVNKGHTDE
12
   CKOLLTLMGIPYVEAPCEAEAQCAALVKAGKVYATATEDMDSLTFGSNVLLRYLTYSEAKKMPIKEFHLD
13
   KILDGLSYTMDEFIDLCIMLGCDYCDTIKGIGAKRAKELIDKHRCIEKVIENLDTKKYTVPENWPYQEAR
   RLFKTPDVADAETLDLKWTQPDEEGLVKFMCGDKNFNEERIRSGAKKLCKAKTGQTQGRLDSFFKVLPSS
15
   KPSTPSTPASKRKVGCIIYLFLYF
```

3.2 Execution

```
user@dijkstra$ ./hw3 -i input.fasta -o output.phy -s 1:-1:-5
```

3.3 Output

```
user@dijkstra$ cat output.phy
        2
             454
              MGIKGLTGLL SENAPKCMKD HEMKTLFGRK VAIDASMSIY QFLIAVRQQD
   gi | 3211
   gi|3212
              MGIKGLTQVI GDTAPTAIKE NEIKNYFGRK VAIDASMSIY QFLIAVRSE-
              GQMLMNESGD VTSHLMGFFY RTIRMVDHGI KPCYIFDGKP PELKGSVLAK
              GAMLTSADGE TTSHLMGIFY RTIRMVDNGI KPVYVFDGKP PDMKGGELTK
8
              RFARREEAKE GEEEAKETGT AEDVDKLARR QVRVTREHNE ECKKLLSLMG
9
              RAEKREEASK OLVLATDAGD AVEMEKMNKR LVKVNKGHTD ECKOLLTLMG
10
11
              IPVVTAPGEA EAQCAELARA GKVYAAGSED MDTLTFHSPI LLRHLTFSEA
12
              IPYVEAPCEA EAQCAALVKA GKVYATATED MDSLTFGSNV LLRYLTYSEA
13
14
              KKMPTSETHI, DVALRDLEMS MDQFTELCTI, LGCDYLEPCK GTGPKTALKI.
15
              KKMPIKEFHL DKILDGLSYT MDEFIDLCIM LGCDYCDTIK GIGAKRAKEL
16
17
              MREHGTLGKV VEHIRGKMAE KAEEIKAAAD EEAEAEAE KYDSDPENEE
18
              IDKHRCIEKV IENL ----- ------ KY-TVPEN --
19
20
              GGETMINSDG EEVPAPSKPK SPKKKAPAKK KKIASSGMQI PEFWPWEEAK
21
22
23
              QLFLKPDVVN GDDLVLEWKQ PDTEGLVEFL CRDKGFNEDR VRAGAAKLSK
24
              RLFKTPDVAD AETLDLKWTQ PDEEGLVKFM CGDKNFNEER IRSGAKKLCK
25
              MLAAKQQGRL DGFFTVKPKE PAAKDAGKGK GKDTKGEKRK AEEKGAAKKK
27
              AKTGQTQGRL DSFFKVLP-- -SSKPS---- TPSTPASKRK V---GCIIYL
28
              TKK-
30
              FI.YF
```