

# Median String and Motif Finding

Using L-mer tree bypassing (Assignment 3 – 291T)

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## Description

This application will find top 5 best median strings in a given file by using Branch and Bound algorithm in which it will bypass visiting few nodes. Later, the application will find the best matching location and score in each of the DNA sequences. Furthermore, it will calculate the consensus string and its score. Lastly, it will print the number of nodes skipped by subtracting number of nodes visited from the total number of nodes ( $4^6 = 4096$ ).

## Application specifications

**Programming language:** JAVA

**Other required installations:** JRE 1.8 to run the application,  
JDK 1.8 to compile the application.

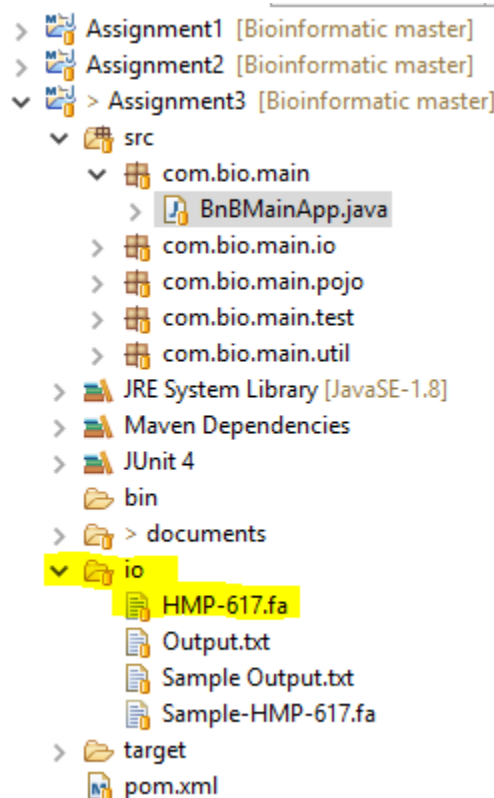
**Version Control:** Git (GitHub) - <https://github.com/momazia/Bioinformatic/tree/master/Assignment3>

**IDE:** Eclipse (Mars 4.5.1)

**Build automation tool:** Maven (Refer to /Assignment3/pom.xml for the list of the libraries used)

## How to execute the program?

In order to run the application, please put the DNA sequence file under /Assignment3/io and point the following constant `com.bio.main.BnBMainApp.DNA_FILE` to the file.



## Output

Median String: GAAAAA (tot\_dist = 309)

Motif consensus string: GAAAAA (consensus\_score = 3393)

Motif positions/string s=(s1..st):

194 (GAAAAA), 962 (GAAAAA), 4 (GCAGAA), 210 (GAAAAA), 35 (GAAAAA), 5 (GTATAA), 482 (GAAAAA), 72 (GAAAAA), 46 (GAAAAA), 12 (GAAAAA), 6 (GAGAAA), 203 (GAAAAA), 80 (GGTAAA), 210 (GAAAAA), 35 (GAAAAA), 170 (GAATAA), 12 (GAAAAA), 46 (GAAAAA), 4 (GAACAA), 408 (GAAAAA), 165 (GAAAAA), 662 (GAAAAA), 819 (GAAAAA), 69 (GAGAAA), 66 (GAGAAA), 313 (GAAAAA), 162 (GAAATA), 473 (TAAAAA), 7 (GAACAA), 2 (GAGTAA), 300 (GAAAAA), 881 (GAAAAA), 216 (GAAAAA), 322 (GAAAAA), 158 (GATAAA), 189 (GAAAAA), 14 (GAAAAA), 140 (GCAAAA), 69 (GAAGAA), 28 (GAAATA), 137 (GCAAAA), 139 (GAAAAA), 2 (GAAAAA), 1085 (GAAAAA), 2 (GAAACA), 479 (GAATAA), 42 (GAAAT), 579 (GAAAAA), 28 (GAAAT), 75 (GAAATA), 2 (GAAAAA), 44 (GACAAA), 2 (GAAGAA), 2 (GAAAAA), 2 (GAAAT), 247 (GAAAAA), 522 (GAAAG), 19 (GAGAAA), 3 (GAAAAA), 317 (GAAAAA), 84 (GCAAAA), 818 (GAAAAA), 34 (CAAAAA), 357 (GAAAAA), 678 (GAAAAA), 210 (GAAAAA), 23 (GCAAAA), 23 (GAAAAA), 125 (GAAAAA), 115 (GCAAAA), 1014 (GAAAAA), 2 (GAACAA), 159 (GAAAAA), 3 (GAAAAA), 317 (GAAAAA), 54 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**Median String: CTGGCG (tot\_dist = 348)**

**Motif consensus string: CTGGCG (consensus\_score = 3354)**

**Motif positions/string s=(s1..st):**

475 (CTGGCG), 525 (CTGGCG), 114 (CTGGCA), 60 (CTGGGG), 19 (CGGGCG), 17 (CAGGCG), 133 (TTGACG), 37 (CTGACG), 94 (CTGGCA), 66 (CTGGAG), 25 (CTAGCG), 564 (CTTGCG), 25 (CTGCCG), 171 (CTGTCT), 19 (CGGGCG), 66 (CTGGCG), 66 (CTGGAG), 27 (CAGGGG), 241 (ATGGCG), 173 (CTGGTG), 69 (CTGGCG), 128 (CTGGGG), 64 (GTGGCG), 40 (CTGCCG), 188 (CTGGCG), 349 (CTGGCA), 42 (CTTGCA), 80 (CTGGGG), 155 (CTGGCA), 36 (CTGGGG), 135 (CTGGCC), 663 (CTGGCG), 71 (CTGGCA), 281 (CTGGCG), 13 (CTGCCG), 1158 (CTGGCG), 20 (CTGGCT), 81 (CTGGTG), 27 (CTGCCG), 176 (CTGGCC), 54 (CTGGGG), 126 (CTGCCG), 414 (CTGGCG), 84 (CTGGCG), 151 (CCGGCG), 180 (CTGGCG), 0 (GTGGCG), 780 (CTGGCG), 298 (CCGGCG), 62 (TTTGCG), 423 (CTGGCG), 66 (CTGGCG), 60 (CTGGCC), 21 (CTGGCG), 94 (GTGGCG), 725 (CTGGCG), 72 (CTGGCG), 26 (GTGCCG), 221 (CTGGCG), 146 (CTGGCT), 161 (CTGGCG), 600 (CTGGCG), 48 (CTGGCA), 1385 (CTGGCG), 1610 (CTGGCG), 202 (CTGGCG), 72 (ATGGTG), 43 (CTGGCG), 21 (CTGGCG), 21 (CTGGCA), 149 (CTGGCG), 78 (CTGGAG), 137 (CTGGGG), 18 (CTGGTG), 146 (CTGGCT), 169 (CTGGCC), 447 (CTGGGG), 162 (CTGGGG), 40 (CTGGCT), 1434 (CTGGCG), 9 (CTGTCT), 453 (CTGACG), 67 (CTGTCT), 22 (CAGGCG), 33 (TTGACG), 54 (CTGGCT), 0 (GTGGCG), 114 (CTGGGG), 593 (CTGGCG), 445 (CTGACG), 261 (CTGGAG), 357 (CAGGCG), 51 (CTGGCT), 140 (CTGGCA), 11 (CTTTCT), 87 (CTGGTG), 128 (CTGGCA), 206 (CTGGCG), 258 (CTGGCG), 309 (CTGGCT), 987 (CTGGCG), 73 (ATGGCG), 120 (CTGGCG), 33 (CTGTCT), 135 (CTTGCG), 121 (CTGGGG), 12 (ATGGTG), 431 (CTGGCG), 936 (CTGGCG), 9 (CTGGCT), 202 (CTGGCG), 53 (CTGGTG), 168 (CTGGCG), 127 (CTGGCG), 36 (GTGGCG), 153 (CTGGCG), 57 (CTGGCG), 111 (CTGGCG), 116 (CTGGAG), 126 (GTGGCG), 41 (CTGGCG), 81 (CCGGCG), 27 (CTCGCG), 551 (CTGGCG), 132 (CTGGCG), 11 (CAGGCG), 42 (CTGGCG), 119 (CTGGCG), 206 (CTGGCG), 87 (CTGGCG), 222 (CTGGCG), 102 (CTGGCG), 79 (CTGGCG), 75 (CAGGCG), 18 (CTGGCA), 81 (CCGGCG), 171 (CTGGGG), 6 (CTGGCT), 20 (CTGGCA), 73 (CTGGCA), 67 (CTGATG), 48 (CTGGCT), 13 (CTGATG), 25 (GTGTCT), 111 (CTGGTG), 278 (CTGGCG), 120 (CTGGAG), 184 (CTGGCG), 273 (CTGGCA), 195 (CTGGCT), 549 (CTGGCG), 28 (CTGCCG), 33 (CAGGCG), 30 (CTGGCG), 968 (CTGGCG), 56 (CTGGGG), 22 (CTGCCG), 300 (CTGCCG), 24 (CTGGCT), 98 (CTGGCA), 189 (CTGGCG), 15 (CTGACG), 63 (CTGGCG), 633 (CTGGCG), 118 (CTGGTG), 42 (CTGGGG), 514 (CTGGCG), 180 (CTGGCG), 924 (CTGGCG), 506 (CTGGCG), 108 (CTGGCG), 126 (CTGGCG), 38 (CTGGTG), 82 (CCGGCG), 51 (CCGGCG), 0 (ATGTCT), 56 (TTGGCG), 41 (CTGGAG), 230 (ATGGCG), 24 (CTGGCC), 48 (CTGACG), 57 (CAGGCA), 102 (CTGGCG), 119 (CTGGCG), 567 (CTGGCG), 304 (CTGGGG), 60 (CAGGCT), 67 (CTGGCA), 317 (CTGGCG), 233 (CTGGCG), 93 (CTGGCG), 45 (CAGGCT),

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**Motif consensus string: CTGGAA (consensus\_score = 3349)**

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**Motif consensus string: TGCTGG (consensus\_score = 3349)**  
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 52 (TGCTGG), 35 (TGCTGC), 124 (TGCTGG), 58 (TGCTGC), 118 (TGCTGG), 37 (TGTTGG), 506 (TGCTGG), 40 (CGCTGG),  
 30 (TGTTGG), 61 (GGCTGG), 49 (TGCTGG), 136 (TGCTGA), 1 (TGATGA), 368 (TGCTGG), 304 (TGCTGG), 88 (TGCTGA),  
 206 (TGCTGA), 112 (TGCTGG), 280 (TGCTGG), 132 (TACTGG), 12 (TGCCGG), 712 (TGCTGG), 92 (TGCTGC),  
 123 (TGCTGG), 127 (TGCTGG), 65 (TGTTGG), 46 (TGGTGG), 17 (TGATGG), 137 (TACTGG), 1039 (TGCTGG),  
 223 (TGCTGG), 202 (TGCTGG), 15 (TGCTGT), 291 (TGCTGG), 166 (GGCTGG), 397 (TGCTGG), 8 (TGCAGG), 67 (TGCTGG),  
 55 (TGCTGG), 3 (TGCTGC), 109 (CGCTGG), 34 (TGCTGG), 148 (TCCTGG), 190 (TGCTGG), 235 (TGCTGG), 59 (TGCTGA),  
 85 (TGCTGG), 262 (TGCTGG), 55 (TGCAGG), 94 (TGCTGA), 388 (TGCTGG), 59 (TGCAGG), 71 (TGCCGG), 354 (TACTGG),  
 61 (TGCCGG), 580 (TGCTGG), 60 (TGCCGG), 6 (GGCTGG), 21 (TGCCGG), 622 (TGCTGG), 37 (AGCTGG), 274 (TGCTTG),  
 624 (TGCTGG), 175 (TGCTGG), 46 (TGCAGG), 53 (TGTTGG), 254 (TGCTTG), 112 (TGCTGG), 89 (TGCTGT),  
 129 (TGGTGG), 39 (CGCTGT), 39 (TGGTGG), 1646 (TGCTGG), 142 (TGCTGG), 142 (TGCTGA), 27 (TGCCGG),  
 483 (TGCTGG), 114 (TGCTGC), 102 (TGCTGT), 72 (TGCCGG), 302 (TGCTGG), 200 (TGCTGG), 5 (TGCTGA), 31 (TCCTGG),  
 476 (TGCTGG), 28 (TGCTCG), 157 (TGCTGG), 325 (TGCTGG), 15 (TTCTGG), 238 (TTCTGG), 41 (TACTGG), 17 (TGCCGG),  
 58 (TCCTGG), 41 (TGCTGT), 43 (CGCTGG), 1007 (TGCTGG), 514 (TGCTGG), 131 (TGCCGG), 127 (TTCTGG),  
 100 (TGCTGG), 236 (TGCTGA), 335 (TGATGG), 389 (TGCTGA), 28 (AGCTGG), 410 (TGCTGG), 131 (TGCTGG),  
 39 (TGGTGT), 3 (TACTGG), 31 (TACTGG), 43 (TGCTGT), 112 (TGCTTG), 156 (TGCTGT), 40 (TGTTGG), 56 (TGCCGG),  
 460 (TGCTGG), 201 (TGCTGG), 655 (TGCTGG), 40 (TTCTGG), 1 (TGCTGA), 568 (TGCTGG), 362 (TGCTGG),  
 502 (TGCTGG), 155 (TGCTGG), 197 (TGCTGG), 46 (TGCTGT), 76 (TGCTGG), 212 (TGCTGC), 1 (TGCTGA), 418 (TGCTGG),  
 241 (TGCTGG), 227 (TGCCGG), 195 (TACTGG), 56 (TGATGT), 119 (AGCTGG), 3 (TGCCGG), 685 (TGCTGG), 82 (TGCTGG),  
 454 (TGCTGG), 418 (TGCTGG), 10 (TGTTGG), 895 (TGCTGG), 415 (TGCTGG), 1 (TGCATG), 1 (TGCATG), 847 (TGCTGG),  
 1289 (TGCTGG), 40 (TGTTGG), 52 (TGATGG), 418 (TGATGG), 62 (TGCAGG), 246 (TGCTGG), 83 (TGCCGG),  
 1003 (TGCTGG), 711 (TGCTGG), 394 (TGCTGG), 49 (TGCCGG), 760 (TGCTGG), 103 (TGCTGG), 169 (TGCTGG),  
 499 (TGCTGG), 298 (TGCTGG), 463 (TTCTGG), 184 (TGCTGG), 133 (TGTTGG), 446 (TGCAGG), 454 (TGCTGG),  
 109 (TGCTGG), 1357 (TGCTGG), 625 (TGCTGG), 224 (TGCTGG), 502 (TGCTGG), 520 (TGCTGG), 538 (TGCTGG),  
 565 (TGCTGG), 757 (TGCTGG), 301 (TGCTGG), 448 (TGCTGG), 10 (TGCTGG), 121 (TGCTGA), 427 (TGCTGG),  
 235 (TGCTGG), 250 (TGCTGG), 55 (TGCTGG), 220 (TGCTGG), 550 (TGCTGG), 76 (TGCTGG), 94 (CGCTGG), 52 (TGCCGG),

11 (TGCTGT), 559 (TGCTGG), 38 (TAATGG), 211 (TGCTGG), 259 (TGCTGG), 17 (ACCTGG), 170 (TGCTGG),  
 325 (TGCTGG), 31 (TGCTGG), 211 (TGCTGG), 154 (TGCTGG), 376 (TGCTGG), 1063 (TGCTGG), 310 (TGCTGG),  
 466 (TGCTGG), 373 (TGCTGG), 496 (TGCTGG), 331 (TGCTGG), 775 (TGCTGG), 538 (TGCTGG), 701 (TGCTGG),  
 532 (TGCTGG), 242 (TGCTGC), 265 (TGCTGG), 175 (TGCTGG), 249 (TTCTGG), 33 (TGCGGG), 511 (TGCTGG),  
 340 (TGCTGG), 464 (TGCTGG), 247 (TGCTGG), 49 (TGCTGG), 34 (TGATGG), 43 (TGCTGG), 88 (TGCTGG), 19 (TACTGG),  
 161 (TGCTGG), 253 (CGCTGG), 854 (TGCTGG), 458 (TGCTGG), 532 (TGCTGG), 25 (TGCTGG), 265 (TGCTGG),  
 112 (TGCTTG), 238 (TTCTGG), 142 (CGCTGG), 160 (TGATGG), 217 (TGCTGG), 2131 (TGCTGG), 121 (TGCTGG),  
 49 (TGCTGG), 667 (TGCTGG), 283 (TGCTGG), 46 (TACTGG), 25 (TGCTGA), 13 (TGCTGC), 399 (TGCTGG), 349 (TGCTGG),  
 121 (TGCTGG), 62 (TGCTGG), 80 (CGCTGG), 257 (TGCGGG), 34 (TGATGG), 64 (TGCTGT), 163 (TGCTTG), 37 (TGCTGG),  
 43 (CGCTGG), 997 (TGCTGG), 121 (TGCAGG), 50 (CGCTGG), 370 (TGCAGG), 301 (AGCTGG), 166 (TGCTGG),  
 379 (TGCTGG), 55 (CGCTGG), 472 (TGCTGG), 478 (TGCTGG), 145 (TGCTGG), 34 (TGCTGG), 187 (TGCTGG),  
 262 (TGCTGG), 22 (CGCTGG), 229 (TGCTGG), 415 (TGCTGG), 43 (TGCTGC), 277 (TGCTGG), 1369 (TGCTGG),  
 154 (TGCTGG), 176 (TGATGG), 109 (TGCTGG), 445 (TGCTGG), 70 (TGCTGG), 32 (GGCTGG), 302 (TGCTGG),  
 241 (TGCTGG), 106 (TGCTGG), 311 (TGCTGG), 84 (CGCTGG), 109 (TGCTGG), 214 (TGCTGG), 31 (TGCTGT),  
 20 (TGCAGG), 56 (TGATGG), 85 (TGCTGG), 230 (TGCTGG), 550 (TGCTGG), 262 (TGCTGG), 226 (TGCTGG),  
 868 (TGCTGG), 1102 (TGCTGG), 1 (TGCTGG), 328 (TGCTGG), 73 (TGCTGA), 76 (CGCTGG), 130 (TGCTGG),  
 197 (TGATGG), 52 (TGATGG), 224 (TGCTGG), 168 (GGCTGG), 208 (TGCTGT), 634 (TGCTGG), 207 (GGCTGG),  
 1 (TGCGTG), 341 (TGCTGG), 22 (TGCTGG), 157 (TGCTGG), 457 (TGCTGG), 340 (TGCTGG), 118 (AGCTGG), 11 (TGCCGG),  
 232 (TGCTGG), 700 (TGCTGG), 193 (TGGTGG), 42 (CGCTGG), 47 (TCCTGG), 166 (GGCTGG), 43 (TGCTTG), 2 (GGCTGG),  
 211 (TGCTGG), 253 (TGCTGG), 115 (TGCTGG), 43 (TGCTGG), 169 (TGCTGG), 271 (TGCTGG), 346 (TGCTGG),  
 163 (TGCTGG), 238 (TGCTGG), 1051 (TGCTGG), 577 (TGCTGG), 61 (TGCTGG), 150 (TGCCGG), 484 (TGCTGG),  
 55 (TGCAGG), 355 (TGCTGG), 11 (TACAGG), 85 (TGCTGA), 115 (TGCTGG), 1215 (TGCTGG), 3337 (TGCTGG),  
 1 (TGCTTC), 16 (TGCTTG), 103 (TTCTGG), 6 (TTCAGG), 406 (TGCTGG), 280 (TGCTGG), 398 (TGATGG), 152 (TGCTGG),  
 343 (TGCTGG), 402 (TGCTGG), 61 (TGCTGG), 21 (TACTCG), 64 (TACTGG), 51 (TGCTTG), 160 (CGCTGG), 229 (TGATGG),  
 484 (TGCTGG), 406 (TGCTGG), 1042 (TGCTGG), 141 (CGCTGG), 185 (TGTTGG), 58 (CGCTGG), 688 (TGCTGG),  
 133 (TACTGG), 1045 (TGCTGG), 156 (TTCTGG), 28 (TGATGG), 220 (TGCTGG), 1 (TGCTGG), 68 (TGCTGG), 80 (TGCAGG),  
 860 (TGCTGG), 30 (TGCGGG), 373 (TGCTGG), 151 (TGCTGG), 124 (TGCTGA), 115 (TGCTGG), 253 (TGCTGG),  
 265 (TTCTGG), 418 (TGCTGG), 154 (TTCTGG), 61 (CGCTGG), 16 (TGCTGG), 884 (TGCTGG), 93 (TTCTGG),  
 163 (GGCTGG), 89 (TGCTGT), 124 (TGCTGG), 91 (TGGTGG), 193 (TGCTGG), 46 (TGCTTG), 228 (TGCTGG), 65 (TGCTGT),  
 67 (TACTGG), 334 (TGCCGG), 68 (TGCTGG), 28 (CGCTGG), 34 (TGATGG), 115 (TGCCGG), 170 (TGCCGG),  
**Number of leafs visited: 1728**  
**Number of leafs skipped: 2368**

## Source code

/Assignment3/src/com/bio/main/BnBMainApp.java

```
package com.bio.main;

import java.io.IOException;
import java.util.List;

import com.bio.main.io.FileProcessor;
import com.bio.main.pojo.Median;
import com.bio.main.pojo.Motif;
import com.bio.main.pojo.Sequence;
import com.bio.main.util.BnBMainUtil;
import com.bio.main.util.MotifUtil;

/**
 * The main application to be executed in order to find top best median strings, motif consensus
 * strings and their scores, locations and each of the tiles in a given
 *
 * DNA sequence and number of leafs visited in BnB approach and how many were skipped. <br>
 *
 * In order to execute the program, put the DNA sequence file under "/Assignment3/io" and run this
 * application. <br>
 *
 * <b>Configurations:</b> <br>
 *
 * 1. DNA_FILE = Name of the file in "/Assignment3/io" folder to read the DNA sequences from <br>
 *
 * 2. K = 4 since there are 4 letters in TGCA.<br>
 *
 * 3. L_MER = 6 in this assignment.
 *
 *
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class BnBMainApp {

    /**
     * Location of DNA sequence file
     */
}
```

```

private static final String DNA_FILE = "HMP-617.fa";

/**
 * In case of DNA (TGCA), always 4
 */
private static final int K = 4;

/**
 * Lmer is 6 according to the assignment 3 requirements.
 */
private static final int L_MER = 6;

/**
 * Main method to run the application.
 *
 * @param args
 */
public static void main(String[] args) {

    try {

        // Reading the DNA sequences from the file
        List<Sequence> sequences =
FileProcessor.getInstance().readSequences(DNA_FILE);

        // Finding medians search using BnB and keeping the top best medians.
        BnBMainUtil mp = new BnBMainUtil(sequences, L_MER, K);
        List<Median> medians = mp.medianSearch();

        // Finding the motifs in the sequences given for the medians found earlier.
        MotifUtil.getInstance().findMotifs(medians, sequences, L_MER);

        // Calculating consensus string and score
        MotifUtil.getInstance().calculateConsensus(medians, L_MER);

        // Prints the result
        print(mp, medians);
    }
}

```

```

        } catch (IOException e) {
            System.out.println("Cannot read the file: " + e.getMessage());
        }

    }

    /**
     * Prints the result according the format given in assignment 3.
     *
     * @param mp
     * @param medians
     */
    private static void print(BnBMainUtil mp, List<Median> medians) {
        for (Median median : medians) {
            System.out.println("Median String: " + median.getStr() + " (tot_dist = " +
median.getTotalDistance() + ")");
            System.out.println("Motif consensus string: " + median.getConsensusStr() + "
(consensus_score = " + median.getConsensusScore() + ")");
            System.out.println("Motif positions/string s=(s1..st):");
            String motifs = " ";
            for (Motif motif : median.getMotifs()) {
                motifs += motif.getLocation() + "(" + motif.getStr() + ")", ";
            }
            System.out.println(motifs);
        }
        System.out.printf("Number of leafs visited: %d\n", mp.getNumOfLeafsVisited());
        System.out.printf("Number of leafs skipped: %d", Double.valueOf(Math.pow(K, L_MER) -
mp.getNumOfLeafsVisited()).intValue());
    }
}

```

```
package com.bio.main.io;

import java.io.IOException;
import java.nio.file.Files;
import java.nio.file.Paths;
import java.util.ArrayList;
import java.util.Iterator;
import java.util.List;

import com.bio.main.pojo.Sequence;

/**
 * The main class in charge of reading from a file.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class FileProcessor {

    /**
     * Default path to read the file from
     */
    public static final String IO_PATH = "../Assignment3/io/";

    private static FileProcessor instance = null;

    /**
     * Not accessible because of Singleton Design Pattern.
     */
    private FileProcessor() {
        super();
    }
}
```

```

public static FileProcessor getInstance() {
    if (instance == null) {
        instance = new FileProcessor();
    }
    return instance;
}

/**
 * For the given file name, it will read the sequences headers and strings from the file
and return them in a list.
 *
 * @param fileName
 * @return
 * @throws IOException
 *         If file cannot be read
 */
public List<Sequence> readSequences(String fileName) throws IOException {

    List<Sequence> result = new ArrayList<>();

    // Reading the whole file line by line
    List<String> lines = Files.readAllLines(Paths.get(IO_PATH + fileName));
    Iterator<String> iterator = lines.iterator();

    while (iterator.hasNext()) {
        result.add(new Sequence(iterator.next(), iterator.next()));
    }

    return result;
}
}

```

```
package com.bio.main.pojo;

import java.util.List;

/**
 * Main POJO which holds the data needed to be shown to the user according.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class Median {

    /**
     * Median string
     */
    private String str;

    /**
     * Total distance of the median string.
     */
    private int totalDistance;

    /**
     * Consensus string
     */
    private String consensusStr;

    /**
     * Consensus score
     */
    private int consensusScore;

    /**
     * List of Motifs found.
     */
    private List<Motif> motifs;
```



```
public Median(String str, int totalDistance) {
    super();
    this.str = str;
    this.totalDistance = totalDistance;
}

public String getStr() {
    return str;
}

public void setStr(String str) {
    this.str = str;
}

public int getTotalDistance() {
    return totalDistance;
}

public void setTotalDistance(int totalDistance) {
    this.totalDistance = totalDistance;
}

public String getConsensusStr() {
    return consensusStr;
}

public void setConsensusStr(String consensusStr) {
    this.consensusStr = consensusStr;
}

public int getConsensusScore() {
    return consensusScore;
}
```

```
public void setConsensusScore(int consensusScore) {  
    this.consensusScore = consensusScore;  
}  
  
public List<Motif> getMotifs() {  
    return motifs;  
}  
  
public void setMotifs(List<Motif> motifs) {  
    this.motifs = motifs;  
}  
}
```

```
package com.bio.main.pojo;

/**
 * Motif holds the data related to the each of the tiles found. It contains a string and its
 * location in the sequence.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class Motif {

    /**
     * Motif string
     */
    private String str;
    /**
     * Motif location in the sequence
     */
    private int location;

    public Motif(String str, int location) {
        super();
        this.str = str;
        this.location = location;
    }

    public String getStr() {
        return str;
    }

    public void setStr(String str) {
        this.str = str;
    }
}
```

```
public int getLocation() {  
    return location;  
}  
  
public void setLocation(int location) {  
    this.location = location;  
}  
}
```

```
package com.bio.main.pojo;

/**
 * DNA Sequence which holds header of each DNA and the string itself.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class Sequence {

    /**
     * Header of the sequence
     */
    private String header;

    /**
     * The contain of the sequence
     */
    private String str;

    public Sequence(String header, String str) {
        this.header = header;
        this.str = str;
    }

    public String getHeader() {
        return header;
    }

    public void setHeader(String header) {
        this.header = header;
    }

    public String getStr() {
```

```
        return str;
    }

    public void setStr(String str) {
        this.str = str;
    }
}
```

```
package com.bio.main.pojo;

/**
 * An enumeration for each of the possible values in DNA.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public enum TCGA {
    A, C, G, T
}
```

```
package com.bio.main.util;

import java.util.ArrayList;
import java.util.Arrays;
import java.util.Comparator;
import java.util.List;
import java.util.PriorityQueue;

import com.bio.main.pojo.Median;
import com.bio.main.pojo.Sequence;

/**
 * Main utility program used to find median using Branch and Bound (BnB) algorithm.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class BnBMainUtil {

    /**
     * Moving index within S
     */
    private int i;

    /**
     * DNA sequences
     */
    private List<Sequence> dnaSeq;

    /**
     * Lmer
     */
    private int l;

    /**
     * TGCA size = 4
     */
}
```



```

    */
    private int k;
    /**
     * The leaf representation in an array of characters.
     */
    private char[] s;
    /**
     * Size of the priority queue
     */
    private static final int PRIORITY_QUEUE_SIZE = 5;
    /**
     * Counter for checking to see how many leafs were visited and skipped.
     */
    private int numOfLeafsVisited = 0;
    /**
     * Priority queue defined by comparing the total distances of each to {@link Median}
objects.
     */
    PriorityQueue<Median> priorityQueue = new PriorityQueue<>(PRIORITY_QUEUE_SIZE, new
Comparator<Median>() {

        @Override
        public int compare(Median o1, Median o2) {
            return Integer.compare(o1.getTotalDistance(), o2.getTotalDistance());
        }

    });

    public BnBMainUtil(List<Sequence> dnaSeq, int l, int k) {
        super();
        this.dnaSeq = dnaSeq;
        this.l = l;
        this.k = k;
    }

```

```

public BnBMainUtil() {

}

/**
 * The main method which triggers the median search and finds the {@link
BnBMainUtil#PRIORITY_QUEUE_SIZE} top medians and return them.
 *
 * @return
 */
public List<Median> medianSearch() {
    // Creating the initial lmer array of strings in '111111' format.
    s = createInitiallmer(1);

    int bestDistance = Integer.MAX_VALUE;

    i = 1;
    while (i > 0) {
        if (i < 1) { // In case of parent nodes.
            String prefix = getActualText(s, i);
            int optimisticDistance = getTotalDistance(prefix);
            if (optimisticDistance > bestDistance) { // If the prefix (parent node)'s
total distance is worse, then we byPass.
                byPass();
            } else { // Otherwise we go to the next vertex.
                nextVertex();
            }

        } else { // In case of leaf nodes.
            String word = getActualText(s);
            // Counting the number of leafs visited.
            numOfLeafsVisited++;
            // Finding the best distance

```

```

        int totalDistance = getTotalDistance(word);
        if (totalDistance < bestDistance) {
            bestDistance = totalDistance;
        }
        // Priority queue takes care of throwing out those which do not have a
high score

        priorityQueue.add(new Median(word, totalDistance));
        nextVertex();
    }
}
// Returning the final result.
return getTopMedians();
}

/**
 * Converts the priority queue's top {@link BnBMainUtil#PRIORITY_QUEUE_SIZE} elements into
a list.
 *
 * @return
 */
private List<Median> getTopMedians() {

    List<Median> result = new ArrayList<>();
    for (int i = 0; i < PRIORITY_QUEUE_SIZE; i++) {
        result.add(priorityQueue.poll());
    }

    return result;
}

/**
 * Gets an array with digits format and convert it into its proper presentation format
('AACCA'). <br>
 * ('11221') to ('AACCA')
 *

```

```

    * @param chr
    * @param to
    * @return
    */
private String getActualText(char[] chr, int to) {
    return getActualText(Arrays.copyOfRange(chr, 0, to + 1));
}

/**
 * By passes a part of the tree by updating s[j] into the next possible character given if
it is possible. Otherwise it will stop (at the end of
 * the tree).
 */
private void byPass() {
    for (int j = i; j >= 1; j--) {
        if (Character.getNumericValue(s[j]) < k) {
            s[j] = nextCharacter(s[j]);
            i = j;
            return;
        }
    }
    i = 0;
}

/**
 * Finds the total distance of a given word from all the DNA sequences.
 *
 * @param word
 * @return
 */
private int getTotalDistance(String word) {

    int totalDistance = 0;

    char[] wordChars = word.toCharArray();

```

```

        for (Sequence sequence : dnaSeq) {

            char[] seqChars = sequence.getStr().toCharArray();
            int bestLocalDistance = Integer.MAX_VALUE;

            // Going through the DNA sequence using a window of lmer.
            for (int seqCharIndex = 0; seqCharIndex < seqChars.length - wordChars.length +
1; seqCharIndex++) {

                char[] sequenceChars = Arrays.copyOfRange(seqChars, seqCharIndex,
seqCharIndex + wordChars.length);

                // Finding the distance between the window and the word given.
                int distance = getDistance(sequenceChars, wordChars);
                if (bestLocalDistance > distance) {
                    bestLocalDistance = distance;
                }
            }
            totalDistance += bestLocalDistance;

        }

        return totalDistance;
    }

    /**
     * Finds the total distance between the two given arrays of characters. If the same
     characters in the array, of the same index, are not the same,
     * that means its distance is added by 1.
     *
     * @param seqChars
     * @param leafChars
     * @return
     */
    private int getDistance(char[] seqChars, char[] leafChars) {

```

```

        int distance = 0;
        for (int i = 0; i < seqChars.length; i++) {
            if (Character.toLowerCase(seqChars[i]) != Character.toLowerCase(leafChars[i]))
{
                distance++;
            }
        }
        return distance;
    }

/**
 * Converts digit formatted arrays into DNA format.
 *
 * @param s
 * @return
 */
public String getActualText(char[] s) {
    String result = "";
    for (int i = 1; i < s.length; i++) {
        switch (s[i]) {
            case '1':
                result += "A";
                break;
            case '2':
                result += "C";
                break;
            case '3':
                result += "G";
                break;
            case '4':
                result += "T";
                break;
        }
    }
}

```

```

        return result;
    }

    /**
     * Moves to the next vertex in the tree.
     */
    private void nextVertex() {
        if (i < 1) { // Parent node
            i++;
            s[i] = '1';
            return;
        } else { // Leaf node
            for (int j = 1; j > 0; j--) {
                if (Character.getNumericValue(s[j]) < k) {
                    s[j] = nextCharacter(s[j]);
                    i = j;
                    return;
                }
            }
        }
        i = 0;
    }

    /**
     * Gives back the next digit in character data format. Example: '1' becomes '2'
     *
     * @param c
     * @return
     */
    public char nextCharacter(char c) {
        return (char) (c + 1);
    }

```

```

/**
 * Creates the initial array of characters in which the index 'i' will move around and the
algorithm is based on.
 *
 * @param l
 * @return
 */
public char[] createInitialLmer(int l) {
    char[] chr = new char[l + 1];

    chr[0] = ' '; // Putting an empty char in the beginning of the char seq since the
indexes start from 0 in JAVA. And in the pseudo code indexes

                // start at 1. This is for readability purposes.

    for (int i = 1; i <= l; i++) {
        chr[i] = '1';
    }
    return chr;
}

public int getNumOfLeafsVisited() {
    return numOfLeafsVisited;
}

public void setNumOfLeafsVisited(int numOfLeafsVisited) {
    this.numOfLeafsVisited = numOfLeafsVisited;
}
}

```



```
package com.bio.main.util;

import java.util.ArrayList;
import java.util.Arrays;
import java.util.HashMap;
import java.util.List;
import java.util.Map;

import org.apache.commons.lang3.mutable.MutableInt;

import com.bio.main.pojo.Median;
import com.bio.main.pojo.Motif;
import com.bio.main.pojo.Sequence;
import com.bio.main.pojo.TCGA;

/**
 * A utility class for Motif finding.
 *
 * @author Mohamad Mahdi Ziaee
 *
 */
public class MotifUtil {

    private static MotifUtil instance = null;

    private MotifUtil() {
        super();
    }

    public static MotifUtil getInstance() {
        if (instance == null) {
            instance = new MotifUtil();
        }
    }
}
```

```

        return instance;
    }

    /**
     * Finds the motifs and put them into medians for the given sequences.
     *
     * @param medians
     * @param sequences
     * @param lmer
     */
    public void findMotifs(List<Median> medians, List<Sequence> sequences, int lmer) {

        for (Median median : medians) {

            List<Motif> result = new ArrayList<>();

            for (Sequence sequence : sequences) {
                Motif motif = findMotif(sequence.getStr().toCharArray(),
median.getStr().toCharArray(), lmer);
                result.add(motif);
            }

            median.setMotifs(result);
        }
    }

    /**
     * For the given median, it will try to find the best local motif based on its score.
     *
     * @param seqChars
     * @param median
     * @param lmer
     * @return
     */

```

```

public Motif findMotif(char[] seqChars, char[] median, int lmer) {

    int bestScore = 0;
    String motifStr = null;
    int location = 0;

    for (int seqCharIndex = 0; seqCharIndex < seqChars.length - median.length + 1;
seqCharIndex++) {

        char[] sequenceChars = Arrays.copyOfRange(seqChars, seqCharIndex, seqCharIndex
+ median.length);

        int score = getScore(sequenceChars, median);

        if (score > bestScore) {
            bestScore = score;
            motifStr = String.valueOf(sequenceChars);
            location = seqCharIndex;
        }
    }

    return new Motif(motifStr, location);
}

/**
 * Gets the score of two given arrays of characters, each matching character is counted as
1. The higher the score, the better the match.
 *
 * @param sequenceChars
 * @param median
 * @return
 */
private int getScore(char[] sequenceChars, char[] median) {
    int score = 0;
    for (int i = 0; i < median.length; i++) {
        if (sequenceChars[i] == median[i]) {

```

```

        score++;
    }
}

return score;
}

/**
 * Calculates the consensus string and score for each of the medians given.
 *
 * @param medians
 * @param lmer
 */
public void calculateConsensus(List<Median> medians, int lmer) {

    for (Median median : medians) {

        String result = "";
        int totalScore = 0;

        for (int i = 0; i < lmer; i++) {

            Map<TCGA, Integer> map = new HashMap<>();

            for (Motif motif : median.getMotifs()) {

                TCGA key =
TCGA.valueOf(String.valueOf(motif.getStr().charAt(i)));

                Integer score = map.get(key);

                map.put(key, score == null ? 1 : score + 1); // If the score does
not exist(is null), then we put 1, otherwise we add 1 to it.

            }

            MutableInt score = new MutableInt(0); // Using Mutable integer since
Java is using pass by value, so that we don't need to create

```

```

//
another wrapper around it.

        TCGA tcga = findConsensus(map, score); // Finding which TCGA holds the
biggest count number.

        result += tcga.toString();
        totalScore += score.getValue();
    }

    median.setConsensusStr(result);
    median.setConsensusScore(totalScore);
}

}

/**
 * For each of the TCGA keys in the map, it finds the one with the highest score.
 *
 * @param map
 * @param score
 * @return
 */
private TCGA findConsensus(Map<TCGA, Integer> map, MutableInt score) {
    TCGA tcga = null;
    for (TCGA key : map.keySet()) {
        if (score.getValue() < map.get(key)) {
            score.setValue(map.get(key));
            tcga = key;
        }
    }
    return tcga;
}
}

```