Central Dogma Script

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A project for Harvard's CS50 python 2023

Description

- The Central Dogma script is a console application crafted to handle the input of a DNA sequence in plain text format, along with its orientation, according to the principles of the Central Dogma of Biology.
- It outputs the corresponding complementary DNA sequence, the equivalent mRNA sequence, and, if applicable, the corresponding polypeptide sequence.

 In addition, the script calculates the number of phosphodiester and hydrogen bonds, as well as the GC content for the double stranded molecule of each DNA sequence.

Usage

python3 project.py [data.file]

Script Files

- 1. **project.py**: It contains the **main()** function, and the rest of the custom functions that compose the procedural part of the script.
- 2. **bio.py**: It contains the translation_table dictionary and the DNA_obj custom class, which is imported in project.py.
- 3. **test_project.py**: It contains the unit tests for the functions (procedural part) and the methods (object oriented part) of the script.

Purpose

- Emulating the Central Dogma of Biology (CDB) procedures.
- Aiding secondary education biology students in understanding and applying the CDB procedural concepts.
- Assisting biology teachers in writing their own practical exercises.

Operation modes

- 1. Manual input
- 2. Data file input

Manual mode output

- 1. On Screen
- 2. Output file dogma_manual.txt

Input is a Coding DNA Sequence

```
PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma> python project.py
Existing output files may be overwritten.
Continue? (Y/N)v
If you want to load a data file for multiple coding sequences run this script as:
python3 central_dogma.py /path/name_of_file.extension
Enter your coding DNA sequence:
ATGCTACAATTATAG
Enter the direction of your sequence:
1 for 5->3
2 for 3->5
Enter your direction: 1
DNA Coding Strand:
                    5' ATG-CTA-CAA-TTA-TAG 3'
DNA Complementary Strand: 3' TAC-GAT-GTT-AAT-ATC 5'
mRNA sequence:
                   5' AUG-CUA-CAA-UUA-UAG 3'
Peptide sequence:
                        H₂N-Met-Leu-Gln-Leu-COOH
Hydrogen bonds = 34
Phosphodiester bonds = 28
The output was added to the dogma_manual.txt file.
Do you want to continue? (Y/N)y
```

Input is a Non Coding DNA Sequence - Inverted Orientation

```
Enter your coding DNA sequence:
ATGCCCATAGCGTGA
Enter the direction of your sequence:
1 for 5->3
2 for 3->5
Enter your direction: 2
DNA Coding Strand: 5' AGT-GCG-ATA-CCC-GTA 3'
DNA Complementary Strand: 3' TCA-CGC-TAT-GGG-CAT 5'
                5' AGU-GCG-AUA-CCC-GUA 3'
mRNA sequence:
Peptide sequence: H<sub>2</sub>N-Non Coding-COOH
Hydrogen bonds = 38
Phosphodiester bonds = 28
GC content = 0.53333333333333333
The output was added to the dogma_manual.txt file.
Do you want to continue? (Y/N)n
PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma>
```

dogma_manual.txt output file sample

```
≡ dogma manual.txt ×

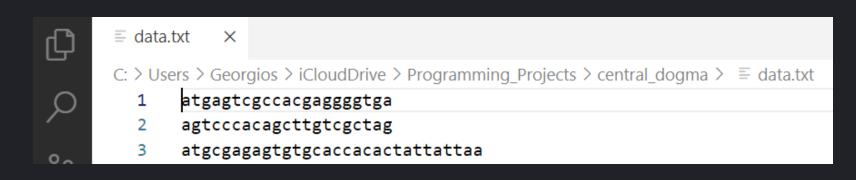
C: > Users > Georgios > iCloudDrive > Programming_Projects > central_dogma > ≡ dogma_manual.txt
                         5' ATG-CTA-CAA-TTA-TAG 3'
      DNA Coding Strand:
      DNA Complementary Strand: 3' TAC-GAT-GTT-AAT-ATC 5'
      mRNA sequence: 5' AUG-CUA-CAA-UUA-UAG 3'
      Peptide sequence: H<sub>2</sub>N-Met-Leu-Gln-Leu-COOH
      Hydrogen bonds = 34
      Phosphodiester bonds = 28
      DNA Coding Strand:
                         5' AGT-GCG-ATA-CCC-GTA 3'
      DNA Complementary Strand: 3' TCA-CGC-TAT-GGG-CAT 5'
      mRNA sequence:
                      5' AGU-GCG-AUA-CCC-GUA 3'
      Peptide sequence: H<sub>2</sub>N-Non Coding-COOH
      Hydrogen bonds = 38
 13
      Phosphodiester bonds = 28
      gc content = 0.5333333333333333
 16
 17
```

Invalid DNA sequence input

```
Windows PowerShell
PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma> python project.py
Existing output files may be overwritten.
Continue? (Y/N)y
If you want to load a data file for multiple coding sequences run this script as:
python3 central_dogma.py /path/name_of_file.extension
Enter your coding DNA sequence:
atgfgtagatga3agatagacg
Enter the direction of your sequence:
1 for 5->3
2 for 3->5
Enter your direction: 2
Traceback (most recent call last):
 File "C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma\project.py", line 175, in <module>
    main()
  File "C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma\project.py", line 60, in main
    dna_object = set_coding_sequence(d_seq, d)
  File "C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma\project.py", line 76, in set_coding_sequence
    dna_obj = DNA_obj(c_seq, direct)
  File "C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma\bio.py", line 73, in __init__
    self.seg = seg.strip().upper()
  File "C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma\bio.py", line 92, in seq
    raise ValueError("Invalid Sequence!")
ValueError: Invalid Sequence!
PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma>
```

Data file input

data.txt input file sample



Data file mode output

- 1. On Screen
- 2. Output files:
 - dogma.txt
 - peptides.csv
 - o peptides_tab.txt

Invalid data filename output

PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma> python project.py wrong_filename.txt Existing output files may be overwritten.
Continue? (Y/N)y
Coding Sequence file not found.

Check that the path and the name of your sequence file are correct, or run the program without arguments and input a coding DNA sequence manually. PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma>

Valid data filename output

PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma> python project.py data.txt

Existing output files may be overwritten.

Continue? (Y/N)y

Your data file exists!

Read the dogma.txt file for Replication, Transcription and Translation data., plus various calculations for each DNA sequence.

Your translation data is written in the peptides.csv file.

For tabular format the peptides_tab.txt was created.

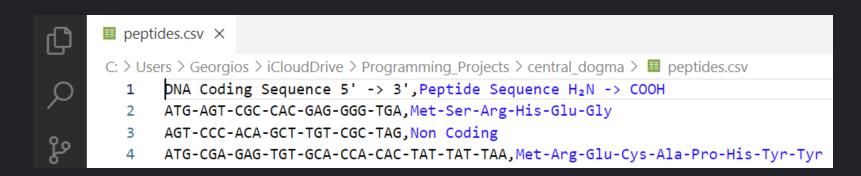
PS C:\Users\Georgios\iCloudDrive\Programming_Projects\central_dogma>

dogma.txt output file sample

```
    ≡ dogma.txt ×

C: > Users > Georgios > iCloudDrive > Programming_Projects > central_dogma > ≡ dogma.txt
       DNA Coding Strand:
                                   5' ATG-AGT-CGC-CAC-GAG-GGG-TGA 3'
       DNA Complementary Strand: 3' TAC-TCA-GCG-GTG-CTC-CCC-ACT 5'
       mRNA sequence:
                                   5' AUG-AGU-CGC-CAC-GAG-GGG-UGA 3'
       Peptide sequence:
                                  H<sub>2</sub>N-Met-Ser-Arg-His-Glu-Gly-COOH
       Hydrogen bonds = 55
       Phosphodiester bonds = 40
       gc content = 0.6190476190476191
       DNA Coding Strand:
                                   5' AGT-CCC-ACA-GCT-TGT-CGC-TAG 3'
       DNA Complementary Strand: 3' TCA-GGG-TGT-CGA-ACA-GCG-ATC 5'
       mRNA sequence:
                                   5' AGU-CCC-ACA-GCU-UGU-CGC-UAG 3'
                                  H<sub>2</sub>N-Non Coding-COOH
       Peptide sequence:
       Hydrogen bonds = 54
       Phosphodiester bonds = 40
       gc content = 0.5714285714285714
 16
       DNA Coding Strand:
                                   5' ATG-CGA-GAG-TGT-GCA-CCA-CAC-TAT-TAT-TAA 3'
       DNA Complementary Strand: 3' TAC-GCT-CTC-ACA-CGT-GGT-GTG-ATA-ATA-ATT 5'
       mRNA sequence:
                                   5' AUG-CGA-GAG-UGU-GCA-CCA-CAC-UAU-UAU-UAA 3'
       Peptide sequence:
                                  H<sub>2</sub>N-Met-Arg-Glu-Cys-Ala-Pro-His-Tyr-Tyr-COOH
       Hydrogen bonds = 72
       Phosphodiester bonds = 58
       gc content = 0.4
```

peptides.csv output file sample



peptides_tab.txt output file sample

Central Dogma of Biology Summary Table (Central Dogma Overview)

Table 2: DNA Coding Sequence R	Replication, Transcription an	d Translation (Central Dogma)
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Procedure	Macromolecule	Starting Edge	Starting Codon	Codon 1	Codon 2	Termination Codon	Ending Edge
	DNA coding	5'	ATG	GAG	CTC	TAA	3'
Replication	DNA complementary	3'	TAC	CTC	GAG	ATT	5'
Transcription	mRNA	5'	AUG	GAG	CUC	UAA	3'
Translation	Polypeptide	H ₂ N	Met	Glu	Leu	-	COOH

Future plans

- Adding non standard genetic tables.
- Introducing a new feature for translating a DNA coding sequence with 2 different genetic tables.
 Then the script will align the 2 corresponding peptides, counting their differences in amino acids.

The End:)