BIOEN 537 Computational System Biology Final Presentation

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Background

What is the problem

- > Current software solutions for nanopore sequencing is not widely available with python.
- No clear guideline for installing the pipelines in python
- > A need for a specialized toolkit that streamlines primer design and sequence alignment, specifically tailored for nanopore sequencing with python.



Use Case

> Laboratory Researchers:

- User will install the package with pip
- Quickly design primers for PCR amplification of specific DNA sequences (prior to Nanopore Sequencing).
- Import data from EPI2ME (official nanopore sequencing software) and align nanopore-sequenced fragments against known reference sequences.

Demo – Primer Design

Primer: TTGACCGATGACCCCGGTTC

Sequence with Primer: TTGACCGATGACCCCGGTTCAGGCTTCACCACAGTGTGGAACGCGGTCGTCTCCGAACTTAACGGCGACC

Primer: AACTGGCTACTGGGGCCAAG

Sequence with Primer: AACTGGCTACTGGGGCCAAGTCCGAAGTGGTGTCACACCTTGCGCCAGCAGAGGCTTGAATTGCCGCTGG

- highlighted_sequence1.fasta
- highlighted_sequence2.fasta
- reference_primer



Demo – Nanopore Sequence Alignment

```
executor > local (24)
[c6/65f505] process > validate_sample_sheet
                                                     [100%] 1 of 1 <
[fd/2368f0] process > fastcat (2)
                                                     [100%] 3 of 3 🗸
[e5/6351e5] process > pipeline:getVersions
                                                     [100%] 1 of 1 🗸
[da/ec30ec] process > pipeline:getParams
                                                     [100%] 1 of 1 🗸
[74/ffa312] process > pipeline:alignReads (3)
                                                     [100%] 3 of 3 🗸
[b1/608882] process > pipeline:mpileup (3)
                                                     [100%] 3 of 3 🗸
[44/d5f883] process > pipeline:whatshap (1)
                                                     [100%] 3 of 3 🗸
[23/ea9ab7] process > pipeline:countReadsRegions (3) [100%] 3 of 3 ✓
[b1/b3b301] process > pipeline:report (1)
                                                     [100%] 1 of 1 <
[0b/fa9009] process > pipeline:reportSingle (1)
                                                     [100%] 1 of 1 🗸
[b2/584306] process > output (4)
                                                     [100%] 4 of 4 🗸
Completed at: 10-Dec-2023 19:18:32
Duration : 1m 25s
CPU hours : 0.1
Succeeded: 24
```

execution Negative.bam Negative.bam.bai Properties: Negative.final.vcf Positive.bam Positive.bam.bai Positive.final.vcf sample1_report.html sample1.bam sample1.bam.bai sample1.final.vcf wf-tb-amr-report.csv wf-tb-amr-report.html



Design

> Primer Design (primerdesign.py):

Generates primers from input DNA sequences.

> Sequence Alignment (nanoAlign.py):

Aligns sequencing data and manages dependencies.

> Interaction:

- Modules interact with the user's input data, processing it according to nanopore-specific algorithms.
- Automated environment setup ensures smooth workflow execution.



Project Structure

> **GitHub Repository:** https://github.com/hgu1uw/UW_BIOEN537.git

docs	-a
nanoporeAlignment	-a
primer_design	-a
test_	-a
.gitignore	Initial commit
LICENSE.txt	-a
README.md	-v3
initpy	-a
setup.py	-a



Lessons Learned and Future Work

> Modularity:

Importance of designing independent, interchangeable modules.

> Documentation:

 Well-documented code and usage instructions are crucial for user adoption and maintenance.

> Future Work:

- Integration of basecalling and more quality control for nanopore sequencing
- For primer design, implement automatic reading of all fasta files in the folder.
- Expanding the toolkit to cover more use cases in nanopore sequencing.

