San Pablo Catholic University (UCSP)
Undergraduate Program in
Computer Science
SILABO

CB309. Bioinformatics (Elective)

2021-I

1. General information		
1.1 School	:	Ciencia de la Computación
1.2 Course	:	CB309. Bioinformatics
1.3 Semester	:	9^{no} Semestre.
1.4 Prerrequisites	:	

- CS212. Algorithm Analysis and Design. (5th Sem)

- MA307. Mathematics applied to computing . (6th Sem)

1.5 Type of course	:	Elective
1.6 Learning modality	:	Virtual
1.7 Horas	:	2 HT; 2 HP; 2 HL;
1.8 Credits	:	4

2. Professors

3. Course foundation

The use of computational methods in the biological sciences has become one of the key tools for the field of molecular biology, being a fundamental part of research in this area.

In Molecular Biology, there are several applications that involve both DNA, protein analysis or sequencing of the human genome, which depend on computational methods. Many of these problems are really complex and deal with large data sets.

This course can be used to see concrete use cases of several areas of knowledge of Computer Science such as Programming Languages (PL), Algorithms and Complexity (AL), Probabilities and Statistics, Information Management (IM), Intelligent Systems (IS).

4. Summary

1. Introduction to Molecular Biology 2. Sequence Comparison 3. Phylogenetic Trees 4. DNA Sequence Assembling 5. Secondary and tertiary structures 6. Probabilistic Models in Molecular Biology

5. Generales Goals

- That the student has a solid knowledge of molecular biological problems that challenge computing.

- That the student is able to abstract the essence of the various biological problems to pose solutions using their knowledge of Computer Science

6. Contribution to Outcomes

This discipline contributes to the achievement of the following outcomes:

a) An ability to apply knowledge of mathematics, science. (**Usage**)

b) An ability to design and conduct experiments, as well as to analyze and interpret data. (**Assessment**)

l) Develop principles research in the area of computing with levels of international competitiveness. (**Usage**)

7. Content

UNIT 1: Introduction to Molecular Biology (4)
Competences:

Content	Generales Goals
- Review of organic chemistry: molecules and macro-molecules, sugars, nucleic acids, nucleotides, RNA, DNA, proteins, amino acids and levels of structure in proteins. - The Dogma of Life: From DNA to Proteins, Transcription, Translation, Protein Synthesis. - Genome study: Maps and sequences, specific techniques	- Achive a general knowledge of the most important topics in Molecular Biology. [Familiarity] - Understand that biological problems are a challenge to the computational world. [Assessment]

Readings: Clote and Backofen (2000), Setubal and Meidanis (1997)

UNIT 2: Sequence Comparison (4)
Competences:

Content	Generales Goals
- Sequences of nucleotides and amino acid sequences. - Sequence alignment, paired alignment problem, exhaustive search, Dynamic programming, global alignment, local alignment, gaps penalty - Comparison of multiple sequences: sum of pairs, complexity analysis by dynamic programming, alignment heuristics, star algorithm, progressive alignment algorithms.	- Understand and solve the problem of aligning a pair of sequences. [Usage] - Understand and solve the problem of multiple sequence alignment. [Usage] - Know the various algorithms for aligning existing sequences in the literature . [Familiarity]

Readings: Clote and Backofen (2000), Setubal and Meidanis (1997), Pevzner (2000)

UNIT 3: Phylogenetic Trees (4)
Competences:

Content	Generales Goals
- Phylogeny: Introduction and phylogenetic relations - Phylogenetic trees: definition, type of trees, problem of search and reconstruction of trees - Reconstruction methods: parsimony methods, distance methods, maximum likelihood methods, confidence of reconstructed trees	- Understand the concept of phylogeny, phylogenetic trees and the methodological difference between biology and molecular biology. [Familiarity] - Understand the problem of the reconstruction of phylogenetic trees, to know and apply the main algorithms for the reconstruction of phylogenetic trees. [Assessment]

Readings: Clote and Backofen (2000), Setubal and Meidanis (1997), Pevzner (2000)

UNIT 4: DNA Sequence Assembling (4)	
Competences:	
Content	**Generales Goals**
- Biological basis: ideal case, difficulties, alternative methods for DNA sequencing - Formal Assembly Models: Shortest Common Superstring, Reconstruction, Multicontig - Algorithms for sequence assembly: representation of overlaps, paths to create superstrings, voracious algorithm, acyclic graphs. - Assembly heuristics: search for overlays, ordering fragments, alignments and consensus.	- Understand the computational challenge of the Sequence Assembly problem. [Familiarity] - Understand the principle of formal model for assembly. [Assessment] - Know the main heuristics for the problem of assembjale of DNA sequences[Usage]
Readings: Setubal and Meidanis (1997), Aluru (2006)	

UNIT 5: Secondary and tertiary structures (4)	
Competences:	
Content	**Generales Goals**
- Molecular structures: primary, secondary, tertiary, quaternary. - Prediction of secondary structures of RNA: formal model, pair energy, structures with independent bases, solution with Dynamic Programming, structures with loops. *Protein folding*: Estructuras en proteinas, problema de protein folding. *Protein Threading*: Definitions, Branch Bound Algorithm, Branch Bound for protein threading. *Structural Alignment*: Definitions, DALI algorithm	- Know the protein structures and the necessity of computational methods for the prediction of the geometry. [Familiarity] - Know the algorithms for solving prediction problems of secondary structures RNA, and structures in proteins. [Assessment]
Readings: Setubal and Meidanis (1997), Clote and Backofen (2000), Aluru (2006)	

UNIT 6: Probabilistic Models in Molecular Biology (4)	
Competences:	
Content	**Generales Goals**
- Probability: Random Variables, Markov Chains, Metropoli-Hasting Algorithm, Markov Random Fields, and Gibbs Sampler, Maximum Likelihood. - Hidden Markov Models (HMM), parameter estimation, Viterbi algorithm and Baul-Welch method, Application in paired and multiple alignments, Motifs detection in proteins, in eukaryotic DNA, in sequences families. - Probabilistic phylogeny: probabilistic models of evolution, likelihood of alignments, likelihood for inference, comparison of probailistic and non-probabilistic methods	- Review concepts of Probabilistic Models and understand their importance in Computational Molecular Biology. [Assessment] - Know and apply Hidden Markov Models for various analyzes in Molecular Biology.. [Usage] - Know the application of probabilistic models in Phylogeny and to compare them with non-probabilistic models[Assessment]
Readings: Durbin et al. (1998), Clote and Backofen (2000), Aluru (2006), Krogh et al. (1994)	

8. Methodology
El profesor del curso presentará clases teóricas de los temas señalados en el programa propiciando la intervención de los alumnos. El profesor del curso presentará demostraciones para fundamentar clases teóricas. El profesor y los alumnos realizarán prácticas Los alumnos deberán asistir a clase habiendo leído lo que el profesor va a presentar. De esta manera se facilitará la comprensión y los estudiantes estarán en mejores condiciones de hacer consultas en clase.

9. Assessment
Continuous Assessment 1 : 20 % **Partial Exam** : 30 % **Continuous Assessment 2** : 20 % **Final exam** : 30 %

References

Aluru, Srinivas, ed. (2006). *Handbook of Computational Molecular Biology.* Computer and Information Science Series. Chapman & Hall, CRC: Boca Raton, FL.

Clote, P. and R. Backofen (2000). *Computational Molecular Biology: An Introduction.* 279 pages. John Wiley & Sons Ltd.

Durbin, R. et al. (1998). *Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids.* Cambridge University Press, p. 357. ISBN: 9780521629713.

Krogh, Anders et al. (1994). "Hidden Markov Models in Computational Biology, Applications to Protein Modeling". In: *J Molecular Biology* 235, pp. 1501–1531.

Pevzner, Pavel A. (2000). *Computational Molecular Biology: an Algorithmic Approach.* The MIT Press: Cambridge, Massachusetts.

Setubal, João Carlos and João Meidanis (1997). *Introduction to computational molecular biology.* Boston: PWS Publishing Company, pp. I–XIII, 1–296. ISBN: 978-0-534-95262-4.