

## Chapter 9

# Evolutionary Computing to Examine Variation in Proteins with Evolution

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### ABSTRACT

*Amino-acid sequences play a pivotal role for the structure of proteins. Alterations in a single amino-acid may vary the protein functioning. Alignment of sequences recognizes evolutionary and structurally related residues in a group of amino-acid sequences. It also aids to perceive the regions that are conserved throughout and are also functionally important. Although protein alignment issue has been studied in the past decades, but computational approaches serves as more accurate to investigate the entire process in a comparably lesser time. Evolutionary algorithms, more specifically, genetic algorithms are very beneficial. It leads to the global optimization of the protein after observance of “the fittest” among the rest. On global optimization, the protein tends to be more stable, thereby, helping the process of interactions among other stable proteins and provides a residue level study. Thus, this state-of-art can be implemented for alignment of macro-molecules, which serves as an essential criterion for further molecular level analyses.*

### INTRODUCTION

Evolutionary computation occupies the zonal study for discerning the part of computer science that indulges with biological evolution to resolve computational issues (Bäck & Schwefel, 1993; Bäck, Fogel & Michalewicz, 1997). Therefore, it serves as a connection in connecting evolutionary biology with computer science. Biological evolution is a serious and efficient cause for the instigation to deal with typical *in silico* issues. The gradual process of “Evolution” aids in bringing in better adaptive characteristics in the population which may be in enormous numbers and ways—the ultimate physical change being the altering of the genes in their sequences and others. That provides also the solutions to new stress or threats from the environment which allow organisms to survive and perpetuate. And,

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scrutinized through a different angle -- the “modalities” involved in evolution are extraordinarily lucid. Species are generated through abrupt variation (including mutation, recombination, and other varied features), preceded by the selection due to natural effects, which ensures “survival of the fittest” and reproduction. In this way, the genetic material is propagated to the next and future generations. This phenomenon is accounted for being conscientious for even some the inexplicably astonishing diversity and intricacy induction, like new species appearance which some time are observed in the biosphere. Moreover, evolutionary studies are essential for studying the intricacy of the biophysical chemistry of proteins contained in a cell. It further includes the responsibility of the self modulations, ensembles in the respective conformations and the supportive adaptations after translational processes; with regard to folding of the proteins, kinetics study of the proteins and protein complexes extending till the liability of the chaperones at a molecular level (Jessica, Johan & David, 2011). The existence of proteins in conformational ensembles includes not only its functional transitions but also its evolutionary shifts (Jessica, Johan & David, 2011). Ahead of thermodynamic concerns of conformational ensembles lies the responsibility of protein kinetics analysis for its specific structure and function. Additionally to an inimitable and steady native condition, structured proteins also preserve pathways via which they tend to abruptly fold to attain a final functional structure (Jessica, Johan & David, 2011). In certain cases, the pathway of their folding might influence the final functional structure into which the sequence folds to (Jessica, Johan & David, 2011). It further implies that the pathway of the folding may serve to be essential for the ultimate fold, thereby leading to an decisive biological function for the protein (Kimchi-Sarfaty, et.al., 2007). Thus it can be documented that pathway of the folding holds prior importance for the protein structure and eventually the protein function that it is highly paramount, evolutionarily. Folding techniques do also hold an important responsibility for preventing the aggregation of protein, with appropriate folding motivated at least partially through the hydrophobic disintegration (Jessica, Johan & David, 2011). Through the evolution, any hindrance in protein stability or folding or its developing phenomena beginning from its sequence to its final structure and function, leads to structural disordered proteins. This is finally emphasized through the identification and analysis of an energy landscape for a particular sequence, and for sequences that are homologous (Jessica, Johan & David, 2011). It further helps to analyze any mutational alterations, if occurred during the evolution of that particular protein. Instantaneously, analysis of protein models via structural biology and biophysical approach will escalate the requisite to precisely take into account the varied evolutionary processes essentially accompanied by the investigation of structural bioinformatics. With these contemplations, protein models will turn out to be, more powerful and effective with the progress of this evolutionary field.

Several approaches are there to follow in the area of developmental studies with *in silico* approach. To resolve evolutionary computational issues, the algorithms with evolutionary approaches are extremely beneficial. The most widely used form of evolutionary algorithm is genetic algorithms (GAs) (Eiben et.al., 1994; Ting & Chaun-Kang, 2005; Akbari & Ziarati, 2010). To study at the genetic level, proteins play an essential role to be observed first with their conservation or alterations throughout the evolution. Evolutionarily, proteins are known to be dynamic in nature. It leads to the fact that significant variations in protein structures can be examined between different varied members of the individual protein groups. For the essentiality of aligning protein sequences, the mission is to recognize associated locations in a group of amino acid sequences which are closer with respect to their evolution or structure. Multiple amino acid sequences are generally studied using the basic multiple sequence alignment (MSA) technique (Wang & Jiang, 1994; Just, 2001; Elias & Isaac, 2006) such as, ClustalW.

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