



Statistical Analysis of Dihedral Angles Perturbation

Golalizadeh, M.*

Department of Statistics, Tarbiat Modares University, Tehran, Iran

*golalizadeh@modares.ac.ir

Abstract: It is known that proteins is not fixed in their forms [1]. Insead, they are varying remarkably. So, to treat the random behavior of them is of great importance from both modeling and application viewpoints [2]. Many signs of progress have been seen from the biological perspective. But, it received less statistical and probabilistic considerations. To predict the protein structure using their random behaviours is usually the source of attention only from the linear statistics viewpoint [3]. It is because the considered variables are the components from some Euclidean spaces. The line of the statistical research in this subject has changed soon after realizing the fact that the dihedral angles well describe the link between atoms. However, due to the periodic properties of these angles, the random perturbation of them should be studied based on the tools from the non-linear statistics [4]. After reviewing fundemantal materials on this innovative topic, we outline the procedures to define proper model to tackle random variation of the dihedral angles on torus. We also present some simulation studies to highlight our main results.

Keywords: Protein structure; Dihedral angles; Non-linear statistics; Torus.

References

- [1] A. Altis, P. Nguyen, R. Hegger, and G. Stock, "Dihedral angle Principal Component Analysis of Molecular Dynamics Simulations", *Journal of Chemical Physics*, 26 (2007) 244111.1-244111.10.
- [2] .THamelryck, K. Mardia and J. Ferkinghoff-Borg, "Bayesian Methods in Structural Bioinformatics", Springer, Berlin, 2012.
- [3] N. Elmaci, R. Berry, "Principal Coordinate Analysis on a Protein Model", *Journal of Chemical Physics*, 110 (1999) 10606-10622.
- [4] K. Mardia, .C Taylor, and G. Subramaniam, "Protein Bioinformatics and Mixtures of Bivariate von Mises Distributions for Angular Data", *Biometrics*, 63 (2007) 505-512.