Generating equilateral random polygons in confinement

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Abstract

One challenging problem in biology is to understand the mechanism of DNA packing in a confined volume such as a cell. It is known that confined circular DNA is often knotted and hence the topology of the extracted (and relaxed) circular DNA can be used as a probe of the DNA packing mechanism. However, in order to properly estimate the topological properties of the confined circular DNA structures using mathematical models, it is necessary to generate large ensembles of simulated closed chains (i.e., polygons) of equal edge lengths that are confined in a volume such as a sphere of certain fixed radius. Finding efficient algorithms that properly sample the space of such confined equilateral random polygons is a difficult problem. In this paper we propose a method that generates confined equilateral random polygons based on their probability distribution. This method requires the creation of a large database initially. However, once the database has been created, a confined equilateral random polygon of length n can be generated in linear time in terms of n. The errors introduced by the method can be controlled and reduced by the refinement of the database. Furthermore, our numerical simulations indicate that these errors are unbiased and tend to cancel each other in a long polygon.

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