A Fast Ergodic Algorithm for Generating Ensembles of Equilateral Random Polygons

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Abstract

Knotted structures are commonly found in circular DNA and along the backbone of certain proteins. In order to properly estimate properties of these three dimensional structures it is often necessary to generate large ensembles of simulated closed chains (i.e. polygons) of equal edge lengths (such polygons are called equilateral random polygons). However finding efficient algorithms that properly sample the space of equilateral random polygons is a difficult problem. Currently there are no proven algorithms that generate equilateral random polygons with its theoretical distribution. In this paper we propose a method that generates equilateral random polygons in a "step-wise uniform" way. We prove that this method is ergodic in the sense that any given equilateral random polygon can be generated by this method and we show that the time needed to generate an equilateral random polygon of length n is linear in terms of n. These two properties make this algorithm a big improvement over the existing generating methods. Detailed numerical comparisons of our algorithm with other widely used algorithms are provided.

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