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A new model for ring polymers with some exact solutions.

A fundamental mathematical problem in the analysis of ring polymers is the efficient generation and analysis of large samples of random closed space polygons. These model polymer configurations in good solvent. The essential question is this: what probability measure should be used to sample polygon space? A number of answers have been proposed for this problem. For instance, if we restrict to the finite set of lattice polygons, there is a natural counting measure on closed lattice walks. Other authors have restricted attention to the space of equilateral closed polygons in space, or to a space of closed polygons where the edgelengths are sampled from a Gaussian distribution. In all these cases, it has not been possible to directly sample the space of closed polygons; existing algorithms use Markov chain methods to converge to a distribution on polygon space. There are no rigorous results on how fast these methods converge to their limiting distributions.

In this talk, we give a new description of polygon space which allows us to give new theoretical and computational results. Our measure is based on a map from the Stiefel manifold of orthonormal 2-frames in complex n-space to the space of closed n-edge space polygons which was constructed by Jean-Claude Hausmann and Allen Knutson in 1997. While Knutson and Hausmann were interested in this map primarily as a way to analyze the symplectic and algebraic geometry of polygon space, we use versions of their map to push forward natural and highly symmetric probability measures to four spaces of polygons: closed and open polygons of n edges and fixed (total) length 2 in space and in the plane.

In the case of an closed equilateral n-edge polygon, our measure restricts to the expected one: it is the subspace measure of n-tuples of vectors in the round S^2 which sum to zero. The constructions restrict from space polygons to the corresponding spaces of planar polygons in a simple way and we will be able to give planar versions of all our theorems.

The most important practical property of these measures is that it is very easy to directly sample n-edge closed polygons in $O(n)$ time (the constant is small), allowing us to experiment with very large and high-quality ensembles of polygons. The most important theoretical property of this measure is that it is highly symmetric, allowing us to prove theorems which match our experiments. We will be able to define a transitive measure-preserving action of the full unitary group $U(n)$ on n-edge closed space polygons of length 2. Using these symmetries, we will be able to explicitly compute simple exact formulae for the expected values of squared chord lengths and radii of gyration for random open and closed polygons of fixed length, with corresponding formulae for equilateral polygons. We can then obtain explicit bounds on how fast the chord lengths of a closed polygon converge to those of an open polygon as the number of edges increases, providing rigorous justification for the intuition that a sufficiently long polygon "forgets" that it is closed.