The Symplectic Geometry of Polygon Space

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The statistical physics of long-chain polymers such as DNA is based on modelling a polymer by a space polygon. Physicists then study the statistics of geometric and topological properties of the polygons with respect to various probability measures on the space of polygons. This is reasonably straightforward for linear polymers, but when the ends of the polymer join together to form a ring polymer, the closure condition imposes subtle global correlations between the individual edges and the analysis becomes considerably more difficult.

Numerical experiments have been the mainstay of this field for several decades (e.g. [7, 9, 12]), but even these experiments are hampered by the state of development of sampling algorithms for equilateral polygons. There exist a number of Markov chain methods (see [1] for a survey) which appear to work fairly well in practice and which have mostly been proved to be ergodic, but their rates of convergence are unknown.

Our basic belief is that geometric structures on the moduli space of polygons can facilitate the search for good sampling algorithms. In earlier work [4] we used methods originally developed by the algebraic geometers Hausmann and Knutson [11] to give a fast new direct sampling algorithm for closed polygons with total length 2 (but varying edgelengths). In addition, this theoretical framework gave us the tools to prove several new exact results on the expectation of physically relevant geometric invariants of these polygons, such as their radius of gyration and total curvature [5].

The present work [6] is focused on fixed edgelength polygons (including equilateral polygons). To set notation, let $\mathrm{Pol}(n;\vec{r})$ be the moduli space of n-gons in $\mathbb{R}^3$ with edgelengths given by the vector $\vec{r} = (r_1, \ldots, r_n)$. The key point is that this space has a natural *symplectic* structure:

Theorem 1 (Kapovich–Millson [13]). $\mathrm{Pol}(n;\vec{r})$ *is the symplectic reduction of* $\prod_{i=1}^{n} S^2(r_i)$ *by the Hamiltonian diagonal* $SO(3)$ *action. In particular,* $\mathrm{Pol}(n;\vec{r})$ *is a* $(2n-6)$*-dimensional symplectic manifold, and the measure induced by the symplectic volume form agrees with the standard measure.*

In fact, Kapovich and Millson proved that any triangulation of the standard n-gon yields a Hamiltonian action of T^{n-3} on $\mathrm{Pol}(n;\vec{r})$ where the angle θ_i acts by folding the polygon around the ith diagonal of the triangulation (called a *bending flow* in symplectic geometry and a *polygonal fold* or *crankshaft move* [1] in random polygons). The induced moment map $\mu : \mathrm{Pol}(n;\vec{r}) \to \mathbb{R}^{n-3}$ records the lengths d_i of the diagonals in the triangulation. If the "fan triangulation" shown in Figure 1 is used, then the inequalities determining the moment polytope are

$$0 \leq d_1 \leq r_1 + r_2 \qquad \begin{matrix} r_{i+2} \leq d_i + d_{i+1} \\ |d_i - d_{i+1}| \leq r_{i+2} \end{matrix} \qquad 0 \leq d_{n-3} \leq r_n + r_{n-1} \tag{1}$$

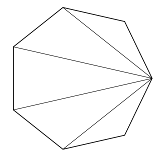

FIG. 1: The fan triangulation of a polygon

The image of the moment map is a convex polytope called the *moment polytope* [3, 10]. Since the torus is half-dimensional (and hence the manifold is *toric*), the Duistermaat–Heckman theorem [8] implies that the pushforward of the symplectic measure on $\mathrm{Pol}(n;\vec{r})$ to the moment polytope is a constant multiple of Lebesgue measure.

We can now give a strategy for sampling fixed edgelength polygons. In general, when M^{2n} is a toric manifold with moment polytope P such that the moment map can be inverted, we can construct a map $\alpha : P \times T^n \to M$ which parametrizes a full-measure subset of M by "action-angle" coordinates. Moreover, this map is measure-preserving. Therefore, a general procedure for sampling a toric symplectic manifold uniformly with respect to its symplectic measure is to sample P and T^n independently and uniformly. In particular, since the symplectic measure and the standard measure agree on $\mathrm{Pol}(n;\vec{r})$, we have

Theorem 2 (with Cantarella [6])**.** *Polygons in* $\mathrm{Pol}(n;\vec{r})$ *are sampled according to the standard measure if and only if the diagonal lengths* $d_1, \ldots, d_{n-3}$ *are uniformly sampled from the moment polytope defined by the inequalities* (1) *and the dihedral angles* $\theta_1, \ldots, \theta_{n-3}$ *are sampled independently and uniformly in* $[0, 2\pi)$.

Note that these uniformity conditions give concrete criteria for evaluating the quality of *any* polygon sampling algorithm.

Since a polygon $P \in \mathrm{Pol}(n;\vec{1})$ is in *rooted spherical confinement* of radius r if each diagonal length $d_i \leq r$, the moment polytope for rooted sphere-confined polygons is determined by the inequalities (1) plus the additional inequalities $d_i \leq r$ for all i. Thus, Theorem 2 easily extends to the case of confined polygons.

For small n the moment polytope can be sampled directly by decomposing it into standard simplices. For large n direct sampling seems challenging, but the moment polytope can certainly be sampled using the hit-and-run algorithm [2], which is a Markov chain algorithm known to produce approximately uniformly distributed sample points on arbitrary convex polytopes in $\mathbb{R}^m$ in time $O^*(m^3)$ [14]. In particular, we can sample fixed edgelength n-gons in any chosen confinement by generating points in the $(n-3)$-dimensional moment polytope using hit-and-run and then pairing each point with $n-3$ independent uniform dihedral angles. Figure 2 shows two equilateral 100-gons (not to scale) sampled using this algorithm.

To close, here are two open questions whose answers would give significant insight into the space of fixed edgelength polygons:

FIG. 2: Two equilateral 100-gons with all edgelengths equal to 1. The 100-gon on the left is completely unconfined, while the 100-gon on the right is confined to a sphere of radius 1.1.

1. Can the volume of the space of confined polygons be bounded below? If so, this should give lower bounds on the probability of complicated knots, since such knots will almost certainly be highly confined.

2. Is there a combinatorial description of the fan triangulation polytope (e.g. a simplicial decomposition)? Such a description would give a *direct* sampling algorithm for fixed edgelength polygons.

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